Proceedings of the 2010 International Conference on Computational and Mathematical Methods in Science and Engineering

Almería (Andalucía), Spain
June 26-30 2010

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Parallel Implementation of a Semi-Implicit 3-D Lake Hydrodynamic Model

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Abstract

The parallel implementation of a three-dimensional (3-D) lake hydrodynamic model in a small commodity cluster of three multi-core nodes is presented. The parallel program uses the three nodes in the cluster (by using the message passing standard MPI) and the four cores in a node (by using the shared memory standard OpenMP). This work analyzes the influence in performance of using different platform configurations, several workload distributions, several parallel implementations, and block-driven processing.

Key words: Parallel processing, Shared memory systems, Distributed memory systems, Hydrodynamics.

1. Introduction

High performance computations are being increasingly demanded in water sciences to get detailed descriptions of the flow fields that develop in natural ecosystems within reasonable lengths of time. It has been through these detailed descriptions of the flow fields, obtained either by means of simulations conducted with three-dimensional (3D) numerical algorithms solving the governing equations of fluid motion (Navier-Stokes equations), or through field observations collected with high-resolution experimental techniques that water scientists have gained, in the last few years, some understanding of transport processes in natural lakes and reservoirs\cite{1},\cite{2}. This understanding, however, is still far from complete.
Many of the 3D hydrodynamic models currently used in lake research are based on the solution of a simplified form of the Navier-Stokes equations, referred to as the shallow water equations (SWE), in which the vertical pressure gradients are assumed hydrostatic. The main state variables in the SWE are the spatially-varying horizontal velocities ($u$, $v$) and the water surface elevation ($\eta$). Being based on a simplified set of equations, SWE models have a moderate computational cost. SWE models, however, are still time and memory consuming when high density spatial grids are used or when they are used to simulate the long-term behavior of natural water systems. High-resolution grids, for example, are needed in order to resolve flow features of small spatial scales, such as near-shore currents, which are important to understand the physical and biogeochemical behavior of large-scale natural water bodies. Long simulation times are unacceptable when the SWE models are part of decision support systems. Model results in these cases are needed much faster than real time so that they can be used to develop and test management strategies aimed at minimizing the effects of natural disasters, such as floods or the introduction of invasive species.

The models in decision support systems are typically run repeatedly, each time with a different set of parameters and/or perturbed boundary conditions, in order to provide predictions of the future state of the flow field with an appropriate degree of uncertainty (see, for example, [3]). Most efforts in the field of environmental fluid modeling, hence, are being directed towards improving the execution time of existing numerical models, especially in inexpensive commodity platforms, so that (1) environmental scientists can build a rigorous and detailed understanding of the physical processes of transport and mixing occurring in inland water bodies and (2) water managers can get accurate predictions of the response of flow systems to external perturbations (e.g. pollution) and management strategies in a timely manner. The goal of this work is to present a parallel implementation of 3D SWE model in a small commodity cluster of three multi-core nodes.

The paper is organized as follows: Section 2 briefly describes the 3-D hydrodynamic model here implemented in parallel; Section 3 deals with related works; Section 4 compares several parallel implementations and data domain decompositions; Section 5 presents the computational platform and discusses some experimental results. Finally, Section 6 summarizes conclusions.

2. Hydrodynamic Model

This work evaluates a parallel implementation of a 3-D SWE model (SI3D, [4]), which has been extensively validated, both against analytical solutions and field data sets collected in a wide range of lake environments [5]. SI3D is based on the numerical solution of the continuity equation for incompressible fluids, the Reynolds-averaged and shallow water form of the Navier-Stokes equations for momentum, the transport equation for temperature, and an equation of state relating temperature to fluid density. The governing equations are first posed in
PARALLEL IMPLEMENTATION OF A LAKE HYDRODYNAMIC MODEL

layer-averaged form by integrating over the height of a series of horizontal layers separated by level planes. The layer-averaged form of the equations is discretized using a semi-implicit, three-level, iterative leapfrog-trapezoidal finite difference algorithm on a staggered Cartesian grid, which introduces little numerical diffusion [4]. The semi-implicit approach is based on treating the gravity wave and vertical diffusion terms implicitly to avoid time-step limitations due to gravity wave Courant–Friedrich–Levy conditions, and to guarantee stability of the method [6]. All other terms (including advection) are treated explicitly. Laplacian operators are used to represent mixing. Constant mixing coefficients are used to parameterize the effect of horizontal eddies. A two-equation turbulence model calculates the vertical eddy coefficients of mixing [7]. Computations in each iteration proceed on a water column-by-water column basis, to assemble a five-diagonal system of equations for water surface elevation η, which is solved using a preconditioned-conjugate gradient solver [4]. Horizontal velocities are recovered from the updated values of η.

3. Related Works

Several SWE models have been implemented in parallel that take advantage of their data parallelism. Implementations that use the message passing paradigm with MPI for both 2-D ([8], with one and also two layers in [9], [10], [11]) and 3-D models ([11]) can be found. The implementation of [10] parallelizes a 3-D lattice Boltzmann model using the shared memory paradigm with OpenMP. These MPI and OpenMP implementations use domain decomposition to divide the workload among processes or threads. Performance can also be increased using SSE instructions either explicitly (manually) or through libraries, or, alternatively, using GPUs. [12], for example, presents results of a SSE optimized implementation of a 2-D SWE-model. [13], in turn, solves a 2-D SWE-model using the Intel Integrated Performance Primitives library. An implementation of a 2-D SWE-model in several GPUs supporting CUDA programming toolkit is presented in [14].

Three-dimensional models, like SI3D, manage larger amounts of data and require higher computer performance. Moreover, distributing workload evenly is more difficult because, to the irregular horizontal dimensions or layer dimensions (first and second dimension), the irregular vertical dimension or depth (third dimension) is added.

Some parallel implementations of a semi-implicit 3-D hydrodynamic model, SI3D, are presented and evaluated here. The parallel implementations of the 3-D model combine both message passing (with MPI) and shared memory paradigms (with OpenMP). Implementations with redundant operations (workload overlapping) are compared to non-redundant implementations. Workload overlapping increases the number of operations and decreases communications. This work also analyzes the influence of different platform configurations (such as simultaneous multithreading, Intel SpeedStep and Turbo Mode technologies, and prefetching hardware), and different domain decompositions have on code
Parallel Implementation of a Lake Hydrodynamic Model

performance. Different compiler optimization options and a block-driven processing implementation were also tested.

4. Implementation

Several parallel SI3D versions have been implemented. The speedup achieved in a parallel implementation of SI3D in which OpenMP construct !$OMP PARALLEL DO- END PARALLEL DO is used to locate parallelism was 1.22 with the four cores of a processor. The performance has been increased when the programmer has also done explicitly these tasks: assign jobs to threads; create and destroy threads; communicate and synchronize threads. Moreover, several parallel versions have been implemented in order to compare implementations with redundant operations, which avoid communications and synchronizations (C/S), with non-redundant operation implementations. The results show that redundant operations improve the MPI version performance of SI3D but the OpenMP version increases performance when the redundant operations are reduced by adding some extra synchronization.

Figure 1 shows a flow diagram of the best SI3D parallel implementation. The stage 2 was not parallelized because it is a 2% of the stages 1 and 3 together in the SI3D sequential version. C/S occur several times per iteration. Process 0 assembles and solves the penta-diagonal matrix for free surface elevation η (stage 2), and scatters the values of η among processes. It also occurs at the end of each iteration, where the processes interchange some data of u, v, and η. In the non-redundant MPI version there are additional data interchanges between processes: four in stage 1 and five in stage 3.

The parallel implementations of SI3D use domain decomposition to divide the workload among processes and threads, as is usually done in Computational Fluid Dynamics applications. Domain decomposition is done previous to the start of the simulations (Figure 1). The criteria followed in determining the best domain decomposition is that all the sub-domains should have the same or similar number of wet cells and that the sub-domain data must be stored in contiguous memory positions.

The overhead of the parallel implementations of SI3D, like in other related applications, is mainly affected by:

- Load unbalance. The irregular grid dimensions make difficult to obtain an even distribution.
- Communication time. It depends both on the number of communications and on the amount of data being transferred in each communication. In the data interchanges between processes, both of them depend on the domain decomposition approach used (most of the C/S are border interchanges between processes).
- Extra operations due to sub-domain overlapping. The number of communications can be reduced by overlapping sub-domains. In these overlapping regions, computations are redundant. The overhead that results
from redundant calculations depends on the extent of overlapping regions, and this, in turn, depends on the particular domain decomposition approach used.

Therefore, domain decomposition affect performance, several approaches are possible in 3-D models. Either horizontal-cut or vertical-cut (depth) decomposition can be applied in these cases. Horizontal-cut decomposition distributes layers among sub-domains, i.e. among processors/cores. The degree of parallelism in this case equals the number of layers and communication depends on the horizontal resolution and the horizontal extent of the lake. Given that large differences exist between the horizontal and vertical dimensions of large-scale geophysical systems, the degree of parallelism in the horizontal-cut decomposition tend to be lower than in a vertical-cut decomposition.

Figure 1. Flow diagram of the best parallel algorithm. The diagram includes the MPI transmission points.
Three types of vertical-cut decomposition (of a river, lake, etc.) are possible (Figure 2). The data interchange between the sub-domains is indicated by the arrows in the Figure 2. The length of the boundaries between any two given sub-domains reflects the amount of data exchanged between them. It is also indicative of the amount of redundant calculations if the number of communications is reduced by overlapping sub-domains. The total length of the sub-domain boundaries will depend on the particular geometry of the water body being simulated, and on how the domain is partitioned among processes. The number of interchange communications is larger if one uses the two-direction cut distribution, as shown in Figure 2(c). The total amount of data exchanged among processes and the number of redundant calculations, though, could be less than in the other two distributions, depending on the particular geometry and number of sub-domains. With this distribution a process can both send to and receive from more than two processes. Both narrow (Figure 2(b)) and wide (Figure 2(a)) cut distributions have the same number of interchange communication operations. A process will send to and receive from just one or two processes. Larger amounts of data are exchanged and more redundant operations are done in the distribution shown in Figure 2(a) (wide-cut distribution). [15] compares the alternatives in Figure 2(b) and Figure 2(c) using MPI in a cluster of four AMD Opteron 2.2 GHz nodes (2 cores each) connected through Gigabit Ethernet. The results for different grid sizes show that better performances are achieved if the decomposition is done using narrow cut distribution compared to the two-direction distribution. [8] compares the alternatives in Figure 2(a) and Figure 2(b) using MPI in a CC-NUMA HP/Convex Exemplar X-Class (SPP2200) with 64 processors distributed in four hyper-nodes. The eight nodes of a hyper-node are connected through a network (switch) of 960 MB/s bandwidth in each link direction [16] (the network of the Exemplar is an implementation of the standard SCI). The results show that narrow-cut distribution reduces execution time compared to wide-cut distribution. Here some tests (Section 5) compare wide and narrow-cut distributions with both message passing and shared memory paradigms in S13D. Note that the alternative in the Figure 2(c) has less data locality compared to the alternatives in (Figure 2(b)) and (Figure 2(a)). The data of a sub-domain in the wide and narrow distribution were stored in disk and memory in contiguous positions in order to improve locality. The lack of locality decreases performance, especially in shared memory implementations.

![Figure 2](image_url)

**Figure 2.** Three domain decomposition alternatives with vertical cut: (a) wide cut distribution, (b) narrow cut distribution, (c) two-direction cut distribution. Arrows show the communication needed among sub-domains in this kind of applications.
A block-driven processing approach was also tested as in the shared memory implementation in [10]. Extra communication and block-driven implementation are also suitable in a process-level parallel implementation when the memory of the processing node is not enough for the application ([17],[9]).

5. Test Results

Platform
The results have been obtained in a small commodity cluster of three nodes connected through a Gigabits Ethernet switch. Each node has 6 GB of memory and a Core i7 CPU 920 (launch date: fourth quarter of 2008). The Core i7 920 has four cores of 2.667 GHz (two threads per core if Hyper-Threading is active), L3 cache of 8 MB shared by all the cores, and QuickPath of 4.8 GT/s. The cluster price was of 3,000 € (first quarter of 2009) approximately with all the components, including the cabinet. It runs Linux Fedora 10 (kernel 2.6.27.41). Cluster communication system has a bandwidth of 113 MB/s, near to the theoretic 125 MB/s.

The program is compiled using Intel Fortran 11.1 compiler. The OpenMP of this compiler is used for the shared memory implementation and MPICH-1.3 for the MPI message passing implementation. The source-code versions implemented were compiled using options that drive classic optimizations and vectorizations. Table 1 summarizes the optimization options checked. Similar execution times are obtained with O2 and O3. When the options ipo and/or SSE4.2 are added to O2 or O3 performance does not improve. PGO does not improve the execution time compared to a version with the same optimization options but without PGO. The executables used in this section have been obtained with O2 and openmp compiler options.

Practical Application
The test application is a simulation of the currents in Lake Tahoe. The ultimate goal of these simulations is to characterize the pathways of transport of young life stages of an invasive species (the bivalve *Corbicula fluminea*, or Asian clam).
from the existing near-shore beds to other sites in the lake and the environmental conditions they would be exposed to en route. Given that \(O(10^2)\) m (hundreds) features of the velocity fields, characteristics of nearshore regions, should be resolved in Lake Tahoe, the computational grid cells should have horizontal dimensions of at least \(O(10)\) m (tens). Simulating a lake of the size of Lake Tahoe (roughly 20 km x 30 km) with \(O(10)\) m horizontal size cell columns, poses a serious computational problem which can only be addressed through the use of parallel computers. For example, the ratio of real to computational time in simulations conducted with 50 m wide grid cells in a single core of the cluster is approximately 1/1. The simulations presented here are conducted in grids with 95 layers of variable thickness and squared columns of 50 m x 50 m in the horizontal. The grid includes 14,654,639 computational cells in 197,781 columns.

**Performance of different platform configurations**

This work analyzes the influence in performance of the multiple cores in a node, the prefetching hardware, the Intel Hyper-Threading technology, and the Intel SpeedStep and Turbo Mode technology.

Hardware prefetcher monitors data access patterns and prefetches data automatically into processor caches. Core i7 cores can track 16 forward streams and 4 backward streams each. Simultaneous multithreading allows the execution of multiple threads in a core; in particular, two threads with Intel Hyper-Threading. Intel SpeedStep Technology allows the operating system to control the core speed. Intel Turbo Mode Technology allows processor cores to run faster than the assigned frequency under specific conditions.

Table 2 shows the seconds per iteration obtained for different platform configurations and different number of processes and threads. The narrow-direction distribution and the MPI redundant operation version have been used. The communication time due to data distribution or collection is not included because it does not depend on the number of iterations. Up to four threads are used to each node; a higher number of threads makes performance worst despite of Hyper-Threading being enabled. The column HSTP shows the results for the default configuration. In the default configuration the BIOS and the operating system have enabled Hyper-Threading (H), SpeedStep (S) and Turbo Mode (T), and prefetching hardware (P). In particular, ondemand is the default CPUfreq governor of the cluster operating system, which means the governor sets the frequency depending on the current usage, between a minimum of 1.6 GHz and a maximum of 2.667 GHz, last one can increase due to Turbo Mode. The time in the default configuration is less reproducible due to the thread distribution of the operating system among the eight logical cores of a node. If Hyper-Threading is disabled (column -STP) performance improves, but if either SpeedStep/Turbo Mode (column ---P) or Prefetching (column -ST-) are also disabled, time increases slightly. The results in the columns -STP and ---P show an increment in the clock frequency due to the Turbo Mode. The results in the columns -STP and -ST- suggest that the prefetching hardware is being weakly used.
Block-driven processing was added to try to reduce cache miss by facilitating data locality. It reduces the execution time by 4% with horizontal cell size of 100 m x 100 m and one process with four threads. Block processing improves only marginally this implementation's performance, although it never makes performance worst as it was observed in the block processing implementation of [10]. The results in [10] are obtained in a platform of IBM with Power5+ 1.9 GHz. For a grid of 1024x1024x10 (=10,485,760 cells), from 1 to 8 processors block-driven processing makes performance worst but from 12 to 16, the maximum number of processors tested, the block-driven implementation improves performance [10].

The results presented in the next subsections are obtained with the configuration –STP and ondemand as the CPUfreq governor.

Comparison of wide-direction and narrow-direction distributions in both MPI versions, with and without redundant operations

Both, wide-direction and narrow-direction distributions, have the same number of communication in both MPI versions, but they are of different sizes. Also, in the MPI version with redundant operations, the wide-direction distribution has more redundant operations than the narrow-direction approach (because it has larger border length).

Table 3 shows the execution time per iteration and speedup for both wide and narrow-direction distribution and both the MPI implementation with redundant operations (R) and the MPI approach with non-redundant operations (NR). As can be observed narrow-cut distribution also improves sequential execution time. The best approach is to use the MPI implementation with redundant operations and the narrow-cut distribution. Speedup improves more with the narrow-cut approach because this approach has lesser border length than the wide-cut approach; the border size is decreased a 25% approximately.

<table>
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<th>No. Processes</th>
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<th>-STP</th>
<th>--P</th>
<th>-ST-</th>
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<tr>
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<td>2.68</td>
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</tr>
</tbody>
</table>

Table 2. Performance of different platform configurations (seconds per iteration). In HSTP, H means Hyper-Threading enable, S means SpeedStep enable, T means Turbo enable, and P mean Prefeching enable. “ -“ means Disable.
6. Conclusion

This work discusses the performance of several thread- and process-level implementations of a semi-implicit 3-D lake hydrodynamic model (SI3D) and the influence of different platform configurations and domain decompositions. It has been found that:

- The program makes a weak use of the prefetching hardware (prefetching decreases execution time by between %5 to %8) and obtains little improvements by using block-driven processing (%4 improvement approximately).
- Intel® Turbo Mode Technology decreases slightly the execution time (by between %3 to 7%).
- Performance is worse if the default BIOS and operating system configuration is used (time increases by between %40 to 60%, depending on the number of processes and threads). This is due to the thread distribution of the operating system among the eight logical cores of a node when Hyper-Threading is enabled. Thread affinity could be used to avoid this problem instead of disable Hyper-Threading.
- Block-driven processing reduces execution time too slightly.
- Process level implementation reduces execution time using overlapping sub-domains (redundant operations).
- With the best parallel implementation and performance configuration, and with narrow-cut domain decomposition the simulation of 24 hours with 50mx50m cell columns in a core of the cluster requires approximately 6 hours.

<table>
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<tr>
<th>Tahoe 50m</th>
<th>Sec./iteration</th>
<th>Speedup</th>
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<td>No. Th</td>
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<td></td>
<td></td>
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<tr>
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<td>3 4</td>
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<td>2.51</td>
</tr>
</tbody>
</table>

Table 3. Wide and narrow distributions in both MPI versions: with (R) and without (NR) redundant operations
with one processor (4 threads) instead of 20 hours and 30 minutes (with 1 thread) and approximately 2 hours and 30 minutes with the three processors (12 threads).

Acknowledgment

This work was partially funded by the project ‘Risk Assessment of Asian clam expansion and potential environmental impacts to Lake Tahoe. Task: Larval Transport Modelling’ funded by Pacific Southwest Research Station, USDA Forest Service.

References


On the Visualization of Honeypot Data through Projection Techniques

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Abstract

A crucial aspect in network monitoring for security purposes is the visual inspection of traffic patterns, which chiefly provides the network manager with a synthetic and intuitive representation of the current situation. In keeping with this idea, neural projection techniques can adaptively map high-dimensional data into a low-dimensional space, for the user-friendly visualization of data collected by different security tools. Different projection methods for the visual inspection of honeypot data are applied in this study, which may be seen as a complementary network security tool that sheds light on internal data structures through visual inspection. Empirical verification of the proposed projection methods was performed in an experimental domain where 1-month data sets were captured and stored for analysis. Experiments showed that whereas an Intrusion Detection System may only identify a low percentage of the malicious traffic, a deeper understanding of attack patterns could easily be gained by means of visual inspections.
On the Visualization of Honeypot Data through Projection Techniques

Keywords: Projection Models, Artificial Neural Networks, Unsupervised Learning, Network & Computer Security, Intrusion Detection, Honeypots.

1. Introduction

A network attack or intrusion will inevitably violate one of the three computer security principles—availability, integrity and confidentiality—by exploiting certain vulnerabilities such as Denial of Service, Modification and Destruction [1]. One of the most harmful issues of attacks and intrusions, which increases the difficulty of protecting computer systems, is precisely the ever-changing nature of attack technologies and strategies.

For that reason alone, among others, Intrusion Detection Systems (IDSs) have become a very necessary asset in addition to the computer security infrastructure of most organizations. In the context of computer networks, an IDS can roughly be defined as a tool designed to detect suspicious patterns that may be related to a network or system attack. Intrusion Detection (ID) is therefore a field that focuses on the identification of attempted or ongoing attacks on a computer system (Host IDS - HIDS) or network (Network IDS - NIDS).

Visual inspection of traffic patterns is an alternative and crucial aspect in network monitoring [2]. Visualization is a critical issue in the computer network defence environment, which chiefly serves to generate a synthetic and intuitive representation of the current situation for the network manager; as a result, several research initiatives have recently applied information visualization to this challenging task [3] [4] [5] [6]. Visualization techniques typically aim to make the available statistics supplied by traffic-monitoring systems more understandable in an interactive way. They therefore focus on traffic data as well as on network topology. Regardless of their specific characteristics, these methods all map high-dimensional feature data into a low-dimensional space for presentation purposes. The baseline of the research presented in this study is that Artificial Neural Networks (ANNs), in general, and unsupervised connectionist models [7, 8], in particular, can prove quite adequate for the purpose of network data visualization through dimensionality reduction. As a result, unsupervised projection models are applied in the present research for the visualization and subsequent analysis of Honeypot data.

The remaining five sections of this study are structured as follows: section 2 contains a brief description of Intrusion Detection (mainly visualization-based). Section 3 presents the approach proposed for ID and the neural projection techniques applied in this work. Some experimental results are presented and described in section 4; the conclusions of this study are discussed in section 5, as well as future work.
On the Visualization of Honeypot Data through Projection Techniques

2. Intrusion Detection and Honeynets

The accurate detection in real-time of computer and network system intrusions has always been an interesting and intriguing problem for system administrators and information security researchers. It may be attributed on the whole to the dynamic nature of systems and networks, the creativity of attackers, the wide range of computer hardware and operating systems and so on. Such complexity arises when dealing with distributed network-based systems and insecure networks such as the Internet.

A honeypot has no authorised function or productive value within the corporate network other than to be explored, attacked or compromised [9]. Thus, a honeypot should not receive any traffic at all. Any connection attempt with a honeypot is then an attack or attempt to compromise the device or services that it is offering—is by default illegitimate traffic. From the security point of view, there is a great deal that may be learnt from a honeypot about a hacker’s tools and methods in order to improve the protection of information systems.

One of the most extended classifications of honeypots takes into account their level of interaction. Low interaction honeypots offer limited interaction with attackers and the most common ones only simulate services and operating systems. High interaction honeypots follow a different strategy: instead of using simulated services and operating systems, real systems and applications are used, usually running in virtual machines.

Somewhere between the two are medium interaction honeypots, which also emulate vulnerable services, but leave the operating system to manage the connections with their network protocol stack. Recently, a new type of honeypot has been proposed as a response to the behavioural change observed in the attackers. Instead of waiting for the attackers to reach traditional honeypots, client side honeypots, also known as honeyclients, scan communication channels looking for malware.

In a honeynet, all the traffic received by the sensors is suspicious by default. Thus every packet should be considered as an attack or at least as a piece of a multi-step attack. Numerous studies propose the use of honeypots to detect automatic large scale attacks; honeyd [10] and nepenthes [11] among others. The first Internet traffic monitors known as Network Telescopes, Black Holes or Internet Sinks were presented by Moore et al. [12].

3. A Visualization-based Approach

This work proposes the application of projection models for the visualization of Honeypot data. Visualisation techniques have been applied to massive datasets, such as those generated by honeynets, for many years. These techniques are considered a viable approach to information seeking, as humans are able to recognize different features and to detect anomalies by inspecting graphs [13]. The underlying operational assumption of the proposed approach is mainly grounded in the ability to render the high-dimensional traffic data in a consistent
yet low-dimensional representation. So, security visualisation tools have to map high-dimensional feature data into a low-dimensional space for presentation. One of the main assumptions of the research presented in this paper is that neural projection models will prove themselves to be satisfactory for the purpose of security data visualisation through dimensionality reduction. This problem of identifying patterns that exist across dimensional boundaries in high dimensional datasets is a challenging task. Such patterns may become visible if changes are made to the spatial coordinates. However, an \textit{a priori} decision as to which parameters will reveal most patterns requires prior knowledge of unknown patterns.

Projection methods project high-dimensional data points onto a lower dimensional space in order to identify "interesting" directions in terms of any specific index or projection. Having identified the most interesting projections, the data are then projected onto a lower dimensional subspace plotted in two or three dimensions, which makes it possible to examine the structure with the naked eye. Projection methods can be smart compression tools that map raw, high-dimensional data onto two or three dimensional spaces for subsequent graphical display. By doing so, the structure that is identified through a multivariable dataset may be visually analysed with greater ease.

Visualisation tools can therefore support security tasks in the following way:

- Visualisation tools may be understood intuitively (even by inexperienced staff) and require less configuration time than more conventional tools.
- Providing an intuitive visualisation of data allows inexperienced security staff to learn more about standard network behaviour, which is a key issue in ID [14]. The monitoring task can be then assigned to less experienced security staff.
- As stated in [3], "\textit{visualizations that depict patterns in massive amounts of data, and methods for interacting with those visualizations can help analysts prepare for unforeseen events}". Hence, such tools can also be used in security training.
- They can work in unison with some other security tools in a complementary way.

As with other machine learning paradigms, an interesting facet of ANN learning is not just that the input patterns may be precisely learned/classified/identified, but that this learning can be generalised. Whereas learning takes place within a set of training patterns, an important property of the learning process is that the network can generalise its results on a set of test patterns that were not previously learnt. The identification of unknown patterns fits the 0-day attack [15] detection. Due to the aforementioned reasons, the present study approaches the analysis of honeynet data from a visualization standpoint. That is, some neural projection techniques are applied for the visualization of such data. The different projection models applied in this study are described in the following sections.
3.1 Principal Component Analysis

Principal Component Analysis (PCA) is a statistical model, introduced in [16] and independently in [17], that describes the variation in a set of multivariate data in terms of a set of uncorrelated variables each, of which is a linear combination of the original variables. Its goal is to derive new variables, in decreasing order of importance, that are linear combinations of the original variables and are uncorrelated with each other. From a geometrical point of view, this goal mainly consists of a rotation of the axes of the original coordinate system to a new set of orthogonal axes that are ordered in terms of the amount of variance of the original data they account for. The optimal projection given by PCA from an $N$-dimensional to an $M$-dimensional space is the subspace spanned by the $M$ eigenvectors with the largest eigenvalues.

According to [18], it is possible to describe PCA as a mapping of vectors $x^d$ in an $N$-dimensional input space $(x_1, ..., x_N)$ onto vectors $y^d$ in an $M$-dimensional output space $(y_1, ..., y_M)$, where $M \leq N$. $x$ may be represented as a linear combination of a set of $N$ orthonormal vectors $W_i$:

$$x = \sum_{i=1}^{N} y_i W_i$$  \hspace{1cm} (1)

Vectors $W_i$ satisfy the orthonormality relation:

$$W_i^T W_j = \delta_{ij}$$  \hspace{1cm} (2)

where $\delta_{ij}$ is the Kronecker delta.

Making use of equation (1), the coefficients $y_i$ may be given by

$$y_i = W_i^T x$$  \hspace{1cm} (3)

which can be regarded as a simple rotation of the co-ordinate system from the original $x$ values to a new set of co-ordinates given by the $y$ values. If only one subset $M < N$ of the basis vectors, $W_i$, is retained so that only $M$ coefficients $y_i$ are used, and having replaced the remaining coefficients by constants $b_i$, then each $x$ vector may be approximated by the following expression:

$$\tilde{x} = \sum_{i=1}^{M} y_i W_i + \sum_{i=M+1}^{N} b_i W_i$$  \hspace{1cm} (4)

Consider the whole dataset of $D$ vectors, $x^d$ where $d = 1, ..., D$.

PCA can be performed by means of ANNs or connectionist models such as [19, 20, 21, 22, 23]. It should be noted that even if we are able to characterize the data with a few variables, it does not follow that an interpretation will ensue.
3.2 Cooperative Maximum Likelihood Hebbian Learning

The Cooperative Maximum Likelihood Hebbian Learning (CMLHL) model [24] extends the Maximum Likelihood Hebbian Learning (MLHL) [25] model, which is based on Exploratory Projection Pursuit (EPP) [26]. The statistical method of EPP was designed for solving the complex problem of identifying structure in high dimensional data by projecting it onto a lower dimensional subspace in which its structure is searched for by eye. To that end, an “index” must be defined to measure the varying degrees of interest associated with each projection. Subsequently, the data is transformed by maximizing the index and the associated interest. From a statistical point of view the most interesting directions are those that are as non-Gaussian as possible.

The MLHL model is based on the Negative Feedback Network and, as the AABP model; it associates an input vector, \( x \in \mathbb{R}^D \), with an output vector, \( y \in \mathbb{R}^Q \). In this case, the output of the network (\( y \)) is computed as:

\[
y_i = \sum_{j=1}^{N} W_{ij} x_j, \forall i
\]  

(5)

where, \( W_{ij} \) is the weight linking input \( j \) to output \( i \).

Once the output of the network has been calculated, the activation (\( e_j \)) is fed back through the same weights and subtracted from the input:

\[
e_j = x_j - \sum_{i=1}^{M} W_{ij} y_i, \forall j
\]  

(6)

Finally, the learning rule determines the way in which the weights are updated:

\[
\Delta W_{ij} = \eta, y_i, \text{sign}(e_j) |e_j|^{p-1}
\]  

(7)

where, \( \eta \) is the learning rate and \( p \) is a parameter related to the energy function.

The main difference between the basic MLHL model and its Cooperative version is the introduction of lateral connections. After the Feed forward step (Eq. 5) and before the Feed back step (Eq. 6), lateral connections between the output neurons are applied as follows:

\[
y_i(t+1) = \left[ y_i(t) + \tau(b - Ay) \right]^+
\]  

(8)

where, \( \tau \) is the “strength” of the lateral connections, \( b \) is the bias parameter and \( A \) is a symmetric matrix used to modify the response to the data. Its effect is based on the relation between the distances among the output neurons.

4. Experiments and Results

The Euskalert project [26] has deployed a network of honeypots in the Basque Country (northern Spain) where eight companies and institutions have installed
one of the project’s sensors behind the firewalls of their corporate networks. The honeypot sensor transmits all the traffic received to a database via a secure communication channel. These partners can consult information relative to their sensor (after a login process) as well as general statistics in the project’s website. Once the system is fully established, the information available can be used to analyse attacks suffered by the honeynet at network and application level. Euskalert is a distributed honeypot network based on a Honeynet GenIII architecture [26]. This honeypot system receives 4000 packets a day on average. All the traffic is analyzed by the Snort IDS, and an alert is launched whenever the packet matches a known attack signature. For this experiment, we have analysed the logs coming from Euskalert and Snort gathered during February 2010. Fig. 1 shows the traffic volume in terms of number of packets received for that period of time.

![Figure 1](image.png)

**Fig. 1.** Temporal distribution of the traffic volume in terms of number of packets captured by Euskalert in February, 2010.

The February 2010 dataset contains a total of 3798 packets, including TCP, UDP and ICMP traffic received by the distributed honeypot sensors. The characterization of the traffic in the dataset is shown in Table 1. The table shows which alerts have been triggered in that period of time and their percentage. Those signatures starting with “Wormledge” are automatically generated and not present in the default signature database.

From this dataset, it may be said that a misuse detection-based IDS such as Snort is only capable of identifying about 10.38% of bad-intentioned traffic. Furthermore, it was demonstrated that only 2% of the unsolicited traffic was identified by the IDS when automatically generated signatures were included from a previous work [27]. Thus, a deeper analysis of the data is needed in order to discover the internal structure of the remaining 90% of the traffic. Explaining the behaviour of the unknown traffic is a difficult task that must be performed to better protect computer networks and systems.
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<th>Signature</th>
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<th>%</th>
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<td>89,62</td>
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<tr>
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<td>3,34</td>
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<td></td>
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</tbody>
</table>
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depicted with different colors and shapes, taking into account the destination port; from 3 to 10371: red circles, from 10371 to 20739: black crosses, from 20739 to 31107: green pluses, from 31107 to 41475: magenta stars, from 41475 to 51843: yellow squares, and from 51843 to 62205: cyan diamonds.

Fig. 2. Projections of data traffic captured by Euskalert, in February, 2010.

5. Conclusions and Future Work

From the projections in Fig. 2 we can conclude that CMLHL provides a more sparse representation that the other two methods. This enables the intuitive visualization of the honeynet, where the general structure of these data can be seen. After getting a general idea of the dataset structure, an in-depth analysis was
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carried out to comprehensively analysed each one of the points in the groups identified by CMLHL. As a result, the following conclusions can be stated for each one of the destination ports in the analysed dataset:

- 8: ICMP ping, used for probing the Internet, looking for victim hosts.
- 22: SSH. It seems to be a traffic flow with many packets coming from one source to one of the honeypot. They correspond to connection attempts by attackers or infected machines.
- 80: HTTP. Attackers try different vulnerabilities against web applications.
- 135: DCE endpoint resolution, used by Microsoft for Remote Procedure Call protocol. It has always been and still is one of the most exploited services by virus and worms.
- 139: NETBIOS Session Service. Plenty of attacks to this Microsoft Windows service can be found.
- 443: HTTP protocol over TLS SSL connection attempts.
- 445: SMB directly over IP. As most of the traffic in the biggest group identified by CMLHL is aimed at this destination port, we can conclude that this is a widely exploited service.
- 1433: Microsoft-SQL-Server, used by the old SQL Slammer worm.
- 1521: Oracle TNS Listener. It seems that attackers try to connect to the honeypot via Oracle service.
- 2967: Symantec System Center. Vulnerabilities have been found on Symantec service, and it is being expiated in the wild.
- 3128: Proxy Server // Reverse WWW Tunnel Backdoor, where the MyDoom worm operates.
- 3389: MS Terminal Services, used for Remote Desktop.
- 4444: This port is a common return port for the rpc dcom.c buffer overflow vulnerability and for the msblast rpc worm.
- 4899: Remote Administrator default port. There is a known remote exploitable vulnerability in radmin server versions 2.0 and 2.1 that allows code execution.
- 5061: SIP-TLS. Used for VoIP communications.
- 5900: Virtual Network Computer or VNC, used also as a remote desktop solution.
- Port 8080: HTTP Alternate, used as an HTTP proxy.
- Port 19765: Used in Kademlia (Bittorrent protocol).

Future work will combine the honeypot data with the output of a signature-based IDS, such as Snort, in the same visualization. This will validate the proposed approach as a complementary tool that can be combined with some other security tools or IDSs.

Acknowledgments

This research has been partially supported through the Regional Government of Castilla y León under Project BU006A08, the Department of Research, Education and Universities of the Basque Government; and the Spanish Ministry of Science.
On the Visualization of Honeypot Data through Projection Techniques and Innovation (MICINN) under projects CIT-020000-2008-2 and CIT-020000-2009-12. The authors would also like to thank the vehicle interior manufacturer, Grupo Antolin Ingenieria S.A., within the framework of the MAGNO2008 – 1028.- CENIT Project also funded by the MICINN.

References

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A Study of Meteorological Conditions by means of Soft Computing Models

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Abstract

In this interdisciplinary study, soft computing models are used to identify typical days in terms of their meteorological conditions. Meteorological and pollution data were taken from a pollution measurement station in the Spanish Autonomous Region of Castile-Leon. In this case, six meteorological variables are considered for the second half of 2006. The relation between the variables and the evolution of its values throughout the day is shown through the application of statistical and soft computing models. Two case studies are analyzed, in an attempt to identify a ‘Typical’ day in Summer and Autumn, 2006. Differences between the various methods are discussed and comparisons drawn with the results of similar studies in other periods.

Keywords: artificial neural networks; soft computing; meteorology; atmospheric pollution

1. Introduction

In recent years, our knowledge of atmospheric pollution and our understanding of its effects have advanced greatly. It has now been accepted for some years that air pollution not only represents a health risk, but that it also reduces, for example, food production and vegetative growth due to its effects on photosynthesis. Other serious consequences may be mentioned such as acid rain, corrosion, climate change and global warming. Thus, all efforts that are directed towards studying
these phenomena may improve our understanding and help to prevent the serious problematic nature of atmospheric pollution.

Finding solutions to current environmental problems constitutes a fundamental step towards life with a sense of sustainability. Fulfilling such a wish is to a great extent determined by the preservation of a clean atmosphere given its impact on the dynamics of the biosphere.

Systematic measurements in Spain, which are usually taken within large cities, are fundamental due to the health risks caused by high levels of atmospheric pollution. Recent trends point to the benefits of continuing to extend the network of atmospheric pollution measurement stations.

The basis of this study is the application of a series of statistical and soft computing models to identify what may be called ‘Typical Days’ in terms of previously selected meteorological variables.

The rest of this study is organized as follows. Section 2 presents the statistical and soft computing methods applied throughout this research. Section 3 details the various case studies and Section 4 describes the experiments and results. Finally, Section 5 sets out the conclusions and future lines of work.

2. Statistical and Soft Computing Models

Several statistical and soft computing models are used in this study, although the results are only shown of those that offer the best performance.

1. Principal Components Analysis (PCA)

PCA [1] gives the best linear compression of the data in terms of least mean square error and can be implemented by several artificial neural networks [2, 3]. The basic PCA network [4] applied in this study is described by the next three equations (Eq.1 to Eq.(3)): an $N$-dimensional input vector at time $t$, $x(t)$, and an $M$-dimensional output vector, $y$, with $W_{ij}$ being the weight linking input $j$ to output $i$, and $\eta$ being the learning rate. Its activation and learning may be described as follows:

Feedforward step, “Eq. (1)”: 
$$y_i = \sum_{j=1}^{N} W_{ij} x_j, \forall i$$  \hspace{1cm} (1)

Feedback step, “Eq. (2)”: 
$$e_j = x_j - \sum_{i=1}^{M} W_{ij} y_i$$  \hspace{1cm} (2)

Change weights, “Eq. (3)”: 
$$W_{ij} = W_{ij} + \eta e_j y_i$$
2. An Exploratory Projection Pursuit Neural Model (EPP)

EPP [2, 3] projects the data onto a low dimensional subspace which allows its structure to be examined by eye. This is done by means of an index that measures the “interestingness” of a given projection, the data for which is then represented by projections that maximize the most “interesting” vectors. “Interesting” structure is usually defined with respect to the fact that most projections of high-dimensional data onto arbitrary lines through most multi-dimensional data give almost Gaussian distributions [2, 5]. Therefore to identify “interesting” features in data, it is important to look for those directions onto which the data-projections are as far from the Gaussian as possible.

3. Cooperative Maximum Likelihood Hebbian Learning (CMLHL)

CMLHL [6, 7] is an extended version of MLHL [6, 8] adding lateral connections which have been derived from the Rectified Gaussian Distribution [9]. The resultant net can find the independent factors of a data set but does so in a way that captures some type of global ordering in the data set.

Consider an $N$-dimensional input vector $x$, an $M$-dimensional output vector $y$ and a weight matrix $W$, where the element $W_{ij}$ represents the relationship between input $x_j$ and output $y_i$, then as is shown in [6, 10], the CMLHL can be carried out as a four-step procedure:

Feed-forward step, outputs are calculated “Eq. (4)”:

$$y_i = \sum_{j=1}^{N} W_{ij} x_j, \forall i$$

(4)

Lateral activation passing step, “Eq. (5)”:

$$y_j(t+1) = [y_j(t) + \tau(b-Ay)]^+$$

(5)

Feedback step, “Eq. (6)”:

$$e_j = x_j - \sum_{i=1}^{M} W_{ij} y_i, \forall j$$

(6)

Weights update step, learn the neural network, “Eq. (7)”:

$$\Delta W_{ij} = \eta y_i \text{sign}(e_j) |e_j|^{p-1}$$

(7)

Where $t$ represents an instant, $[ \cdot ]^+$ is necessary to ensure that the $y$-values remain in the positive quadrant, $\eta$ is the learning rate, $\tau$ is the "strength" of the lateral connections, $b$ the bias parameter, $p$ a parameter related to the energy function, and $A$ is a symmetric matrix used to modify the response to the data. The effect of this matrix is based on the relation between the distances separating the output neurons.
3. **Case of Study. Identifying the Typical Day in Summer and Autumn**

This study presents interesting results related to the evolution of different meteorological parameters using the records of an air quality control station (made available by the Department of the Environment-Directorate of Environmental Quality of the Government of the Spanish Autonomous Region of Castile-Leon) [11, 12]. The aforementioned station is situated in the urban area of the Spanish city of Burgos. The study was conducted over approximately half a year in 2006.

In this study, the following variables were analyzed: wind direction (degrees), wind speed (m/s), dry temperature (Cº), relative humidity (%), atmospheric pressure (mbar) and solar radiation (W/m²).

The general characteristics of the site where the measurement station used in the study is situated are as follows: Burgos, a city in the north-centre of Spain with a population of around 170,000 inhabitants and a total municipal area of approximately 107 km². The city of Burgos is 854 masl (meters above sea level) at latitude (N) 42º20’ and longitude (W) 3º42’. The measurement station is located within the city and may be classified as an urban station.

The aim of the present study is to identify the existence of ‘Typical’ meteorological days or at least to find some kind of associated patterns, for which purpose several statistical and soft computing methods were used. Only the results of applying PCA and CMLHL are shown. This is because PCA (Section 2.1) is the statistical method which offers a vision of the internal structure of the information and CMLHL (Section 2.3) is a Soft Computing Model which provides the best results in terms of identifying internal structure.

4. **Experiments and Results**

As stated, the aim of this study is to identify the ‘Typical Day’ in Summer and the ‘Typical Day’ in Autumn for 2006.

The study, which forms part of a more ambitious project [13, 14], is based on a file containing meteorological and pollution data sets recorded at fifteen-minute intervals: a daily total of 96 records for the second part of 2006, referring to six variables, as explained in Section 3.

The information represented at each point is visually labelled from Fig. 1 to Fig. 2, which shows the record number, (from record numbered as 1.-0:00 AM, to record numbered as 96.-23:45 PM). All data was normalized for the study.

1. **Typical Day in Summer**

The graphical results obtained in this study for a Typical Day in Summer are presented (Figure 1) and analyzed as follows.
A Typical Day in Burgos, Summer 2006, according to the results of applying PCA to the meteorological variables, is shown in Figure 1(a). Two data clusters are identified. $C_2$ is related to samples with the highest values of solar radiation and temperature which correspond to the records taken around midday and the early afternoon, from 12:00PM to 16:00PM approximately. Cluster $C_1$ is related to samples with the lowest values which correspond to the rest of the day. Cluster $C_2$ contains fewer samples than $C_1$. These are the general characteristics of a Typical Day in Summer: variations between the different Typical Days are explained by the lowest values of the most representative variables -temperature and solar radiation- for the day being found among the earliest or the latest records of the day. But this is not enough, it is necessary to study the samples contained into the cluster $C_1$, for this reason it is important to apply soft computing models in order to obtain finer a response.

Figure 1(b) is obtained by applying CMLHL to the data set. Cluster $C_2$ contains the same samples as in Figure 1(a). In this case CMLHL is able to identify three clusters instead of two, achieving a sparser representation. Cluster $C_1$ in Figure 1(a) contains the same samples as clusters ($C_{1a}$ and $C_{1b}$). Cluster $C_{1a}$ contains samples from late evening, just before sunset, and cluster $C_{1b}$ contains the samples belonging to the night-time, at which time solar radiation is almost null.

2. Typical Day in Autumn

The graphical results obtained in this study for a Typical Day in Autumn are presented (Figure 2) and analyzed below.
Figure 2. Typical Day in Autumn. (a) PCA Projections (b) CMLHL Projections

Figure 2(a) shows the results of applying a PCA model to identify a Typical Day in Autumn, which once again highlights two clusters (C₁ and C₂) in a similar way to Figure 1. Cluster C₂ is again related to samples with the highest values of solar radiation and temperature, which correspond to the records taken around midday and the early afternoon. In this case, C₂ in Figure 2 contains fewer samples than it does in Figure 1. This is because sunset is earlier in the day. A further difference is that the C₂ cluster is closer to cluster C₁ in Figure 2 than it is in Figure 1, which is because there is not so much variability in autumn data values throughout the day as they are in the Summer period.

Figure 2(b) shows the graphical results of applying CMLHL. Cluster C₂ contains the same samples as in Figure 1(a), but in a more grouped form. Again, in this case, CMLHL is able to identify three clusters instead of two. Cluster C₁ in Figure 1(a) contains the same samples as in Figure 2 (C₁a and C₁b). Cluster C₁a contains most of the samples, and cluster C₁b contains few samples belonging to the night, where a significant variability of the wind direction is observed. The detection of this effect is an interesting example of how a model like CMLHL can help us to analyze complex data sets.

5. Conclusions and Future Works

In this study it has been possible to demonstrate the validity of soft computing models for the identification of the so-called “Typical Day” of Summer and Autumn in 2006, as it was possible in 2007 [15].

PCA provides a first approximation to the internal structure of the data, but other soft computing models provide a top response, discovering new clusters of information which represent extra information. Several soft computing models were applied, and in this case only the results of PCA and CMLHL are shown.
The Typical Day in Summer in the city of Burgos is characterized by sudden changes in temperature and in solar radiation. Due to these factors, it is easy to identify a cluster corresponding to the central hours of the day, as temperature decreases very quickly at sunset.

In contrast, the variability of solar radiation and temperature is smoother in the Typical Day in Autumn in the city of Burgos. The clusters are not so clearly identified due to the evolution of the data values throughout the day.

In [15], a similar study was undertaken in 2007. The results of both studies are consistent. In subsequent studies, other seasons and annual periods will be analyzed, and a meticulous comparison will be made between those studies and public information on atmospheric pollution and meteorological conditions.

Acknowledgments. This research has been partially supported through projects BU006A08 and BU035A08, both of the JCyL, and project CIT-020000-2008-2 of the Spanish Ministry of Education and Innovation. The authors would also like to thank the vehicle interior manufacturer, Grupo Antolín Ingeniería, S.A., within the framework of the project MAGNO2008 - 1028.- CENIT Project funded by the Spanish Ministry.

6. References


Orthogonal Zero-Interpolants: Properties & Applications

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Abstract

This paper deals with the notion of “Orthogonal Zero Interpolants” (OZI) which have several properties similar to the classical orthogonal polynomials. OZI are constructed in such a way that they interpolate the “Zero Function” at a finite number of pre-assigned nodes, even of multiple orders, in the sense of Hermite. These polynomials are also determined by the 3-term recurrence relation. We shall discuss structure and some properties of OZI along with their applications to certain approximation and boundary value problems.

Key words: $L^2$-approximation, Hermite interpolation, Orthogonal Zero Interpolants, Erdos-Turan theorem, 3-term recurrence relation, Two-point boundary value problem.

1. Introduction

Solution of several approximation problems and quite a few numerical solutions of boundary value problems (BVP) are based on orthogonal polynomials with respect to Jacobi weight functions $\omega_{\alpha,\beta}(x) := (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$ over $[-1,1]$. These polynomials, in general, are not suitable for determining solution of the problems subject to constraints. Here, we present some problems and discuss their solutions by a specific class of polynomials which we shall refer to as orthogonal zero interpolants. In order to avoid repetition, we list below some notations which will be frequently used in this paper:

$\omega(t) :=$ Positive weight function defined on $[c,d]$

$L^2_{\omega}[c,d] :=$ Class of functions $f$ with $\|f\|_{\omega[c,d]} := \int_c^d |f(t)|^2 \omega(t) dt < \infty$
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\[ \pi_n := \text{Class of all polynomials of degree } \leq n \]

\[ \langle g, h \rangle_{\omega_{[c,d]}} := \int_c^d g(t)h(t)\omega(t)\,dt \]

\[ I[g, \omega] := \int_c^d g(t)\omega(t)\,dt \]

\[ L_n (., Z_{n+1}, f) : \text{Lagrange polynomial of degree } n \text{ which interpolates } f \]

at the \( n + 1 \) points of \( Z_{n+1} \)

\[ \{f_0, f_1, ..., f_n \} : \text{Vector space generated by } f_0, f_1, ..., f_n \]

With the notations given above, we look into the following problems:

A. Least squares approximation problem [1]
Given \( f \in L^2_{\omega}[c,d] \) and a finite data \( \{(x_{i,j}, y_{i,j})\}_{i=1,j=1}^{k,n-1} \) with distinct \( x_i \)'s, can we find \( p^* \in \pi_m \) that minimizes the error \( \|p - f\|_{\omega_{[c,d]}} \) over all \( p \in \pi_m \) subject to the constraints: \( p^{(j)}(x_i) = y_{i,j}, i = 1, ..., k; j = 0, 1, ..., n_i - 1 \) ?

B. Lagrange interpolants in Erdos-Turan theorem
A result due to Erdos-Turan [4] states that \( \lim_{n \to \infty} \|L_n (., Z_{n+1}, f) - f\|_{\omega_{[c,d]}} = 0 \) where the set \( Z_{n+1} \) consists of the \( n + 1 \) zeros of an \( (n + 1) \) degree orthogonal polynomial with respect to \( \omega(x) \) over \([c,d]\). An extension of this problem may be posed as follows: Given a finite data \( \{(x_{i,j}, f^{(j)}(x_i))\}_{i=1,j=0}^{k,n-1} \) with distinct \( x_i \)'s lying outside the interval \([c,d]\), can we modify the interpolating polynomial \( L_n (., Z_{n+1}, f) \) to one which interpolates the additional data and preserves the convergence property over the interval \([c,d]\)?

C. Numerical Solution of BVP by collocation method
When determining a numerical solution of boundary value problems by collocation method, the Gaussian nodes are usually regarded as a best choice [6]. Can we determine their appropriate replacement by certain orthogonal points with partial freedom of choice without compromising the quality of numerical solution?

To answer these questions, we slightly change the structure of classical orthogonal polynomials by appending a finite number of pre-assigned zeros. The modified polynomials will be referred to as \( OZI \). The suggested polynomials convert certain constrained approximating problems to unconstrained ones by
modifying their approximating set. In addition, the zeros of OZI in some cases have some advantage over the Gaussian nodes in collocation methods.

2. Orthogonal Zero Interpolants (OZI)

The structure of OZI, in general, is based on a given data \( \{(x_i, n_i)\}_{i=1}^{k} \) where \( x_i \)'s are distinct real numbers and \( n_i \)'s are positive integers. These interpolants arise from a sequence of polynomials \( \psi_j(x), j = 0,1,2,..... \), which is constructed by the 3-term recurrence relation [5] as follows:

\[
\psi_{j+1}(x) = (x - \alpha_j)\psi_j(x) - \beta_j\psi_j(x), \quad j = 1,2,.....
\]

(1)

with \( \psi_0(x) = \prod_{i=1}^{k} (x - x_i)^{n_i} \) and \( \psi_1(x) = (x - \alpha_0)\psi_0(x) \). The recursion coefficients in (1) are given by

\[
\alpha_j = \frac{I[x\psi_j^2, \omega]}{I[\psi_j^2, \omega]}, \quad j = 0,1,....
\]

\[
\beta_j = \frac{I[\psi_j^2, \omega]}{I[\psi_{j-1}^2, \omega]}, \quad j = 1,2,....
\]

(2)

where the notation \( I[h, \omega] \) stands for \( \int_{c}^{d} h(x)\omega(x)dx \).

**Definition 1.** The polynomials \( \psi_j(x), j = 0,1,2,..... \), generated from relation (1) will be referred to as orthogonal zero interpolants relevant to the data \( \{(x_i, n_i)\}_{i=1}^{k} \).

**Some properties of OZI.** It is obvious that the OZI \( \psi_n(x) \) is a polynomial of degree \((n+N)\) with \( N = \sum_{i=1}^{k} n_i \) and that \( \psi_0(x) = \prod_{i=1}^{k} (x - x_i)^{n_i} \) is a factor of this polynomial. Also, \( \psi_l^{(i)}(x_i) = 0 \) for \( i = 1,.....,k; l = 0,1,2,....,n_i - 1 \). The polynomials \( \psi_i(x), i = 0,1,2,..... \) are monic and mutually orthogonal w.r.t. the weight function \( \omega(x) \) over the interval \([c,d]\), i.e., \( I[\psi_j\psi_l, \omega] = 0 \) for \( j \neq l \). Besides the fixed zeros each \( \psi_n(x) \) has exactly \( n \) real and distinct zeros in the open interval \((c,d)\). We shall denote these zeros by \( z_{i,n}, i = 1,2,....,n \), in the sequel. Thus, \( \psi_n(x) = \psi_0(x)Q_n(x) \) where

\[
Q_n(x) := \prod_{i=1}^{n} (x - z_{i,n})
\]

(3)

Also, the coefficients \( \beta_0 \) in (1) are positive. As a custom, we set \( \beta_0 = I[\psi_0^2, \omega] \).
Remark 1. The vector space \( \{ x^i \psi_0 : i = 0,1,...,n \} \) which will be denoted by \( \pi_n(\psi_0) \) is an \( (n+1) \)-dimensional subspace of \( \pi_{n+N} \) where \( N = \sum_{i=1}^{k} n_i \). Also, \( \{ \psi_0, \psi_1, \psi_2,...,\psi_n \} \) is an orthogonal bases \( \pi_n(\psi_0) \). Thus, \( \psi_n \perp \pi_r(\psi_0) \) for \( 0 \leq r \leq n - 1 \).

3. Problem A: Formulation, solution and convergence

We reformulate Problem (A) as follows [1]: Find a polynomial \( p_m^* \in \pi_m \) which minimizes \( \| p - f \|_{\omega_{\lambda[d,a]}} \) over all \( p \in \pi_m \) satisfying \( p^{(r)}(x_i) = y_{i,j}, \quad i = 1,2,...,k, \quad j = 0,1,...,n_i - 1. \)

Because of the number of interpolatory conditions, \( m \) can not be less than \( N - 1 \). We solve the reformulated problem by converting it to an unconstrained minimization problem. To do so, first we set

\[
 f_{H}(x) = f(x) - H_{N-1}(x,Y),
\]

(4)

where \( H_{N-1}(x,Y) \) is the polynomial of degree \( N-1 \) satisfying \( N \) interpolation conditions: \( H^{(r)}_{N-1}(x,y_i) = y_{i,j}, \quad i = 1,2,...,k; \quad j = 0,1,...,n_i \). In terms of \( f_{H}(x) \) and \( \pi_m(\psi_0) \), we state an equivalent form of Problem (A):

**Problem (A\(^*\):** Find a polynomial \( \phi_m \in \pi_m(\psi_0) \) which solves the problem:

\[
 \min_{\phi \in \pi_m(\psi_0)} \| \phi - f_{H} \|_{\omega_{\lambda[d,a]}}. \]

(5)

**Solution of Problem (A):** By Riesz-Fischer Theorem, we note that the solution of (4) is given by \( \phi_m(x) = \sum_{i=0}^{m} \left( \frac{f_{H}, \psi_i}{\psi_i, \psi_i} \right) \psi_i(x) \). Thus, \( p_m^*(x) = H_{N-1}(x,Y) + \phi_m(x) \) is the solution of Problem (A).

**Convergence.** If \( f \) is at least \( N^* \)-times continuously differentiable where \( N^* = \max(n_i - 1) \), we can prove:

**Theorem 1** [1]. If \( y_{i,j} = f^{(r)}(x_i), \quad i = 1,...,k; \quad j = 0,1,...,n_i \) in the set-up of Problem (A), then \( \lim_{m \to 0} \| p_m^* - f \|_{\omega_{\lambda[d,a]}} = 0 \).
Remark 2. The OZI’s considered in the solution of Problem (A) satisfy the Parseval equality for all \( f \in C^{\infty}([a,b]) \), i.e.,

\[
\langle f_H, f_H \rangle = \sum_{i=0}^{\infty} \langle f_H, \psi_i \rangle^2 / \langle \psi_i, \psi_i \rangle.
\]

4. Problem B: Formulation, solution and convergence

Problem (B) can be elaborated as follows [3]: Let \( f : [a,b] \to \mathbb{R} \) with \([c,d] \subseteq [a,b]\). Assuming that \( \Delta_k = \{x_i, x_2, \ldots, x_k\} \subseteq [a,b] \setminus (c,d) \), find a polynomial \( P_{n,k} \in \pi_{n+k-1} \) satisfying the following properties:

(i) The polynomial \( P_{n,k} \) emerges from an interpolation scheme based on distinct \((n+1)\) zeros of certain orthogonal polynomial with respect to \( \omega \) over \([c,d]\),

(ii) \( P_{n,k}^{(j)}(x_i) = f^{(j)}(x_i), \quad x_i \in \Delta_k, \quad j = 0,1,\ldots,n_i-1, \)

(iii) \( \lim_{n \to \infty} \|P_{n,k} - f\|_{\omega[c,d]} = 0. \)

Like Problem (A), this problem is also based on the data \( \{(x_i, f^{(j)}(x_i))\}_{i=1,j=0}^{k, n_i-1} \). In order to construct \( P_{n,k} \), we find an orthogonal polynomial which has \( n + 1 \) free nodes in the open interval \((c,d)\) and \( k \) pre-assigned nodes \( x_i \) of multiplicity \( n_i \), \( i = 1, 2, \ldots, k \), lying outside \((c,d)\).

Choice of orthogonal polynomials. The requirements (i) and (ii) are met by the OZI \( \psi_n \) which can be determined by the 3-term recurrence relation (1) with

\[
\psi_n(x) = \prod_{i=1}^{k} (x-x_i)^{n_i}.
\]

Thus, (cf (3)):

\[
\psi_{n+1}(x) = \psi_n(x) Q_{n+1}(x).
\]  

As before, we set \( f_H(x) = f(x) - H_{N-1}(x,f) \) where \( H_{N-1}(x,f) \) is the polynomial of degree \( N-1 \) which interpolates \( f \) in the sense of Hermite at \( k \) pre-assigned nodes \( x_i \) of multiplicity \( n_i \), \( i = 1, 2, \ldots, k \). With \( N := \sum_{i=1}^{k} n_i \), Problem (B) is reformulate in terms of \( f_H(x) \) and \( \pi_{n+1}(\psi_0) \):

**Problem B*. Find a polynomials \( P_n^* \in \pi_n(\psi_0) \) which interpolate \( f_H \) at the \( N + n + 1 \) zeros of \( \psi_{n+1} \). Moreover, \( \lim_{n \to \infty} \|P_n^* - f_H\|_{\omega[c,d]} = 0. \)
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Existence of $P_n^*$. Set $\Delta_k := \{x_1, x_2, \ldots, x_k\}$ and define $f_{H, \Delta_k} : [a, b] \to \Re$ as follows:

$$f_{H, \Delta_k}(x) = \begin{cases} 
\frac{f_H(x)}{\psi_0(x)}, & \text{if } x \notin \Delta_k \\
\lim_{t \to x} f_H(t), & \text{if } x \in \Delta_k.
\end{cases}$$

With $Z_{n+1} = \{z_{1,n+1}, \ldots, z_{n+1,n+1}\}$ (cf (3)) define $P_n^*(x) = \psi_0(x)L_n(x, Z_{n+1} f_{H, \Delta_k})$. It may be noted that $P_n^*(x) = f_{H, \Delta_k}(x)$ if $x \in Z_{n+1}$, and $P_n^{(j)}(x_i) = 0 = f_{H}^{(j)}(x_i)$ for $i = 1, \ldots, k$, $j = 0, 1, \ldots, n_i - 1$.

Convergence. Set $p_{n,N}^* (x) := P_n^*(x) - H_{N-1}(x, f)$. Then with suitable differentiability conditions on $f$ we have

**Theorem 2 [3]**: \[ \lim_{n \to \infty} \|p_{n,N}^* - f\|_{\infty[a,b]} = 0. \]

**Remark 3.** Theorem 2 is an extension of a result due to Erdos and Turan [4].

5. **Problem C: Formulation, solution and computational aspect [2]**

Problem C addresses the nature of collocation points required in the collocation solution of boundary value problems ($BVP$). Here, we shall notice certain advantage of the zeros of $OZI$'s over the Gaussian points when used as collocation points. This phenomenon is explained by a two-point linear $BVP$

$$y'' + \alpha(t)y' + \beta(t)y = f(t) : y(a) = 0, y(b) = 0,$$

with $\alpha(t) = 0, \beta(t) = -1, f(t) = \cos t$ and $a = 0, b = 1$. The exact solution of (7) is given by

$$y(t) = \frac{e^{-t} - \cos(1) + \cos(1) - e^{-t}}{2(e^{-1} - e)} - \frac{1}{2} \cos t.$$

We shall compute collocation solutions of this problem by using a three dimensional solution space $S_3 = \langle \phi_1, \phi_2, \phi_3 \rangle$ where each polynomial $\phi_i$ vanishes at 0 and 1. The collocation solution in this setup will be of the form [6] $\zeta = c_1\phi_1 + c_2\phi_2 + c_3\phi_3$ where the unknowns are retrieved by solving the linear system.
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\[
\begin{bmatrix}
L\phi(t_1) & L\phi(t_2) & L\phi(t_3) \\
L\phi(t_2) & L\phi(t_3) & L\phi(t_1) \\
L\phi(t_3) & L\phi(t_1) & L\phi(t_2)
\end{bmatrix}
\begin{bmatrix}
c_1 \\
c_2 \\
c_3
\end{bmatrix} =
\begin{bmatrix}
f(t_1) \\
f(t_2) \\
f(t_3)
\end{bmatrix},
\]

(8)

Here, \( L := D^2 + a(x)D + b(x) \). If \( \phi_1, \phi_2, \phi_3 \) are linearly independent and the points \( t_1, t_2, t_3 \) are distinct, then the coefficient matrix \( \begin{bmatrix} L\phi(t_j) \end{bmatrix}_{i,j=1}^3 \) is always nonsingular. Therefore, a unique solution of (8) does exist.

Our aim is discuss the collocation solutions based on different sets \( \{t_1, t_2, t_3\} \) which consist of either the Gaussian nodes or the zeros of OZI's, and then compare the resulting errors.

We have selected two different basis polynomials for \( S_3 \):

- **B-1**: \( \phi_1(t) = t(1-t), \quad \phi_2(t) = t^2(1-t), \quad \phi_3(t) = t^2(1-t)^2 \),
- **B-2**: \( \phi_1(t) = t(1-t), \quad \phi_2(t) = t^2(1-t), \quad \phi_3(t) = t^3(1-t) \).

For collocation points, we have considered different sets consisting of zeros of OZI's of the form “\( \psi_2(t) = \psi_3(t)Q_2(t) \)” where \( Q_2 \in \pi_2 \) and \( \psi(t) = t - t_1 \). Having fixed different values of \( t_1 \in [0,1] \), the remaining two zeros, \( t_2 \) and \( t_3 \), are determined from \( Q_2(t) \) (cf (3)). We have constructed eight sets of collocation points (Cpt) with different choice of \( t_1 \in [0,1] \). These are:

- **Cpt-1**: \( t_1 = 0 \), \( t_2 = 4.5585 \times 10^{-1} \), \( t_3 = 8.7749 \times 10^{-1} \),
- **Cpt-2**: \( t_1 = 1.5000 \times 10^{-1} \), \( t_2 = 4.8928 \times 10^{-1} \), \( t_3 = 8.8543 \times 10^{-1} \),
- **Cpt-3**: \( t_1 = 3.0000 \times 10^{-1} \), \( t_2 = 2.3246 \times 10^{-1} \), \( t_3 = 8.7315 \times 10^{-1} \),
- **Cpt-4**: \( t_1 = 4.5000 \times 10^{-1} \), \( t_2 = 1.1607 \times 10^{-1} \), \( t_3 = 8.8529 \times 10^{-1} \),
- **Cpt-5**: \( t_1 = 6.0000 \times 10^{-1} \), \( t_2 = 1.1897 \times 10^{-1} \), \( t_3 = 8.6954 \times 10^{-1} \),
- **Cpt-6**: \( t_1 = 7.5000 \times 10^{-1} \), \( t_2 = 1.2662 \times 10^{-1} \), \( t_3 = 6.6825 \times 10^{-1} \),
- **Cpt-7**: \( t_1 = 9.0000 \times 10^{-1} \), \( t_2 = 1.2906 \times 10^{-1} \), \( t_3 = 5.0097 \times 10^{-1} \),
- **Cpt-8**: \( t_1 = 1.0000e+00 \), \( t_2 = 1.2251 \times 10^{-1} \), \( t_3 = 5.4415 \times 10^{-1} \).

Two collocation solutions based on B-1 and B-2 each with three Gaussian points

- **Gpt**: \( t_1 = 5.0000 \times 10^{-1} \), \( t_2 = \left(1 - \sqrt{3}\right)/2 \), \( t_3 = \left(1 + \sqrt{3}\right)/2 \)

are also computed for the sake of comparison.

**Accuracy.** The level of accuracy of the resulting collocation solutions is determined by considering maximum error \( \text{M-Err} = \max_{1 \leq i \leq n} \left| y(t_i) - \zeta_{(K,L)}(t_i) \right| \), and
the root mean squared error: \( \text{RMS} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (t_i - \hat{y}_i)^2} \). These errors are computed over \( n = 101 \) uniform mesh points of \([-1,1]\). Here, \( \hat{y}_{(K,L)} \) denotes the collocation solution corresponding to basis \( B_{K,L} \), \( K = 1, 2 \) and collocation points \( C_{pt-L}, L = 1, 2, \ldots 8 \). The errors corresponding to each solution are tabulated below.

Table 1: Comparison of errors based on B-1 polynomials

<table>
<thead>
<tr>
<th>( t_1 )</th>
<th>( \zeta_{(1,1)} )</th>
<th>( \zeta_{(1,2)} )</th>
<th>( \zeta_{(1,3)} )</th>
<th>( \zeta_{(1,4)} )</th>
<th>( \zeta_{(1,5)} )</th>
<th>( \zeta_{(1,6)} )</th>
<th>( \zeta_{(1,7)} )</th>
<th>( \zeta_{(1,8)} )</th>
<th>( \zeta_{(1,Gpt)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 0 )</td>
<td>1.6248 ( \times 10^{-3} )</td>
<td>7.8463 ( \times 10^{-6} )</td>
<td>4.8222 ( \times 10^{-6} )</td>
<td>8.8012 ( \times 10^{-6} )</td>
<td>5.7026 ( \times 10^{-6} )</td>
<td>9.8077 ( \times 10^{-6} )</td>
<td>1.8457 ( \times 10^{-5} )</td>
<td>8.5202 ( \times 10^{-6} )</td>
<td></td>
</tr>
<tr>
<td>( 0.15 )</td>
<td>1.0982 ( \times 10^{-3} )</td>
<td>4.9540 ( \times 10^{-6} )</td>
<td>2.6670 ( \times 10^{-6} )</td>
<td>6.1676 ( \times 10^{-6} )</td>
<td>7.0045 ( \times 10^{-6} )</td>
<td>6.7537 ( \times 10^{-6} )</td>
<td>7.0045 ( \times 10^{-6} )</td>
<td>5.9790 ( \times 10^{-6} )</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Comparison of errors based on B-2 polynomials

<table>
<thead>
<tr>
<th>( t_1 )</th>
<th>( \zeta_{(2,1)} )</th>
<th>( \zeta_{(2,2)} )</th>
<th>( \zeta_{(2,3)} )</th>
<th>( \zeta_{(2,4)} )</th>
<th>( \zeta_{(2,5)} )</th>
<th>( \zeta_{(2,6)} )</th>
<th>( \zeta_{(2,7)} )</th>
<th>( \zeta_{(2,8)} )</th>
<th>( \zeta_{(2,Gpt)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 0 )</td>
<td>2.5382 ( \times 10^{-3} )</td>
<td>2.5583 ( \times 10^{-3} )</td>
<td>2.6814 ( \times 10^{-3} )</td>
<td>2.5888 ( \times 10^{-3} )</td>
<td>2.4589 ( \times 10^{-3} )</td>
<td>2.5547 ( \times 10^{-3} )</td>
<td>2.5248 ( \times 10^{-3} )</td>
<td>2.2997 ( \times 10^{-3} )</td>
<td>2.5449 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>( 0.15 )</td>
<td>1.7835 ( \times 10^{-3} )</td>
<td>1.7960 ( \times 10^{-3} )</td>
<td>1.8829 ( \times 10^{-3} )</td>
<td>1.8177 ( \times 10^{-3} )</td>
<td>1.7253 ( \times 10^{-3} )</td>
<td>1.7933 ( \times 10^{-3} )</td>
<td>1.7722 ( \times 10^{-3} )</td>
<td>1.6125 ( \times 10^{-3} )</td>
<td>1.7865 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

The graphs of error functions for each basis polynomials are given in Figures 1 and 2. Each figure involves three error functions corresponding to Gaussian points and the sets of the zeros of two different OZI’s. In case of OZI’s, we have selected one set resulting to a superior solution and the other one resulting to inferior when compared with the solution based on Gaussian nodes.
Conclusions. The performance of collocation methods, as already known, depends on the choice of collocation points and the nature of basis functions of the solution space. From the tables, we note that the zeros of several OZI’s provide a better solution to the one based on the Gaussian points. However, we could not figure out any criterion that determines a better choice of OZI for a specific basis of a collocation solution space.

Acknowledgement. The author acknowledges the research facilities availed at King Fahd University of Petroleum & Minerals during the preparation of this paper.

6. References

Fitting a straight line to a Normal Q-Q Plot. R Script

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Abstract
In this contribution we present different proposals of straight lines and develop an R Script to fit these lines to a Normal Quantile-Quantile Plot (Q-Q Plot), which can be chosen among six possibilities.

Key words: Normal Q-Q Plot, R Script, straight line.

1. Introduction
In Statistics, there are many studies in which it is necessary to verify if the data set comes from a Normal distribution.

The Normal Quantile-Quantile Plot (Q-Q Plot) is a popular and useful tool for assessing the normality of a data set. This plot compares the ordered distribution of a sample with the quantiles of the Standard Normal distribution indicated by the straight line. If the sample is normally distributed, the points will lie along this line.

Given a set of ordered observations $x_{(1)}, x_{(2)}, \ldots, x_{(n)}$, a Normal Q-Q Plot is constructed by plotting the pairs $\left(\Phi^{-1}(p_i), x_{(i)}\right)$, where $\Phi$ represents the standard normal cumulative distribution function (with zero mean and unit variance) [1] and $p_1, p_2, \ldots, p_n$ are appropriate plotting positions [2]. In this paper, we will use the definition of plotting position proposed by Hazen [3] in 1930, which is defined as:

$$p_i = \frac{i - 0.5}{n}, \quad i = 1, 2, \ldots, n$$
2. Fitting a straight line to a Normal Q-Q Plot

The Normal Q-Q Plot graphically compares the distribution of a given variable with the Normal distribution, represented by a straight line, though not necessarily the straight line $y=x$.

The value of the straight line on the point of abscissas zero, will provide estimation of the population average, and the value of the straight line on the point of abscissas one, will show the value of the sum of the average and the standard deviation. We may use this to provide estimation of the population mean and the standard deviation.

Moreover, what adjusts of the straight line to the Normal Q-Q Plot is an important aspect to consider. In this paper we develop an R script [4] through which we can choose a desired straight line (among six possible alternatives).

3. Possible straight lines in a Normal Q-Q Plot

In a Normal Q-Q Plot there exists the possibility of representing diverse straight lines for these pairs of points, since for each of the straight lines we will obtain different population parameters for the average and the standard deviation.

We will study the following straight lines:

1. Straight line that passes through the first and third quartiles.
2. Straight line that passes through the 10 and 90 percentiles.
3. Straight line fitted by the method of least squares.
4. Tukey’s resistant line [5].
5. Theil’s line [6].
6. Straight line with slope ‘$s$’ and constant the average of the data set.

4. R Script

The basic content of the R script that we propose to select the different straight lines in a Normal Q-Q Plot, is the following:

```r
lines <- function(x)
{
  x <- sort(x)
  n <- length(x)
  phazen <- ((1:n)-0.5)/n
  ejex <- qnorm(phazen)
  print("To key in definition’s number of straight line, where: ")
```


Fitting a straight line to a normal Q-Q plot. R script

print("1:'First and Third quartiles' ; 2:'10 and 90 percentiles' ; 3:'Method of least squares' ; 4:'Tukey’s resistant line' ; 5:'Theil’s line' ; 6:'Slope ‘s’ and constant average")
line <- scan(file="", what=integer(0), n=1, quiet=TRUE)
if (line<1 || line>6) print("You must key a number between 1 and 6") else
qqnorm(x, xlab="Quantiles N(0,1)", ylab="Observations")

if (line==1) qqline(x)
if (line==2)
{  
p10x <- quantile(ejex,0.1)
p90x <- quantile(ejex,0.9)
p10y <- quantile(x,0.1)
p90y <- quantile(x,0.9)
pte <- (p90y-p10y)/(p90x-p10x)
cte <- p10y-(pte*p10x)
abline(a=cte,b=pte)
}

if (line==3) abline(lm(x~ejex))
if (line==4)
{  
library("LearnEDA")
Tukey <- rline(ejex,x)
abline(a=Tukey$a, b=Tukey$b)
}
if (line==5)
{  
library("mblm")
Theil <- mblm(x~ejex)
abline(a=Theil$coefficients[1], b=Theil$coefficients[2])
}

if (line==6) abline(a=mean(x), b=sd(x))

5. Example

An application of the previous R script is represented in the following example, where we use simulated observations of a Chi-Square distribution.
In Figure 1 we can observe how the choice of the adjustment method of a straight line is fundamental in a Normal Q-Q Plot, since there are differences in the straight lines represented in the plot.

6. References

Evolutionary strategies of thermal adaptation to parasite load in a heterogeneous habitat

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Abstract

By evolutionary game theory, we can study the pressure of biotic factors on strategies adopted by predators and prey. Here, we show an analysis of a thermal game between predators and prey, where the habitat is composed of hotter and colder areas. In these areas, predators choose patches based on prey density and prey choose based on operative temperature and on the parasite load.

Key words: game theory, thermoregulation, temperature, parasite load

1. Introduction

Mathematical models about the behavioural regulation of temperature were pioneered by Huey and Slatkin [6]. In these models we formulate how phenotypes are dependent on thermal environments. This means that we evaluate the cost and benefit to be in a specific thermal environment, finding the optimal solutions. Importantly, these models generate hypotheses that can be investigated experimentally, leading to a possible cycle of improvements. Models of interacting predators and preys, with pressure from abiotic factors, are still lacking, but, more recently, effort has been done to further expand the field [3,9].

There are evidences of interaction between biotic factors and thermoregulation. For example: different preference for microclimates in the presence of competitors [5, 4]; reduced time of basking, in ectotherms, in situations of higher risk of predation [7, 8], avoidance of thermal favourable waters [1].
2. Thermal game

In this model we use a thermal game, where the prey has the ability to choose the patch that confers a specific energetic gain and a specific risk of predation. Besides that, we simulate a natural situation, where the patch with higher temperature will boost the immune system, being more advantageous for preys with some parasite load. If the prey chooses the patch with higher energetic gain, most of the time, it will lead to a distribution of predators around that some patch, and vice-versa. So, some trade-off must occur, where the need for a high energetic gain is counterbalanced by an evolutionary strategy that minimizes the risk of predation. However, in our model, a broader distribution of the prey will lead to more time spent in less favourable patches for the immune system functions.

3. Model

Our model has a habitat that is divided in two patches, a hotter and a colder, where the hotter one gives a higher energetic gain \( e \) for the prey. This higher energetic gain will lead to a faster growth rate, and a faster rate of reproduction and, consequently, to a higher fitness \( G \) of the prey. The fraction of time spent by the prey, in the colder patch will be \( t_1 \) and in the hotter one \( t_2 \). Similarly, for the predator, the fraction of time spent in the colder patch will be \( u_1 \) and \( u_2 \) for the hotter patch.

The fitness of the prey is defined as the product of fecundity \( F \) and probability to survive to maturity \( S \) [3, 2]:

\[
G = FS
\]

where we assume that fecundity increases monotonically with the energetic state of the prey \( X \).

The energetic state of the prey will be defined as the energetic gain of each patch multiplied by the fraction of time spent on it and taking into account the parasite load \( I \). We assume that the parasite load (that it also is the fraction of the population infected) only affects the energetic gain on the colder patch, while on the hotter patch the boosted immune system lowers the parasite load to minimal levels. So, it follows that:

\[
X(t_1, t_2, I) = [e_1 t_1 (1 - I) + e_2 t_2]
\]

where \( I \) is the parasite load.

For the survival of the prey, we assume that it declines exponentially over time [brown], as a function of rate of predation. This rate depends on the encounters of the prey with predators and on the lethality of that encounter \( l \). So, the fitness of the prey can be described as:
THERMAL ADAPTATION TO PARASITE LOAD

\[ G(t_1, t_2, u_1, u_2) = F[e_1 t_1 (1 - I) + e_2 t_2] e^{-l_p(u_1 t_1 + u_2 t_2) - l_i(u_2 t_2)} \] (3)

where \( l_p \) is the lethality due to normal predation and \( l_i \) is the increased lethality that an infected prey has due to different behavior when infected. For example, infected ectotherms tend to increase their basking time to maintain a higher body temperature, which leads to an increased probability of being spotted by predators. The predator’s fitness depends on the number of preys that it consumes the efficiency of conversion of the preys and on the time it allocates to each patch. In this model we assume that there is no significant difference for the energetic gain of the predator.

\[ H(t_1, t_2, u_1, u_2, N) = \pi N \left[ 1 - e^{-(u_1 t_1 + u_2 t_2) - l_i(u_2 t_2)} \right] \] (4)

In equation 4, \( N \) is the number of preys in the range of the predator, at the beginning of the season and \( p_i \) is the efficiency to which the predator converts prey to offspring.

4. Equilibrium

For a strategy of allocation of time to a patch by the prey, there will be an optimum allocation of time for the predator, in order to optimize its fitness. Likewise, for a given allocation of time by the predator, there will be a best strategy of allocation for the prey. The intersection of these set of responses gives us the combination of strategies that the predator and prey can not change unilaterally so that they can achieve greater fitness.

To find the set of strategies above, we study the limit cases for \( t_1, t_2 \) and \( u_1, u_2 \), when their values are 0 or 1, and evaluate the rate of fitness gain (\( \partial H/\partial u_i \) or \( \partial G/\partial t_i \)). Besides the limit cases, we also evaluate on the range between these limits. If the higher rate of fitness gain is not found in one of the limits above, there will be an equilibrium, where the fitness gain, by changing \( t_1 (u_1) \), will be the same as the fitness gain by changing \( t_2 (u_2) \), on the opposite direction, as follows:

\[
\left. \frac{\partial H}{\partial u_1} \right|_{u_1^*} = \left. \frac{\partial H}{\partial u_2} \right|_{u_2^*}
\] (5)

where \( u_1^* \) and \( u_2^* \) are the values at equilibrium.

For the predator, the patches confer equal rates of fitness gain if the prey spends time in the patches, following the equation:
As $t_2$ can be evaluated knowing that $t_2 = 1 - t_1$, by equation 6, we see that the allocation of time giving equal fitness gain, to the predator, in the two patches, is only dependent on the parasite load, the risk of predation and the increased risk of predation by the parasite load, on the hotter patch. It does not depend on the decrease on the energetic state, by the prey, due to the parasite load on the colder patch.

For the prey fitness gain equilibrium, we have a more complex formulation:

$$u_1 = \frac{e_1 (1 - I) - e_2}{(2l_p + l_p^2)} + \frac{l_p + l_p I}{2l_p + l_p}$$

From equation 7, the fitness gain equilibrium of the prey is shown to depend on $t_1, t_2, e_1, e_2, l_p, l_i$ and $I$.

If we use equation 6 and equation 7 to draw the curves (lines) that define the equilibrium for the predator and for the prey, we can find the behavioural Nash equilibrium, where these two curves intercept. In figure 1 we can evaluate the impact of raising the parasite load, from left to right, from 0 to 0.5. As the parasite load rises, predators spend more time on the warm patch. The preys start to spend more time on the colder patch (figure 1b), but as $I$ increases, they allocate more of their time to the warm patch.

Increasing the lethality of predation, for preys with or without parasite load, leads to more time allocated to the colder patch, for the prey and for the predator, as can be seen in figure 2.
The allocation of time of the prey in the colder patch \( (t_1) \) and of the predator \( (t_2) \). From the bottom, for the curves: \( l_1=0, \ l_p=0.5; \ l_1=0.25, \ l_p=0.5; \ l_1=0.5, \ l_p=0.5; \ l_1=0, \ l_p=1; \ l_1=1.0, \ l_p=1.0 \). The vertical lines correspond to the allocation of time for the prey, for the corresponding curves of the same color. From left to right, \( t_1=0.5, \ t_1=0.52 \) and \( t_1=0.55 \). For all, \( l=0.2, \ e_1=0.75, \ e_2=1.0 \).

These results reinforce that it is necessary to take into account biotic factors to understand the thermoregulation. Particularly, parasite load, in this model, was responsible for a shift in the behaviour of preys. For higher values of parasite load, the prey allocates more time to the warm patch, opposing the strategy of allocating more time to the colder patch when the parasite load is not so severe. The increase in the lethality of predation, due to an increased parasite load, leads to an increase in the time allocated to the colder patch.

References


Modeling a P-FAIMS with COMSOL

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Abstract

A micro Planar high-Field Asymmetric waveform Ion Mobility Spectrometer (P-FAIMS) has been simulated in air at ambient pressure using COMSOL Multiphysics software. Targeted analytes used in simulations are vapor phase compounds for security applications. In P-FAIMS target ions are discriminated by the application of the proper separation voltages to the electrodes of the system. By modeling, optimum voltages for achieving the proper sensitivity have been obtained and dual detection is achieved for ions with opposite charges.

Key words: FAIMS; FEM Gas Simulation; COMSOL

1. Introduction

Ion Mobility Spectrometry (IMS) is an analytical technique based on ion separation in gaseous phase due to an electric field. The IMS technology has fundamental advantages: high resolution (~ppb) and fast measurements (~ms). Also, ionization and characterization of the sample in IMS instruments occurs at ambient pressure[1], allowing a smaller analytical unit, lower power requirements, lighter weight and easier use for field applications. IMS instruments have a typical minimum volume of 40 cm³, but due to the trend toward miniaturization of ion mobility spectrometer, smaller volumes (~mm³) are being explored [2-4]. These advantages make IMS a rapidly advancing technique with a wide spectrum of applications, including detection of chemical warfare agents’ and explosives [5].
2. P-FAIMS working principle

In presence of an electric field, ions with different collision cross-sections temporally separate based on the frequency of ion-neutral interactions. The continual micro-scale acceleration and scattering collisions deceleration of ions results in a constant average velocity, the drift velocity \( v_d \) (m/s); that is directly proportional to the magnitude of the applied electric field strength \( E \) (V/cm): \[1\]:

\[ v_d = K E \]

where \( K(\text{cm}^2/\text{Vs}) \) is the ion mobility coefficient. This parameter is characteristic of each ion and each medium, and is the basis for its identification. The mobility of a given ion at constant temperature and pressure with gas density \( N \) (m\(^{-3}\)) through a drift gas under the influence of a high electric field can be expressed by [6]:

\[ K(E/N) = K(0) \cdot [1 + \alpha(E/N)] = K(0) \cdot [1 + \alpha_2(E/N)^2 + \alpha_4(E/N)^4 + ...] \] \[2\]

where \( K(0)=K(E/N)_{E=0} \) is the ion mobility at low electric field at \( N \); and \( \alpha(E/N) \) describes ion mobility dependence on the electric field at a constant density of drift gas at atmospheric pressure and constant temperature. \( E/N \) is the electric field in Townsend (1 Td = 10^{-17} \text{Vcm}^2) units. Equation 2 is a convenient mathematical expression for the alpha function [7]. \( K(0), \alpha_2, \) and \( \alpha_4 \), are characteristic of each ion and are obtained experimentally. When electric field exceeds 10000 V/cm \( (E/N \sim 40 \text{Td}) \) the mobility of some ions increase, decrease or remains unchanged.

A high radio frequency (RF) asymmetric electric field is applied to a narrow gap between two parallel plates, while ions are carried between them by a gas flow and undergo oscillations, i.e. perpendicular to gas flow as shown in Fig. 1. One of the plates is grounded and the other is biased at high voltage with an asymmetric waveform, \( V_{RF}(t) \), satisfying that its integration over a period has to be zero. While all ions interact with the applied RF field and are drawn towards the drift channel walls, selected ions can be kept in the flowing gas by applying particular low DC voltage or compensation voltage \( (V_C) \), prevents the ion migration towards either electrode. Thus, a selected ion passes through the filter electrodes and reaches the detector being this \( V_C \) voltage a characteristic of each ion species.

3. Two Dimensional Modeling Planar-FAIMS

COMSOL Multiphysics software is used to simulate the behavior of three different vapor ions in a P-FAIMS. The software takes into account nonlinear combined effects of different forces and concentrations fields. Created model combines fluid dynamics and electric field which have been found to be the most significant effects. Other effects such as electric repulsion in ion cloud due to space charge have been found to be considerably less significant (for the low concentration level simulated, 1ppm) and thus were not included in the simulations presented [8]. A 2D schema of the drift channel model used in the simulations is shown in Fig. 1.
Fig. 1. Schematic of a drift channel defined by P-FAIMS and detector electrodes. Ion paths are schematized under the influence of RF and DC fields for the filtering region and the detector fields for detection region.

The P-FAIMS electrodes of 13×5 mm² separated by 0.5 mm gap, are used to produce the alternating electric field in the gap. A two-harmonics asymmetric waveform is applied to the top electrode while the bottom electrode is grounded. The VC is applied to the top electrode too. Detector electrodes (charge collectors) of 5×5 mm² are placed after P-FAIMS electrodes to collect ions and generate the $V_C$ spectrum. Drift gas and ions enter the P-FAIMS from the left, passes through the P-FAIMS electrodes and only ‘selected’ ions reach the detector electrodes. Ions are introduced from the centre of the channel high at the beginning of the P-FAIMS electrodes with a spatial distribution specified as $\Delta y = 0.02$ mm, while air gas flows over all the channel height.

Model assumptions are resumed in Fig. 2. Drift gas velocity in the P-FAIMS gap has been calculated using the Navier-Stokes module for air. Electric potentials applied to the P-FAIMS and detector electrodes are calculated using the conductive media DC module and, the movement of ions is calculated with electrokinetic flow module, which takes into account of ions behavior.

The modeled ions correspond to a vapor phase compounds: 1) positive and negative reactant ions in purified air identified as protonated water clusters $H^+(H_2O)_n$ and $O_2^-(H_2O)_n$, 2) a chemical warfare agent simulant positive ion monomer: DMMPH⁺ that emulates gas sarin. Ions modeled are listed in Table 1 and have been selected because their main properties: $K_0$, $\alpha_2$ and $\alpha_4$ are available in the literature [7].

Fig. 2. Block diagram of key computational steps involved in modeling P-FAIMS with COMSOL Multiphysics software. Straight squares indicate main modules and dashed squares indicate variables needed for the modules.
Table 1: Parameters used in simulations for the studied compounds [7].

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Ion Acronym</th>
<th>$K_0$ (10^4 m^2/V·s)</th>
<th>$\alpha_2$ (Td^2)</th>
<th>$\alpha_4$ (Td^4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positive Reactant Ion</td>
<td>H+(H₂O)_n</td>
<td>2.34</td>
<td>1.78·10^3</td>
<td>-4.91·10^{10}</td>
</tr>
<tr>
<td>Negative Reactant Ion</td>
<td>O²⁻(H₂O)_n</td>
<td>2.13</td>
<td>1.93·10^3</td>
<td>-4.30·10^{10}</td>
</tr>
<tr>
<td>Dimethyl methylphosphonate (DMMP)</td>
<td>DMMPH⁺</td>
<td>1.94</td>
<td>5.09·10^6</td>
<td>-1.58·10^{19}</td>
</tr>
</tbody>
</table>

To simplify numerical simulations, following assumptions are made: 1) All ions are singly charged 2) Ions are assumed to be free from clusters - from water vapor and nitrogen in the ionization process - 3) Ions do not interact with one another, so that interactions resulting from space charging do not occur 4) Ions are created immediately upon entering the analyzer 5) The type of ionization is not considered 6) Reactant ions and product ions are not present in the system 7) Ions do not have dipolar moment.

4. Results and Discussion

For low RF electric fields ($E/N < 40$ Td) there is no dependence of mobility with electric field, therefore $V_C = 0$ V for all ions. Increasing electric field they can be separated due to their differences on mobility coefficients.

In Fig. 3, concentrations of the H+(H₂O)_n and DMMPH⁺ ions are presented for an $E/N$ of 60Td, showing that with the proper selection of the applied compensation voltage $V_C$ it is possible to obtain a good separation. As could be seen in this case of DMMPH⁺, ion reach the detector for a $V_C$=-1.35V. For the same compensation voltage, the positive reactant ion peak H+(H₂O)_n ion dose not reach the detector. Differentiation is achieved.

![Fig. 3. Concentrations for a separation field of $E/N = 60$ Td, of LEFT) DMMPH⁺ ions and RIGHT) H⁺(H₂O)_n ions; showing that for the same $V_C$=-1.35V only the DMMPH⁺ ion reaches the detector electrode. Differentiation is achieved.](image)

For an $E/N$=60Td showed, the positive reactant ion H⁺(H₂O)_n is detected for $V_C$=-4.6V, and the negative reactant ion O²⁻(H₂O)_n is detected for $V_C$=-5.5V. Therefore, differentiation is also obtained for the three compounds studied.
Results obtained from simulations showed that ion detection could be achieved with COMSOL software. Obtained intensities for initial concentrations of 1ppm, are in all cases of the order of nA.

5. Conclusions and Prospect
Simulations of a P-FAIMS have been done with COMSOL Multiphysics software for three compounds in vapor phase that could be considered representative for security applications.

Reactant ion peaks has been shown that can be separated from ions of dimethyl methylphosphonate positive monomer ion DMMPH$^+$ applying a determinate $V_C$ that makes ions pass through the drift channel and reach the detector.

From the good simulation results, the fabrication of the P-FAIMS instrument device will be addressed using micro-electro-mechanical systems fabrication techniques.

Acknowledgment
This work has been financially supported by the Spanish Ministry of Education and Science MEC-TEC2007-67962-C04-01 project.

References
Mathematical model for a temporal-bounded classifier in security environments

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Abstract

Security is a major concern when web applications are implemented. This has led to the proposal of a variety of specifications and approaches to provide the necessary security for these environments. SQL Injection attacks on web applications have become one of the most important information security concerns over the past few years. The purpose of this article is to present an adaptive and intelligent mechanism that can handle SQL injection attacks and real time. Our approach is based on a real time classifier agent that incorporates a mixture of experts to choose a specific classification technique depending on the feature of the attack and the time available to solve the classification. This research presents a case study to evaluate the effectiveness of the approach and also presents the preliminary results obtained with an initial prototype.

Key words: Case-Based Reasoning, Support Vector Machine, Artificial Neural Network, SQL Injection, Intrusion Detection

1. Introduction
Mathematical model for a temporal-bounded classifier in security environments

In recent years, Internet attacks have increased due to the large number of information systems connected to the Internet. One of the most serious security threats around Web application and databases has been the SQL Injection attack [1]. This attack takes place at the database layer when a user request that has been sent through an HTTP request is executed without prior validation. Confidentiality, integrity and availability are the main objectives of any information security model [2]. Various approaches have attempted to deal with the problem of SQL injections [3] [4] [5] [6] [7]. However, the biggest inconvenience of these solutions is their inability to adapt to the rapid changes in attack patterns, which renders them a bit inefficient in the long term. More complex SQL attacks are characterized by the various techniques used for remaining undetected by existing security solutions. Finally, none of these approaches consider the limitations or restrictions in response time. Response time is a critical aspect in the majority of Internet security systems. With systems requiring a response to be given before a specific deadline, as determined by the system needs, it is essential that the execution time for each of the tasks carried out by the system is predictable and capable of guaranteeing correct execution within the time needed for the given response. Furthermore, the system providing the service and the security analysis must both have the necessary mechanisms for executing tasks in a predictable framework, that is, the agent must be prepared for its execution in a real time environment. A Real-Time Agent may have its interactions bounded; a modification that will affect all the communication processes in the Multi-Agent system where the Real-Time Agent is located. Some examples of real time agents are: The ARTIS agent specifically designed to develop Real-Time Systems [8] [9] [10], The ObjectAgent Architecture developed by Pinceton Satellites in 2001 [9] and time-aware agents proposed by Prouska et al. in 2002 [10].

This study presents a new agent model with a novel perspective for analyzing and classifying SQL injections in real time. The agent’s internal structure, an integrated mixture of an Artificial Neural Network (ANN) and a Support Vector Machine (SVM) is used as a classification mechanism. By using this mixture, it is possible to exploit the advantages of both strategies in order to classify the SQL queries in a more reliable way. The internal structure of the agent is based on the Case-Base Reasoning (CBR) model, with the main difference being that the different CBR phases are time-bounded, thus enabling its use in real time. CBR can be very suitable for application in agent reasoning, where similar problems should have similar solutions. However, few of the existing approaches cope with the problem of applying CBR as deliberative engine for agents in MAS with real-time constraints. Additionally, the adaptation phase in the CBR system integrated in the agent proposes a new analysis classification model that is carried out by a mixture of experts. The concept of a mixture of experts was first proposed by[11]. It involves a system that contains a series of input data that is distributed over a set of expert classifiers. Depending on the time available for performing classification, a set of experts is selected to perform the different analyses. The experts are selected with a multiple method model [12]. Finally the different
Mathematical model for a temporal-bounded classifier in security environments selected experts generate the predictions and the outputs are fused to generate a new unique result [13] [25].

The paper is structured as follows: Section 2 presents the problem that has prompted most of this research work. Section 3 describes the SQL attack problem. Section 4 shows a general view of the temporal bounded CBR used as deliberative mechanism in the classifier agent. Section 5 describes a set of tests to evaluate our proposal.

2. **Real Time Agent and Case-Based Reasoning (CBR)**

A real time agent is one that is able to support tasks that should be performed within a restricted period of time [14]. This characteristic justifies its use in real time systems. In this type of environment, the validity of the solution is determined not only by its correct execution, but by its ability to be carried out within the allotted time frame [15].

The main problem in the architecture of a Real Time Agent (RTA) is with the deliberation process. This process may use Artificial Intelligence (AI) techniques as problem-solving methods to compute more intelligent actions. If this is the case, it is difficult to know the time required, because it can either be unbounded or have a high variability. If the agent has to operate in a real-time environment, the agent complexity required to achieve any or all of these features is greatly increased. Thus a RTA requires an efficient integration of high-level, deliberative processes within reactive processes. When using AI methods, it is necessary to provide techniques that allow their response times to be bounded. These techniques are mainly based on well-known Real-Time Artificial Intelligence System (RTAIS) techniques[16][17].

![TB-CBR cycle](image)

**Figure 1. TB-CBR cycle**
Mathematical model for a temporal-bounded classifier in security environments

Figure 1 shows the reasoning cycle for a TB-CBR system. The TB-CBR cycle starts at the learning stage, where it checks to see if there are previous cases waiting to be revised and possibly stored in the case-base. In our model, the plans provided at the end of the deliberative stage will be stored in a solution list while feedback about their utility is received. When each new TB-CBR cycle begins, this list is accessed. If there is enough time, the learning stage is implemented for those cases whose solution feedback has been recently received. If the list is empty, this process is omitted.

The next stage to be implemented is the deliberative stage. The retrieval algorithm is used to search the case-base and retrieve a case that is similar to the current case (i.e. one that characterizes the problem to be solved). Each time a similar case is found, it is sent to the reuse phase where it is transformed into a suitable plan for the current problem by using a reuse algorithm. Therefore, at the end of each iteration of the deliberative stage, the TB-CBR method is able to provide a plan for the problem at hand, although this plan can be improved in subsequent iterations if the deliberative stage has enough time to perform them.

Hence, the temporal cost of executing the cognitive task is greater than or equal to the sum of the execution times of the learning and deliberative stages (as shown in equation 1):

\[ t_{\text{cognitiveTask}} \geq t_{\text{learning}} + t_{\text{deliberative}} \]
\[ t_{\text{learning}} \geq (t_{\text{revise}} + t_{\text{retain}}) \times n \]
\[ t_{\text{deliberative}} \geq (t_{\text{retrieve}} + t_{\text{reuse}}) \times m \]

where \( t_{\text{cognitiveTask}} \) is the maximum time available for the agent to provide a response, \( t_{\text{learning}} \) and \( t_{\text{deliberative}} \) are the total execution time of the learning and deliberative stages; \( t_x \) is the execution time of the phase \( x \) and \( n \) and \( m \) are the number of iterations of the learning and deliberative stages respectively.

This algorithm can be launched when the real-time agent considers it appropriate and there is enough time for it to be executed. The real-time agent indicates to the TB-CBR the maximum time (\( t_{\text{max}} \), where \( t_{\text{max}} \geq t_{\text{cognitiveTask}} \)) that is available to complete its execution cycle. The time \( t_{\text{max}} \) must be divided between the learning and the deliberative stages to guarantee the execution of each stage. The designer can assign more time to the learning stage if it desires a real-time agent with a greater capacity to learn.

The anytime behaviour of the TB-CBR is achieved through the use of two loop control sequences. The loop condition is built using the \( \text{enoughTime} \) function, which determines if a new iteration is possible according to the total time that the TB-CBR has to complete each stage.

The first phase of the algorithm executes the learning stage. This stage is executed only if the agent has the solutions from previous executions stored in the
Mathematical model for a temporal-bounded classifier in security environments solutionQueue. The solutions are stored just after the end of the deliberative stage. The deliberative stage is only launched if the agent has a problem to solve in the problemQueue. This configuration allows the agent to launch the TB-CBR in order to only learn (no solution is needed and the agent has enough time to reason previous decisions), only deliberate (there are no previous solutions to consider and there is a new problem to solve) or both.

2. SQL attack

A SQL injection attack takes place when a hacker changes the semantic or syntactic logic of a SQL text string by inserting SQL keywords or special symbols within the original SQL command that will be executed at the database layer of an application [18]. A SQL injection attack can cause serious damage to an organization, including financial loss, breach of trust with clients, among others. There have been many proposed solutions for SQL injection attacks, including some Artificial intelligence techniques. One of the approaches is WAVES (Web Application Vulnerability and Error Scanner)[22]. This solution is based on a black-box technique. WAVES is a web crawler that identifies vulnerable points, and then builds attacks that target those points based on a list of patterns and attack techniques. WAVES monitors the response from the application and uses a machine learning technique to improve the attack methodology. WAVES cannot check all the vulnerable points like the traditional penetration testing. The strategy used by the intrusion detection systems has also even been implemented to deal with some SQL injection attacks. Valeur [21] presents an IDS approach that uses a machine learning technique based on a dataset of legal transactions. These are used during the training phase prior to monitoring and classifying malicious accesses. Generally, IDS systems depend on the quality of the training set; a poor training set would result in a large number of false positives and negatives. Skaruz [19] proposes the use of a recurrent neural network (RNN). The detection problem becomes a time serial prediction problem. The main problem with this approach is the large number of false positives and false negatives.

Other strategies based on string analysis techniques and the generation of dynamic models have been proposed as solutions to SQL injection attacks. Halfond and Orso [18] propose AMNESIA (Analysis and Monitoring for Neutralizing SQL Injection Attacks). Kosuga et al. proposes SANIA (Syntactic and Semantic Analysis for Automated Testing against SQL Injection) [20]. With only slight variations of accuracy in the models, these strategies have as drawback their meaningful rate of false positives and negatives.

2. SQL-TB-CBR agent classifier

In this section the new SQL-TB-CBR agent is presented, with special attention paid to its internal structure and the classification mechanism of SQL attacks. This mechanism combines the advantages of CBR systems, such as learning and adaptation, real time, with the predictive capabilities of ANNs and SVMs.
Mathematical model for a temporal-bounded classifier in security environments

In terms of CBR, the case is composed of elements of the analysed SQL Query described as follows:

- **Problem**: describes the initial information available for generating a plan. The problem description consists of: case identification, user session and SQL query elements.
- **Solution**: states the action carried out in order to solve the problem. In this case, the applied prediction models.
- **Final State**: describes the state achieved after that the solution has been applied.

The fields defining a case are as follows: *IdCase, Session, User, IP_Address, Query_SQL, Affected_table, Affected_field, Command_type, Word_GroupBy, Word_Having, Word_OrderBy, Numer_And, Numer_Or, Number_literals, Number_LOL, Length_SQL_String, Start_Time_Execution, End_Time_Execution, and Query_Category*. Additionally, the information related to the prediction models used is stored as well.

In Fig. 1, the different stages applied in the reasoning cycle can be seen.

![Figure 2. TB-CBR cycle and classification mechanism of the SQL-TB-CBR agent](image)

In the retrieval stage, there is a selection of queries sorted by type and by the memory’s classification models. In the reuse phase, as seen in Fig. 1, a Multilayer Perceptron (MLP) and/or an SVM are applied to carry out the prediction of the new query. Subsequently, a new inspection is performed which can be done automatically or by a human expert. In the case of the query resulting as suspicious, further inspection will be carried out manually by a human expert. During learning, memory information regarding the cases and models will be
Mathematical model for a temporal-bounded classifier in security environments updated. Below, the different stages of the CBR reasoning cycle associated with the system are described in more detail.

**Retrieve**

In the Retrieve phase, the real time agent recovers the cases that it will use to perform classification. The time needed to recover the different cases to be used is clearly defined and temporally bounded. The retrieval time for the cases depends on the number of cases in the case base. If the number is known, it is easy to predict how much execution time will be used to recover the cases. The asymptotic cost is linear (O(n)).

The retrieve phase is broken down into two phases; case retrieval and model retrieval. Case retrieval is performed by using the Query_Category attribute which retrieves queries from the case memory (Cr) which were used for a similar query in accordance with attributes of the new case \( c_n \). Subsequently, the models for the multilayer perceptron and/or SVM associated with the recovered cases are retrieved. The recovery of these memory models allows the improvement of the system’s performance so that the time necessary for the creation of models will be considerably reduced, mainly in the case of the ANN training.

**Reuse**

The SQL injection in our proposal can be analyzed by two different techniques. Execution time in both cases is known, since previous stored models as used. The first is known as the Light technique Support Vector Machine (SVM) and is usually a detection algorithm with a low temporal cost, but of low quality as well. Using the Heavy technique, Multiplayer Perceptron, the result of the analysis is much more exact, but it requires a much higher amount of execution time. The inputs of the MLP are: Query_SQL, Affected_table, Affected_field, Command_type, Word_GroupBy, Word_Having, Word_OrderBy, Numer_And, Numer_Or, Number_literals, Number_LOL, and Length_SQL_String. The number of neurons in the hidden layer is \( 2n+1 \), where \( n \) is the number of neurons in the input layer. Finally, there is one neuron in the output layer. The activation function selected for the different layers has been the sigmoid. Taking into account the activation function \( f_j \), the calculation of output values are given by the following expression

\[
y_j^p = f_j\left(\sum_{i=1}^{N} w_{ji}(t) x_i^p(t) + \theta_j\right)
\]

The outputs correspond to \( x_r \). As the neurons exiting from the hidden layer of the neural network contain sigmoidal neurons with values between \([0, 1]\), the incoming variables are redefined so that their range falls between \([0.2, 0.8]\). This transformation is necessary because the network does not deal with values that fall outside of this range. The outgoing values are similarly limited to the range of \([0.2, 0.8]\) with the value of 0.2 corresponding to a non-attack and the value of 0.8
Mathematical model for a temporal-bounded classifier in security environments corresponding to an attack. The network training is carried out through the error Backpropagation Algorithm [23].

The light algorithm SVM represents an extension of nonlinear models [24]. SVM also allows the separation of element classes which are not linearly separable. To do so, the space of initial coordinates is mapped in a high dimensionality space through the use of functions. Due to the fact that the dimensionality of the new space can be very high, it is not feasible to calculate hyperplanes that allow the production of linear separability. For this reason, a series of non-linear functions called kernels is used.

Let us consider a set of patterns \( T = \{(x_1, y_1), (x_2, y_2), ..., (x_m, y_m)\} \) where \( x_i \) is a vector of the dimension \( n \). The idea is to convert the elements \( x_i \) in a space of high dimensionality through the application of a function, in such a way that the set of original patterns is converted into the following set \( \Phi(T) = \{(\Phi(x_1), y_1), (\Phi(x_2), y_2), ..., (\Phi(x_m), y_m)\} \) that, depending on the selected function \( \Phi(x) \), could be linearly separable. To carry out the classification, this equation sign is studied [16]:

\[
\text{class}(x_k) = \text{sign} \left( \sum_{i=1}^{m} \lambda_i y_i \Phi(x_i) \Phi(x_k) + b \right)
\]

The selected kernel function in this problem was polynomial. The values used for the estimation are dominated by decision values and are related to the distance from the points to the hyperplane.

If there is enough time for carried out both techniques, the mixture is performed in such a way that the higher value is selected for both methods. This is done in order to avoid false negatives.

**Revise and Retain**

The revise phase can be manual or automatic depending on the output values. The automatic review is given for non-suspicious cases during the estimation obtained for the reuse phase. For cases detected as suspicious, with output values determined experimentally in the interval \([0.35, 0.6]\), a review by a human expert is performed.

The learning phase updates the information of the new classified case and reconstructs the classifiers offline to leave the system available for new classifications. The ANN classifier is reconstructed only when an erroneous classification is produced. In the case of a reference to inspection of suspicious queries, information and classifiers are updated when the expert updates the information.
2. Results and Conclusions

This article has presented a novel proposal for detecting SQL injections in real time. The article proposes a new vision in which each attack mechanism is individually analyzed. It also makes it possible to obtain better classification results with regard to both the effectiveness of the classification process and the response time, since all classification mechanism tasks are temporally bounded.

In order to validate the initial prototype, we proposed a benchmark case study that contains 705 SQL queries (437 legal queries and 268 attacks). The tests were conducted with a simple web application with database access, MySQL 5.0. The entries were automated by using the SQLMap 0.6.3 tool, with which an initial case base was established for training the SQL-TB-CBRClassifier.

Prior to initiating the tests, the attack classification mechanisms were analyzed for each use of a Light or Heavy technique and other classifiers. To analyze the successful rates, a test of the classification of queries was conducted, taking into account the following classifiers: Bayesian Network, Naive Bayes, AdaBoost M1, Bagging, DecisionStump, J48, JRIP, LMT, Logistic, LogitBoost, MultiBoosting AdaBoost, OneR, SMO, light planner, heavy planner. The different classifiers were applied to 705 previously classified queries.

<table>
<thead>
<tr>
<th>Method</th>
<th>Total number of hits</th>
</tr>
</thead>
<tbody>
<tr>
<td>BayesNet</td>
<td>638</td>
</tr>
<tr>
<td>Bagging</td>
<td>684</td>
</tr>
<tr>
<td>JRIP</td>
<td>692</td>
</tr>
<tr>
<td>LogitBoost</td>
<td>680</td>
</tr>
<tr>
<td>SMO</td>
<td>685</td>
</tr>
<tr>
<td>Naive Bayes</td>
<td>666</td>
</tr>
<tr>
<td>DecisionStump</td>
<td>598</td>
</tr>
<tr>
<td>LMT</td>
<td>693</td>
</tr>
<tr>
<td>MultiBoostAB</td>
<td>666</td>
</tr>
<tr>
<td>light</td>
<td>696</td>
</tr>
<tr>
<td>AdaBoostM1</td>
<td>665</td>
</tr>
<tr>
<td>J48</td>
<td>689</td>
</tr>
<tr>
<td>Logistic</td>
<td>688</td>
</tr>
<tr>
<td>OneR</td>
<td>622</td>
</tr>
<tr>
<td>heavi</td>
<td>702</td>
</tr>
</tbody>
</table>

The analysis demonstrated that the use of Heavy techniques provided a better classification, but with a greater temporal cost. The average execution time for the queries, and the worst time used for the light and heavy techniques were respectively 0.013/0.051 and 0.28/1.07 ms.

For the second test a set of 50 queries were selected and then classified according to different pre-determined deadlines. The number of executions and errors obtained for each of the classifiers are shown in Figure 3. The x axis represents the average time between queries and the deadline, while the y axis represents the number of queries executed. As can be seen, the number of executions for the mixture increased as the execution time between queries increased.
Figure 3. Queries made for each combination according to time.

The proposed SQL-TB-CBR agent is capable of detecting SQL injections with low error rates compared with other existing techniques, as shown in table 1. Moreover, it is possible to provide a real-time classifier mechanism, with a high level of confidence to identify legal queries and attacks. The combination of different Artificial Intelligence paradigms allows the development of a hybrid intelligent system with characteristics such as the capacity for learning and reasoning, flexibility and robustness which make the detection of SQL injection attacks possible.

Acknowledgements

This work has been supported by the MICINN TIN 2009-13839-C03-03 project and the Professional Excellence Program 2006-2010 IFARHU-SENACYT-Panama.

References


Mathematical model for a temporal-bounded classifier in security environments


Mathematical model for a temporal-bounded classifier in security environments


Implementation in Chimère of a conservative solver for the advection equation

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Abstract

Extensive research has been performed to solve the advection equation and different numerical methods have been proposed. Most part of these methods including semi-lagrangian methods are not conservative. In this paper we present the implementation in the European scale Eulerian chemistry transport model CHIMERE of an exactly conservative method for the advection equation. The results of the method are compared with a set of observation sites in the area of Madrid (Spain).

Key words: advection equation, conservative scheme, rational interpolation
MSC2000: AMS Codes (optional)

1. Introduction

Accurate numerical simulation of tropospheric air pollution phenomena has become a major challenge in atmospheric science. The advection equation is important for the study of the dynamics of flows, as well for the development of new numerical schemes that are applied to more complex models. Semi-
Lagrangian schemes have gathered a wide acceptance for solving advection dominated problems, especially in the atmospheric sciences [1]. Most part of these methods are not conservative. Apart from the corrective methods different approaches have been developed to generate an inherently conservative solution of advection equation. The conservative methods are used in meteorological simulations as very accurate methods for explicitly computing the transport of rain water.

Our main goal of this research is to improve the transport module in the European scale Eulerian chemistry transport model CHIMERE by implementing a conservative rational scheme. The results of the method are compared with a set of observation sites in the area of Madrid (Spain).

Section 2 introduces the conservative methods. Section 3 gives a description of the rational interpolation and Section 4 introduces the conservative formulation. In section 5 we introduce the European-scale chemistry-transport model (CHIMERE). The comparison of observed and modeled data is given in Section 6, and finally some conclusions are given in Section 7.

2. Conservative methods

One of the main drawbacks of the semi-Lagrangian method is the lack of conservation properties in its original formulation. Therefore, several authors presented stable semi-Lagrangian schemes that were modified such that conservation properties hold [2, 3].

Some authors have recently succeeded in developing new conservative semi-Lagrangian schemes. The schemes conserve the mass using an additional constraint of the value integrated over neighbouring two grid points, this value is introduced as a new model variable that is updated for the advection equation by a flux-form formulation. Then the mass can be exactly conserved. One of these conservative methods, developed by Xiao and Pen [4], is based in rational interpolation. In this scheme a constraint of the conservation relation for cell-integrated average is imposed at the stage to determine the piecewise rational interpolation function. The method conserves exactly the cell-integrated average of the transported field. In this paper we have implemented this conservative method in the European-scale chemistry transport model (CHIMERE). We have adopted the dimensional splitting to extend the scheme to multi-dimensions.

We describe the numerical formulation for the scalar conservative advection transport equation as follows:

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0$$

(1)

where \(f(x,t)\) is the advected quantity, and \(u\) is the advecting current. This is a linear, first-order, partial differential equation with a constant coefficient namely...
u (velocity). When the velocity is constant, the solution of equation (1) gives a simple translational motion of field \( f \) with velocity \( u \).

The value of \( f \) in \( (n+1) \) step is readily obtained by shifting the profile by \( u_i \Delta t \), so that:

\[
f(x_{i+1}, t + \Delta t) = f(x_{i+1} - u_i \Delta x, t) = F_i^n(x_{i+1} - u_i \Delta x)
\]

(2)

where \( F \) is an interpolation function which depends on the conservative algorithm we are using.

### 3. Rational conservative interpolation

Normally the interpolation function is based on polynomials. The main disadvantage of the polynomial interpolation is that can be unstable on the most common grid - equidistant grid. The rational interpolation consists of the representation of a given function as the quotient of two polynomials. The rational interpolation is an alternative for the polynomial interpolation. Its advantages are the high accuracy and absence of the problems which are typical for polynomial interpolation, such as the typical oscillations. However new difficulties can appear in the rational interpolation due to the existence of the poles.

The conservative interpolation is based on the concept of the conservation of the integral of the function, using an additional constraint of the value integrated over neighbouring two grid points. Both properties can be used at the same time in the piecewise rational conservative interpolation.

The rational interpolation function \( F_i \), is expressed in a generic mesh element with boundaries \( x_{i-\frac{1}{2}} \) and \( x_{i+\frac{1}{2}} \) and considering the velocity \( u < 0 \) as

\[
F_i(x) = \frac{a_i + 2b_i(x - x_{i-\frac{1}{2}}) + \beta_i(x - x_{i-\frac{1}{2}})^2}{1 + \beta_i(x - x_{i-\frac{1}{2}})^2}
\]

(3)

where \( a, b, \) and \( \beta \) are the coefficients of the interpolation function which are obtained by using the constraint conditions, where the constraint conditions are given in \( [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \) by

\[
F_i(x_{i-\frac{1}{2}}) = f^n_{i-\frac{1}{2}}
\]

\[
F_i(x_{i+\frac{1}{2}}) = f^n_{i+\frac{1}{2}}
\]

(4)

\[
\frac{1}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} F_i(x) dx = \rho^n_i \quad \text{where} \quad \Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}
\]
Then by solving the three equations we obtain the coefficients of the rational interpolation.

\[ a = f_{i+1/2}^{n-1} \]

\[ b_i = \beta_i \rho_i^n + \frac{1}{\Delta x_i} (\rho_i^n - f_{i-1/2}^n) \]

\[ \beta_i = -\Delta x_i^{-1} \left[ \frac{f_{i+1/2}^n - \rho_i^n}{\rho_i^n - f_{i+1/2}^n} - 1 \right] \]  

(5)

This last expression is corrected according with Xiao and Peng[4], to avoid division by zero as follows

\[ \beta_i = -\Delta x_i^{-1} \left[ \frac{f_{i+1/2}^n - \rho_i^n + 10^{-20}}{\rho_i^n - f_{i+1/2}^n + 10^{-20}} - 1 \right] \]  

(6)

4. **Conservative Formulation.**

For the pollution problem, it is appropriate to use finite volume method. We divide the spatial domain in cells called finite or control volumes \( C_i \), this corresponds in one dimension to a partition of a bounded domain by intervals, see Fig. 1.

![Control volumes](image)

**Fig. 1 Control volumes**

On the other hand one built discrete equations from the integral form of the advection equation. The integral form of the conservation law is given by

\[ \frac{d}{dt} \int_{C_i} f(x,t) \, dx = g(f(x_{i-1/2},t)) - g(f(x_{i+1/2},t)) \]  

(7)
being \( g(f(x_{i-(1/2)},t)) \), \( g(f(x_{i+(1/2)},t)) \) the fluxes in the cell.

By integrating in the time
\[
\int_{C_i} f(x,t+\Delta t)dx - \int_{C_i} f(x,t)dx = \int_{t}^{t+\Delta t} g(f(x_{i-(1/2)},t))dt - \int_{t}^{t+\Delta t} g(f(x_{i+(1/2)},t))dt
\]

we can put this expression as
\[
\rho_{i}^{n+1} = \rho_{i}^{n} - (g_{i+\frac{1}{2}}^{+} - g_{i-\frac{1}{2}}^{-})/\Delta x_{i}
\]

where
\[
g_{i+\frac{1}{2}} = \frac{a_{i+\frac{1}{2}} + b_{i+\frac{1}{2}}^{2}}{1 + \beta_{i+\frac{1}{2}}^{2}} = \text{Flux across boundary } x = x_{i+\frac{1}{2}} \text{ during } t^{n+1} - t^{n}
\]

Finally we shall need to interpolate in the next time step to determine interface values as a function of the cell averages.
\[
f_{i+\frac{1}{2}} = \frac{1}{2}(\rho_{i} + \rho_{i+1}) - \frac{1}{6}(\delta f_{i} - \delta f_{i-1})
\]

For the rational function we calculate the average slope in a cell \( \delta f_{i} \) as
\[
\delta f_{i} = \begin{cases} 
\min(|\delta f_{i}|,3|\rho_{i+1} - \rho_{i}|,3|\rho_{i} - \rho_{i-1}|) \text{sgn}(\delta f_{i}), & \text{si } \rho_{i+1} - \rho_{i} > 0 \\
0, & \text{otherwise}
\end{cases}
\]

being \( \delta f_{i} = (\rho_{i+1} - \rho_{i-1})/2 \)

By using time-splitting the method can be easily extended to solve advection equation in two and three dimensions. For example in two dimensions the time splitting is equivalent to do the transport of particles to the direction (Ox) and then according to the other direction (Oy).

5. Model description
Chimère is based on the mass continuity equation for the concentrations of chemical species in every box of a given grid:

\[
\frac{\partial f}{\partial t} + \nabla \cdot (uf) = \nabla \cdot (kf) + P - L \tag{12}
\]

In this equation, characteristic for the Eulerian approach, \(f\) is a vector containing the concentrations of all model species for every grid box, \(u\) is the three dimensional wind vector, \(k\) the tensor of eddy diffusivity and \(P\) and \(L\) represent production and loss terms due to chemical reactions, emissions and deposition.

The numerical method for the temporal solution of the stiff system of partial differential equations (12) is adapted from the second-order TWO-STEP algorithm originally proposed by [5] for gas phase chemistry only. It is based on the application of a Gauss-Seidel iteration scheme to the 2-step implicit backward differentiation (BDF2) formula:

\[
f^{n+1} = \frac{4}{3} f^n - \frac{1}{3} f^{n-1} + \frac{2}{3} \Delta t R f^{n+1} \tag{13}
\]

With \( f^n \) being the vector of chemical concentrations at time \( t^n \). At the time step leading from time \( t^n \) to \( t^{n+1} \) and \( R(f) = P(f) - L(f) \) the temporal evolution of the concentrations due to chemical production and emissions (P) and chemical loss and deposition (L). Note that L is a diagonal matrix here. After rearranging and introducing the production and loss terms this equation reads

\[
f^{n+1} = \left( I + \frac{2}{3} \Delta t L f^{n+1} \right)^{-1} \left( \frac{4}{3} f^n - \frac{1}{3} f^{n-1} + \frac{2}{3} \Delta t P f^{n+1} \right) \tag{14}
\]

The implicit nonlinear system obtained in this scheme can be solved pertinently with a Gauss-Seidel method [5].

We can find a more complete description and evaluation of the Chimère model designed for seasonal simulations and real time forecasts without the use of supercomputers in [6], where details about the implementation and evaluations of the modeling are given.

### 6. Numerical results

Simulations of photochemical compounds were carried out using the regional V200603par-rc1 version of the CHIMERE model for August 2003. This version calculates the concentration of 44 gaseous species and both inorganic and organic aerosols of primary and secondary origin, including primary particulate matter, mineral dust, sulfate, nitrate, ammonium, secondary organic species and water. Numerical resolution scheme was analyzed for a domain centred on Madrid (MAD in Figure 2), with a similar set up to that used in [7]. This area is one of the most populated areas in Spain, with more than 6 millions of inhabitants. High ozone level episodes are quite frequent over this area. This domain at a horizontal resolution of 0.07 degrees and 14 vertical sigma-pressure levels extending up to 500 hPa, was nested to a coarser one, covering the Iberian Peninsula (SP in Figure...
1) at a 0.2 degree resolution. This second domain was also nested to a European scale domain (EUR1 in Figure 2), ranging from 10.5W to 22.5E and from 35N to 57.5 N and a 0.5 degree horizontal resolution. A one-way nesting procedure was used; coarse-grid simulations forced the fine-grid ones at the boundaries without feedback.

Boundary conditions for the coarsest domain were provided from monthly 2003 climatology from LMDz-INCA model [8] for gases concentrations and from monthly 2004 GOCART model [9] for particulate species, as described in [10].

Emissions for all the simulations were derived from the annual totals of the EMEP database for 2004 [11]. Original EMEP emissions were disaggregated taking into account land use information (Global Land Cover Facility, GLCF, http://change.gsfc.nasa.gov/create.html) in order to get higher resolution emission data. For each SNAP activity sector, the total NMVOC emission was split into emissions of 227 real individual NMVOC according to the AEAT speciation [12]. These species were then aggregated into the CHIMERE model ones.

The MM5 model was used to obtain the meteorological input fields. The simulations were carried out also for three domains, with respective resolutions of 36 Km, 19 Km and 7 km. The two coarsest MM5 simulations were forced by the National Centres for Environmental Prediction model (GFS) analyses. The finest domain was nested to a 21 km resolution MM5 simulation.

The quality of model predictions obtained with the implementation of the rational conservative formulation (RCF) was analyzed by comparing it to observations at the monitoring sites. Figure 3 shows the location of the NO\textsubscript{2}, SO\textsubscript{2} and O\textsubscript{3} monitoring stations located inside the Madrid domain. Figure 4 gives the location of a common monitoring station 280974 and figures 5, 6 and 7 present the numerical results of ozone, NO\textsubscript{2}, and SO\textsubscript{2} in this monitoring station. Also the corresponding observed concentrations with RCF numerical model between 1\textsuperscript{st} August 2003 and 5\textsuperscript{th} August 2003 for this common monitoring station are presented in Figure 5, 6 and 7.
Fig. 3. Distribution map of NO$_2$, SO$_2$ and O$_3$ monitoring stations in the area of Madrid (Spain).

Fig. 4: Location of the monitoring station 280974

Fig. 5: Observed and simulated concentration of NO$_2$ at station 2807924

Fig. 6: Observed and simulated concentration of SO$_2$ at station 2807924

Fig. 7: Observed and simulated concentration of O$_3$ at station 2807924
In order to evaluate the performance of the CHIMERE model with RCF some statistics were calculated. Table 1 presents the metrics used and their definition. Parameters such as mean bias ($B_{MB}$), mean normalized bias ($B_{MNB}$), mean normalized absolute error ($E_{MNAE}$), root mean square error ($E_{RMSE}$) and root mean normalized square error ($E_{RMNSE}$) were estimated for $O_3$, $NO_2$ and $SO_2$. Regarding ozone, only statistics for moderate-to-high ozone concentration cases (more important for human health protection) were considered by selecting predicted-observed value pairs when hourly observations were equal to or greater than the cutoff of 80 $\mu gm^{-3}$. For $NO_2$ and $SO_2$ a cutoff value of 5 $\mu gm^{-3}$ was used. 39 air quality sites were taken into account to estimate ozone statistics. For $NO_2$ and $SO_2$ evaluation information from 10 stations was considered.

### Table 1. Definition of the metrics used in the evaluation of the CHIMERE model performance

<table>
<thead>
<tr>
<th>Metric</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean bias ($B_{MB}$)</td>
<td>$\frac{1}{N} \sum (M_i - O_i) = \overline{M} - \overline{O}$</td>
</tr>
<tr>
<td>Mean normalized bias ($B_{MNB}$)</td>
<td>$\frac{1}{N} \sum \left( \frac{M_i - O_i}{O_i} \right) = \left( \frac{1}{N} \sum \frac{M_i}{O_i} - 1 \right)$</td>
</tr>
<tr>
<td>Mean normalized absolute error ($E_{MNAE}$)</td>
<td>$\frac{1}{N} \sum \left( \frac{</td>
</tr>
<tr>
<td>Root mean square error ($E_{RMSE}$)</td>
<td>$\left[ \frac{1}{N} \sum (M_i - O_i)^2 \right]^{1/2}$</td>
</tr>
<tr>
<td>Root mean normalized square error ($E_{RMNSE}$)</td>
<td>$\left[ \frac{1}{N} \sum \left( \frac{M_i - O_i}{O_i} \right)^2 \right]^{1/2}$</td>
</tr>
</tbody>
</table>

N: pairs of modeled and observed concentrations $M_i$ and $O_i$. The index $i$ is over time series and over all the locations in the domain.

Statistical results for ozone, nitrogen dioxide and sulfur dioxide are presented in Table 2.
Table 2. Statistics for ozone, nitrogene dioxide and sulfur dioxide evaluation for august 2003. Based on hourly values higher than 80 µgm$^{-3}$, 5 µgm$^{-3}$ and 5 µgm$^{-3}$ respectively.

<table>
<thead>
<tr>
<th>Statistical measure</th>
<th>O$_3$</th>
<th>NO$_2$</th>
<th>SO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean bias (µg m$^{-3}$)</td>
<td>-11.2043</td>
<td>-2.6061</td>
<td>-6.7785</td>
</tr>
<tr>
<td>Mean normalized bias</td>
<td>-0.0839</td>
<td>-0.3402</td>
<td>-0.6879</td>
</tr>
<tr>
<td>Mean normalized absolute error</td>
<td>0.1844</td>
<td>0.6285</td>
<td>0.7054</td>
</tr>
<tr>
<td>Root mean square error (µg m$^{-3}$)</td>
<td>25.486</td>
<td>5.8845</td>
<td>8.3290</td>
</tr>
<tr>
<td>Root mean normalized square error</td>
<td>0.2277</td>
<td>0.7728</td>
<td>0.7322</td>
</tr>
</tbody>
</table>

The plots showing the mean normalized absolute error for the individual stations and for the three contaminants are presented in Figures 8, 9 and 10.

![NO$_2$: Mean Normalized Absolute Error](image)

Fig. 8. NO$_2$ Mean normalized absolute error

![SO$_2$: Mean Normalized Absolute Error](image)

Fig. 9. SO$_2$ Mean normalized absolute error

![O$_3$: Mean Normalized Absolute Error](image)

Fig. 10. O$_3$ Mean normalized absolute error
7. Conclusions

In this paper we have presented the implementation in the European scale Eulerian chemistry transport model CHIMERE of an exactly conservative method for the advection equation. The advantage of these methods is that the cell-integrated average is predicted via a flux formulation, thus the mass is exactly conserved. The results of the method for ozone, nitrogen dioxide and sulfur dioxide statistics have been compared with a set of observation sites in the area of Madrid (Spain). The mean normalized bias and the mean normalized absolute error present values, that are inside the range to consider an accurate model performance.

Acknowledgements

This study was supported by Ministerio de Ciencia y Tecnología of Spain under the project CGL2008-1757/CLI.

References


IMPLEMENTATION IN CHIMERE OF A CONSERVATIVE …


Modelling of the advection-diffusion equation with a meshless method without numerical diffusion

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Abstract

A comprehensive study is presented regarding the stability of the forward explicit integration technique with generalized finite difference spatial discretizations, free of numerical diffusion, applied to the advection-diffusion equation. The modified equivalent partial differential equation approach is used to demonstrate that the approximation is free of numerical diffusion. Two-dimensional results are obtained using the von Neumann method of stability analysis. Numerical results are presented showing the accuracy obtained.

Key words: advection-diffusion, generalized finite difference
MSC2000: AMS Codes (optional)

1. Introduction

With the development of modern industry, various pollulants discharge in the air, rivers, lakes and oceans. The changes of pollulants in the air or in the water consist of the physical, chemical and biochemical process and so on. The physical changes of pollution involve two main important processes, that is, advection and diffusion. The mathematical model describing these two processes is the well known advection-diffusion equation. In two dimensions this equation is as follows
MODELLING OF THE ADVECTION-DIFFUSION

\[
\frac{\partial U}{\partial t} + \beta_x \frac{\partial U}{\partial x} + \beta_y \frac{\partial U}{\partial y} = \alpha_x \frac{\partial^2 U}{\partial x^2} + \alpha_y \frac{\partial^2 U}{\partial y^2} ; t > 0, \quad x, y \in \Omega
\]

with the initial condition:

\[ U(x, 0) = f(x) \quad (1) \]

and the boundary conditions:

\[ aU_{x_0, t} + b \frac{\partial U}{\partial n} = g(t) \quad \text{in} \ \Gamma \]

being \( f(x) \) and \( g(t) \) two known functions, \( a, b \) are constants, \( \Gamma \) is the boundary of \( \Omega \), \( U(x, y, t) \) is a transported (advected and diffused) scalar variable, \( \beta_x > 0, \beta_y > 0 \) are constant speeds of advection and \( \alpha_x > 0, \alpha_y > 0 \) are constant diffusivities in the x- and y- direction respectively.

Various numerical techniques can be used to solve this partial differential equation with the associated initial and boundary conditions \[1\]. An active field of research is the use of meshless methods. An evolution of the method of finite differences has been the development of generalized finite difference method (GFDM) that can be applied as a meshless or meshfree method to irregular grids or clouds of points. Benito, Ureña and Gavete have made interesting contributions to the development of this method \[2-7\]. This paper shows the application of the generalized finite difference method to solve the advection-diffusion equation by an explicit method.

The paper is structured in six sections. In section 2, we describe briefly the GFDM. In section 3 we describe the explicit scheme used to approximate the advection-diffusion equation. In section 4 we study the truncation error and the stability. In Section 5 an error analysis is done comparing with a test case. Section 6 contains concluding remarks.

2. The Generalized finite difference method

In the GFDM the intention is to obtain explicit linear expressions for the approximation of partial derivatives in the points of a domain. First of all, an irregular grid or cloud of points is generated in the domain \( \Omega \cup \Gamma \). On defining the central node with a set of nodes surrounding that node, the star of nodes then refers to a group of established nodes in relation to a central node. Each node in the domain has an associated star assigned to it.

We define the following function based in the approximation of second order in Taylor series

\[
B(u) = \sum_{j=1}^{N} \left( u_j - u_i + h_j \frac{\partial \bar{U}^0}{\partial x} + k_j \frac{\partial \bar{U}^0}{\partial y} \right) \left( h_j \frac{\partial \bar{U}^0}{\partial x} + k_j \frac{\partial \bar{U}^0}{\partial y} \right) \left( h_j \frac{\partial \bar{U}^0}{\partial x} + k_j \frac{\partial \bar{U}^0}{\partial y} \right) \right)^2
\]
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where \( u_0 \) is the approximated value of the function at the central node of the star, \((x_0, y_0)\), \( u_j \) are the function values of the rest of the nodes, \( h_j = x_j - x_0 \), \( k_j = y_j - y_0 \) and \( w(h_j, k_j) \) is the denominated weight function.

If the function (2) is minimized with respect to the partial derivatives, the following linear equation system is obtained

\[
\mathbf{A} \mathbf{D}_u = \mathbf{b} = \left\{ \sum_{j=1}^{N} \xi_j u_0 + u_j \left( \frac{h_j^2}{2} w^2 \right) \right\}^T
\]

\[
\mathbf{D}_u = \left\{ \frac{\partial U_0}{\partial x}, \frac{\partial U_0}{\partial y}, \frac{\partial^2 U_0}{\partial x^2}, \frac{\partial^2 U_0}{\partial y^2}, \frac{\partial^2 U_0}{\partial x \partial y} \right\}^T
\]

on solving the system (3) the explicit finite difference formulae are obtained.

\[
\begin{align*}
Y_{k} & = -u_0 \sum_{i=1}^{5} M_{ki} c_i + \sum_{j=1}^{5} u_j \left( \sum_{i=1}^{5} M_{ji} d_{ji} \right), \quad k = 1,...,5 \\
\mathbf{D}_a & = \frac{1}{q_{ik}} \left( Y_{k} - \sum_{i=1}^{5} q_{i+1,k} \mathbf{D}_a \right), \quad k = 1,...,5
\end{align*}
\]

where

\[
M_{ij} = \begin{cases} 
-1^{i-j} \sum_{k=j-i}^{i+j-1} q_{i+k} & \text{for } j < i, \quad i = 1,...,5 \quad j = 1,...,5 \\
\frac{1}{q_{ii}} & \text{for } j = i, \quad i = 1,...,5 \quad j = 1,...,5 \\
0 & \text{for } j > i, \quad i = 1,...,5 \quad j = 1,...,5 
\end{cases}
\]

with \( \delta_{ij} \) the Kronecker delta function, and:

\[
c_i = \sum_{j=1}^{5} d_{ji}
\]

\[
d_{ji} = h_j w^2; d_{j2} = k_j w^2; d_{j4} = \frac{h_j^2}{2} w^2; d_{j5} = \frac{k_j^2}{2} w^2; d_{j6} = h_j k_j w^2
\]

3. The advection-diffusion GFDM explicit scheme

On including the explicit expressions for the values of partial derivatives (5) in the differential equation of problem, we obtain the star equation (explicit difference scheme)(6):

\[
\mathbf{Y} k = u_0 \sum_{i=1}^{5} M_{ki} c_i + \sum_{j=1}^{5} u_j \left( \sum_{i=1}^{5} M_{ji} d_{ji} \right), \quad k = 1,...,5
\]

\[
\mathbf{D}_a = \frac{1}{q_{ik}} \left( \mathbf{Y} k - \sum_{i=1}^{5} q_{i+1,k} \mathbf{D}_a \right), \quad k = 1,...,5
\]
MODELLING OF THE ADVECTION-DIFFUSION

\[
\frac{\partial U_0}{\partial t} = \frac{u_{0}^{n+1} - u_{0}^{n}}{\Delta t}
\]

\[
\frac{\partial U_0}{\partial x} = -\lambda_0 u_0^n + \sum_{j=1}^{N} \lambda_j u_j^n
\]

\[
\frac{\partial U_0}{\partial y} = -\mu_0 u_0^n + \sum_{j=1}^{N} \mu_j u_j^n
\]

\[
\frac{\partial^2 U_0}{\partial x^2} = -m_0 u_0^n + \sum_{j=1}^{N} m_j u_j^n
\]

\[
\frac{\partial^2 U_0}{\partial y^2} = -\eta_0 u_0^n + \sum_{j=1}^{N} \eta_j u_j^n
\]

\[
u_0^{n+1} = u_0^n - \Delta t \left[ \beta_x \left( -\lambda_0 u_0^n + \sum_{j=1}^{N} \lambda_j u_j^n \right) + \beta_y \left( -\mu_0 u_0^n + \sum_{j=1}^{N} \mu_j u_j^n \right) \right] + \Delta t \left[ \alpha_x \left( -m_0 u_0^n + \sum_{j=1}^{N} m_j u_j^n \right) + \alpha_y \left( -\eta_0 u_0^n + \sum_{j=1}^{N} \eta_j u_j^n \right) \right]
\]

with: \( \lambda_0 = \sum_{j=1}^{N} \lambda_j \); \( \mu_0 = \sum_{j=1}^{N} \mu_j \); \( m_0 = \sum_{j=1}^{N} m_j \); \( \eta_0 = \sum_{j=1}^{N} \eta_j \)

This scheme uses the forward-difference form for the time derivative and generalized finite difference forms for all spatial derivatives.

By using the modified equivalent partial differential equation approach of Warming and Hyett [8], we obtain the following expansion equation

\[
\frac{\partial U}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 U}{\partial t^2} + \frac{(\Delta t)^2}{6} \frac{\partial^3 U}{\partial t^3} + \frac{(\Delta t)^3}{24} \frac{\partial^4 U}{\partial t^4} + \beta_x \left( \frac{\partial U}{\partial x} + \sum_{j=1}^{N} \gamma_{1,j} h_j k_j \frac{\partial^3 U}{\partial x^3} + ... \right)
\]

\[
+ \beta_y \left( \frac{\partial U}{\partial y} + \sum_{j=1}^{N} \gamma_{2,j} h_j k_j \frac{\partial^3 U}{\partial y^3} + ... \right) - \alpha_x \left( \frac{\partial^2 U}{\partial x^2} + \sum_{j=1}^{N} \gamma_{3,j} h_j k_j \frac{\partial^3 U}{\partial x^3} + ... \right)
\]

\[
- \alpha_y \left( \frac{\partial^2 U}{\partial y^2} + \sum_{j=1}^{N} \gamma_{4,j} h_j k_j \frac{\partial^3 U}{\partial y^3} + ... \right) = 0
\]

and the modified equation

\[
\frac{\partial U}{\partial t} + \beta_x \frac{\partial U}{\partial x} + \beta_y \frac{\partial U}{\partial y} - \left( \alpha_x - \frac{\beta_x^2}{2} \Delta t \right) \frac{\partial^2 U}{\partial x^2} - \left( \alpha_y - \frac{\beta_y^2}{2} \Delta t \right) \frac{\partial^2 U}{\partial y^2} + \ldots = 0
\]

This method incorporates numerical diffusion.

A new GFD scheme free of numerical diffusion can be created as follows
MODELLING OF THE ADVECTION-DIFFUSION

\[ u_0^{n+1} = u_0^n - \Delta t \left[ \beta_x \left( -\lambda_0 u_0^n + \sum_{j=1}^{N} \lambda_j u_j^n \right) + \beta_y \left( -\mu_0 u_0^n + \sum_{j=1}^{N} \mu_j u_j^n \right) \right] + \]

\[ \Delta t \left[ \left( \alpha_x + \frac{\beta_x^2}{2} \Delta t \right) \left( -m_0 u_0^n + \sum_{j=1}^{N} m_j u_j^n \right) + \left( \alpha_y + \frac{\beta_y^2}{2} \Delta t \right) \left( -\eta_0 u_0^n + \sum_{j=1}^{N} \eta_j u_j^n \right) \right] \]

with: \( \lambda_0 = \sum_{j=1}^{N} \lambda_j \); \( \mu_0 = \sum_{j=1}^{N} \mu_j \); \( m_0 = \sum_{j=1}^{N} m_j \); \( \eta_0 = \sum_{j=1}^{N} \eta_j \)

Then by using the modified equivalent partial differential equation approach of Warming and Hyett [8] we obtain the following expansion equation

\[ \frac{\partial U}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 U}{\partial t^2} + \frac{(\Delta t)^2}{6} \frac{\partial^3 U}{\partial t^3} + \frac{(\Delta t)^3}{24} \frac{\partial^4 U}{\partial t^4} + \beta_x \left( \frac{\partial U}{\partial x} + \sum_{j=1}^{N} \gamma_{1,j} h_j k_j \frac{\partial^3 U}{\partial x^3} + \ldots \right) + \]

\[ \beta_y \left( \frac{\partial U}{\partial y} + \sum_{j=1}^{N} \gamma_{2,j} h_j k_j \frac{\partial^3 U}{\partial y^3} + \ldots \right) - \left( \alpha_x + \frac{\beta_x^2 \Delta t}{2} \right) \left( \frac{\partial^2 U}{\partial x^2} + \sum_{j=1}^{N} \gamma_{3,j} h_j k_j \frac{\partial^4 U}{\partial x^4} + \ldots \right) - \left( \alpha_y + \frac{\beta_y^2 \Delta t}{2} \right) \left( \frac{\partial^2 U}{\partial y^2} + \sum_{j=1}^{N} \gamma_{4,j} h_j k_j \frac{\partial^4 U}{\partial y^4} + \ldots \right) = 0 \]

and the modified equation

\[ \frac{\partial U}{\partial t} + \beta_x \frac{\partial U}{\partial x} + \beta_y \frac{\partial U}{\partial y} - \alpha_x \frac{\partial^2 U}{\partial x^2} - \alpha_y \frac{\partial^2 U}{\partial y^2} + \ldots = 0 \]

The modified equivalent partial differential equation of this method shows that this GFD formula (9) is free of numerical diffusion.

4. Convergence

According to Lax’s equivalence theorem, if the consistency condition is satisfied, stability is the necessary and sufficient condition for convergence. In this section we study firstly the truncation error of the advection-diffusion equation, and secondly consistency and stability.

We split the truncation error (TTE) in time derivative error (TE_t) and space derivatives error (TE_x). As the first order time derivative is given by

\[ \frac{\partial U}{\partial t} x_{0,t} = \frac{U x_{0,t} + \Delta t - U x_{0,t}}{\Delta t} - \frac{\Delta t}{2} \frac{\partial^2 U}{\partial t^2} x_{0,t} + O \Delta t^2 \quad \forall t < t_i < t + \Delta t \]
then the truncation time error is given by

\[ \text{TE}_t = -\frac{\Delta t}{2} \frac{\partial^2 u(x_0, y_0, t_f)}{\partial t^2} + \Theta((\Delta t)^2), \quad t < t_f < t + \Delta t \]  

(12)

In order to obtain the truncation error for space GFD derivatives, Taylor’s series expansion including higher order derivatives is used and then higher order function \( B^*(u) \) is obtained

\[ B^*(u) = \sum_{j=1}^{N} \left[ u_0 - u_i + h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} + \frac{1}{2} \left( h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} \right)^2 + \right] \right]^2 w(h_j, k_j) \]

(13)

If \( B^*(u) \) is minimized with respect to the partial derivatives up to second order, the following linear equation system is defined

\[ A D_u = \begin{cases} \sum_{j=1}^{N} \Xi h_j \sum_{j=1}^{N} \Xi k_j \sum_{j=1}^{N} \Xi h_j^2 \sum_{j=1}^{N} \Xi k_j^2 \sum_{j=1}^{N} \Xi h_j k_j \end{cases} \]

(14)

where

\[ \Xi = \left( u_0 - u_i - \frac{1}{6} \left( h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} \right)^3 - \frac{1}{24} \left( h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} \right)^4 - \right) w(h_j, k_j) \]

with \( N=8 \), and then

\[ \text{TE}_{(x,y)} = \mathbf{CA}^{-1} \left( \sum_{j=1}^{N} \gamma h_j \sum_{j=1}^{N} \gamma k_j \sum_{j=1}^{N} \gamma h_j^2 \sum_{j=1}^{N} \gamma k_j^2 \sum_{j=1}^{N} \gamma h_j k_j \right) \]

where

\[ \gamma = \left( - \frac{1}{6} \left( h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} \right)^3 - \frac{1}{24} \left( h_j \frac{\partial U_0}{\partial x} + k_j \frac{\partial U_0}{\partial y} \right)^4 - \right) w(h_j, k_j) \]

(14)
MODELLING OF THE ADVECTION-DIFFUSION

\[
A = \begin{pmatrix}
\sum_{j=1}^{N} h_j^2 w^2 & \sum_{j=1}^{N} h_j k_j w^2 & \sum_{j=1}^{N} h_j^3 w^2 & \sum_{j=1}^{N} \frac{h_j k_j}{2} w^2 & \sum_{j=1}^{N} h_j^2 k_j w^2 \\
\sum_{j=1}^{N} k_j^2 w^2 & \sum_{j=1}^{N} h_j^2 k_j w^2 & \sum_{j=1}^{N} h_j^3 w^2 & \sum_{j=1}^{N} \frac{h_j k_j}{2} w^2 & \sum_{j=1}^{N} h_j k_j w^2 \\
\sum_{j=1}^{N} h_j^4 w^2 & \sum_{j=1}^{N} \frac{h_j k_j}{4} w^2 & \sum_{j=1}^{N} h_j^2 k_j w^2 & \sum_{j=1}^{N} \frac{h_j k_j}{4} w^2 & \sum_{j=1}^{N} \frac{h_j^2 k_j}{2} w^2 \\
\sum_{j=1}^{N} \frac{k_j^4}{4} w^2 & \sum_{j=1}^{N} \frac{h_j k_j}{4} w^2 & \sum_{j=1}^{N} \frac{h_j^2 k_j}{2} w^2 & \sum_{j=1}^{N} \frac{k_j^4}{4} w^2 & \sum_{j=1}^{N} \frac{h_j^2 k_j}{2} w^2 \\
\sum_{j=1}^{N} h_j^2 k_j w^2 & \sum_{j=1}^{N} \frac{k_j^4}{4} w^2 & \sum_{j=1}^{N} \frac{h_j^2 k_j}{2} w^2 & \sum_{j=1}^{N} \frac{k_j^4}{4} w^2 & \sum_{j=1}^{N} \frac{h_j^2 k_j}{2} w^2 \\
\end{pmatrix}
\]

\[
C = \begin{pmatrix}
-\beta_x & -\beta_y & -(\alpha_x + \frac{\beta_x^2 \Delta t}{2}) & -(\alpha_y + \frac{\beta_y^2 \Delta t}{2}) & 0 \\
\end{pmatrix}
\]

where

\[
w^2 = w(h_j, k_j)^2
\]

Then by solving (14), we obtain

\[
TE(x,y) = -\beta_x \left[ \sum_{j=1}^{N} \left( \psi_{1,j} \frac{\partial^3 U}{\partial x^3} + \psi_{2,j} \frac{\partial^3 U}{\partial x^2 \partial y} + \psi_{3,j} \frac{\partial^3 U}{\partial x \partial y^2} + \psi_{4,j} \frac{\partial^3 U}{\partial y^3} + \ldots \right) \right] - \\
- \beta_y \left[ \sum_{j=1}^{N} \left( \psi_{5,j} \frac{\partial^3 U}{\partial x^3} + \psi_{6,j} \frac{\partial^3 U}{\partial x \partial y^2} + \psi_{7,j} \frac{\partial^3 U}{\partial x^2 \partial y} + \psi_{8,j} \frac{\partial^3 U}{\partial y^3} + \ldots \right) \right] - \\
\left( \alpha_x + \frac{\beta_x^2 \Delta t}{2} \right) \left[ \sum_{j=1}^{N} \left( \psi_{9,j} \frac{\partial^3 U}{\partial x^3} + \psi_{10,j} \frac{\partial^3 U}{\partial x^2 \partial y} + \psi_{11,j} \frac{\partial^3 U}{\partial x \partial y^2} + \psi_{12,j} \frac{\partial^3 U}{\partial y^3} + \ldots \right) \right] - \\
\left( \alpha_y + \frac{\beta_y^2 \Delta t}{2} \right) \left[ \sum_{j=1}^{N} \left( \psi_{13,j} \frac{\partial^3 U}{\partial x^3} + \psi_{14,j} \frac{\partial^3 U}{\partial x^2 \partial y} + \psi_{15,j} \frac{\partial^3 U}{\partial x \partial y^2} + \psi_{16,j} \frac{\partial^3 U}{\partial y^3} + \ldots \right) \right] + \Theta \mathbf{j}_x k_j
\]

(15)

where \( \psi_{i,j}(h_j, k_j) \) are second-order rational functions and \( \Theta h_j, k_j \) is a series of third- and higher-order functions.

The total truncation error for advection-diffusion equation is

\[
TTE = TE_t + TE(x,y)
\]

(16)

By considering bounded derivatives in \( TTE \), we have consistency

\[
\lim_{\Delta t \to 0} \lim_{h_j, k_j \to 0, 0} TTE = 0
\]

(17)
"Boundary conditions are neglected by the von Neumann method which applies in theory only to pure initial value problems with periodic initial data. It does however provide necessary conditions for stability of constant coefficient problems regardless of the type of boundary condition" [9].

From the previously obtained formula (9)

\[
u_{n+1}^a = \left(1 + \Delta t \left[ \beta_x \lambda_0 + \beta_y \mu_0 - (\alpha_x + \beta_x^2 \frac{\Delta t}{2}) m_0 - (\alpha_y + \beta_y^2 \frac{\Delta t}{2}) \eta_0 \right] \right) u_0^n - \\
\Delta t \left[ \beta_x \sum_{j=1}^{N} \lambda_j u_j^n + \beta_y \sum_{j=1}^{N} \mu_j u_j^n - (\alpha_x + \beta_x^2 \frac{\Delta t}{2}) \sum_{j=1}^{N} m_j u_j^n - (\alpha_y + \beta_y^2 \frac{\Delta t}{2}) \sum_{j=1}^{N} \eta_j u_j^n \right]
\]  \hspace{1cm} (18)

For the stability analysis a harmonic decomposition is made of the approximate solution at grid points at a given time level \( n \)

\[
u_0^n = \xi e^{i(\kappa_0 x_0 + \kappa_0 y_0)}; u_j^n = \xi e^{i(\kappa_j x_0 + h_j + \kappa_0 y_0 + k_j)}
\]

where \((x_0, y_0)\) are the coordinates in the central node of the star, and \((h_j, k_j)\) are the coordinates of the other nodes of the star with respect to the central node.

\[
\xi = \left(1 - \Delta t \sum_{j=1}^{N} \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) m_j + \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) \eta_j - \beta_x \lambda_j - \beta_x \mu_j \right) 1 - \cos(\kappa_j h_j + \kappa_j k_j)
\]

\[
+i \Delta t \sum_{j=1}^{N} \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) m_j + \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) \eta_j - \beta_x \lambda_j - \beta_x \mu_j \right) \sen(\kappa_j h_j + \kappa_j k_j)
\]

Taking into account that the stability condition is \( \|\xi\| \leq 1 \), then

a) \( |\text{Real}(\xi)| < 1 \)

\[
\left(1 - \Delta t \sum_{j=1}^{N} \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) m_j + \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) \eta_j - \beta_x \lambda_j - \beta_x \mu_j \right) 1 - \cos(\kappa_j h_j + \kappa_j k_j) < 1
\]

\[
-1 < \left(1 - \Delta t \sum_{j=1}^{N} \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) m_j + \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) \eta_j - \beta_x \lambda_j - \beta_x \mu_j \right) 1 - \cos(\kappa_j h_j + \kappa_j k_j) < 1
\]

\[
\Delta t \left[ -\beta_x \lambda_0 - \beta_x \mu_0 + \left( \alpha_x + \beta_x^2 \frac{\Delta t}{2} \right) m_0 + \left( \alpha_y + \beta_y^2 \frac{\Delta t}{2} \right) \eta_0 \right] \leq 1
\]  \hspace{1cm} (19)

b) \( \|\xi\| \leq 1 \)
Both formulae (19) and (20) give us the conditions for the stability.

5. Numerical results

In order to illustrate the application of the numerical explicit GFD scheme developed previously, a problem for which an exact solution is available is required so that approximate results obtained can be compared with an exact solution. The problem to be solved is

$$\frac{\partial U}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial U}{\partial y} = 0.1\left( \frac{\partial U^2}{\partial x^2} + \frac{\partial U^2}{\partial y^2} \right)$$

(21)

$$t > 0, \quad 9 < x^2 + y^2 < 25$$

The exact solution is
MODELLING OF THE ADVECTION-DIFFUSION

\[ U(x, y, t) = e^{-1.8t \cdot x \cdot y} \]

\[
\begin{align*}
\text{Initial conditions: } & U(x, 0) \\
\text{Dirichlet boundary conditions at } & 9 = x^2 + y^2 = 25
\end{align*}
\]

The weight function is:
\[ w(x_j, y_j) = \frac{1}{\sqrt{x_j^2 + y_j^3}} \]  \hspace{1cm} (22)

The global error is evaluated in the last step considered, using the following formula:
\[
\text{global error} = \sqrt{\frac{\sum_{i=1}^{M} |\text{sol}(i) - \text{exac}(i)|}{\text{exac}_{\text{max}}}} \hspace{1cm} (23)
\]

where \( \text{sol}(i) \) is the GFDM solution at the node \( i \), \( \text{exac}(i) \) is the exact value of the solution at the node \( i \), \( |\text{exac}_{\text{max}}| \) is the maximum value of the exact solution in the cloud of nodes considered and \( M \) is the total number of nodes of the domain.

In this problem we consider different irregular clouds of points as given in Fig. 1.

![Different irregular clouds of points.](image)

Fig. 1. Different irregular clouds of points.
The influence on global error of using different number of nodes is given in Fig. 2.

![% GLOBAL ERROR (with Δt = 0.0005)](image)

Fig. 2 Global error versus the number of nodes.

Also we consider for the irregular cloud of 1248 nodes the influence on global error versus different values of time increment in Fig.3.

![% GLOBAL ERROR (1248 nodes)](image)

Fig. 3 Global error versus the time increment.

As it is shown in Fig.2 and 3, the global error decreases by increasing the number of nodes or decreasing the time increment.

6. Conclusions

An explicit solution of advection-diffusion equation has been presented for the case of using the GFDM over irregular grids. We have defined the truncation
MODELLING OF THE ADVECTION-DIFFUSION

eq

error of the scheme in the case of irregular grids of nodes. Then, we have established the consistency and stability (following the von Neumann stability analysis) criteria for this scheme. An academic test has been presented to illustrate the application of this method.
The fully explicit generalized finite difference schemes are simple to implement and economical to use. They are very efficient and very quick. They are conditionally stable.
The modified equivalent partial differential equation approach of Warming and Hyett[8] has been employed which permits to demonstrate that the GFD scheme is free of numerical diffusion.

Acknowledgements
The authors acknowledge the support from Ministerio de Ciencia e Innovación of Spain, research project CGL2008-01757/CLI.

References
Wireless teleoperation system for vehicles based on automaton and secure communications

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Abstract

We present a teleoperation system via radio for vehicles of combustion engine or electric, designed for using in which human presence is not adequate, such as access to dangerous sites after catastrophes, spraying tasks in farming environments, road rollers, etc. The system has been developed by means of a radio modem of specific purpose that interchanges digital information of commands from the console to the vehicle and states from the vehicle to the console. A security system prevents against non-desired functioning in case of loss of communication or outsider intromissions. This system has been implemented and successfully tested in a prototype of vehicle used for spraying tasks.

Key words: Telecontrol, finite automaton, secure communications

1. Introduction

There exist several control systems of vehicles for several usings. On one hand we have autonomous functioning vehicles such as those described in [1] and [2]. This type of vehicles does not need an operator and have autonomy for the followed route. They are based on a navigation schedule. Therefore autonomous systems present as main problems the necessity of information a priori about the work environment and possible changes in such environment, taking decisions in non-expected situations and a big complexity of the sensorial system that allows the autonomous functioning, including a local computer with high capability of...
calculus and information storing, usually by means of a hard disk. By the precedent, autonomous systems need a complex and delicate control system.

On the other hand, well-known classical telecontrolled systems require a permanent attention and direct observation of the behaviour of the vehicle by the operator. The solution of events such as loss of communication may cause serious consequences in these systems or in the environment. The system that we introduce and have implemented is based on that the operation console interprets what is the desired action to be developed and, by means of a dialogue of operative commands and state responses, the vehicle carries out the desired tasks, solving, automatically, possible problems of the classical case such as loss of communication and decreases the bandwidth of the communication channel. Moreover, our system allows taking pre-programmed decisions in case of non-expected events, such as automatic detention in case of loss of communication or proximity to an obstacle in its trajectory. This system is adequate for controlling vehicles that can be directly watched by the operator or monitored by video cameras in the vehicle. Security of communications is also important depending on the purposes of the vehicle. We have used a novel key selection method for real time communications based on a Linear Feedback Shift Register which allows selecting keys from a list in a pseudorandom manner.

1.1 Technology

The digital communication system has been implemented by means of bidirectional narrow band radio-modems, in the band of 400-470 MHz. The modulation is 4L-DFSK with a speed of 9600 bits/s, which is enough since the control system in the vehicle is continuously attended by a local control and the communication system only transfers operative commands from the operation console to the local control. The vehicle has incorporated as local control a system based on a microcontroller of the family MCS-51 with the embedded program in flash memory. The system has digital outputs by means of drivers of solid state, relay outputs and analogical power outputs with PWM technology to act on the elements of control of the vehicle. The operation console has a joystick in order to input the information about motion, stop or motion directions by the operator. It also has lightning indicators that inform the operator about the state of the vehicle in what concerns to actions developed by the vehicle in real time. The console system has been implemented by means of an embedded microcontroller, taking into account a low consume in order to be supplied with batteries.
2. System Design

Our system, Figure 1, is formed by two interconnected subsystems via the wireless communication device (radiomodem). The first one is constituted by the operation console and the other one is located in the vehicle and corresponds to the control system of drivers of the engines, direction control and additional functionalities, such as a spraying system control, cameras, etc.

![Fig. 1 Block diagram of the system](image)

2.1 Console

The console is formed by a couple of joysticks, a speed selector, interrupters for activation of mechanisms in the vehicle such as spraying functions in the case of a vehicle with farming purposes, and lightning indicators of the state of the vehicle, that inform about the state of communications and actions that are being carried out by the vehicle. The system in charge of the reading of the console controls is based on a microcontroller of the family MS51 whose functioning is as follows. A finite automaton, Figure 2 implemented in the microcontroller makes the functions of reading and encodes as input all possible combinations of the console controls, that jointly with the information of the previous state, allow interpreting the action that the operator wants to carry out. This action is encoded as the output of the following state. The outputs of the states are transmitted to the
control system of the vehicle by means of the communication system (narrowband radiomodem) as packets with a ratio of two packets per second. After emitting each packet, the console receives a packet coming from the vehicle with information about its state. This state is shown on the lighting indicators. This ratio is adequate for tracked vehicles since they manoeuvre slowly. For other kind of vehicles with more speed and that require a faster response time this system allows to increase what needed the packets ratio for a right functioning.

The codification system that is described corresponds to a model implemented on a tracked vehicle with spraying purposes. This vehicle moves at slow or moderated speeds and it was checked that 4 speeds (vslow, slow, middle, high) and the stop state are enough for its manoeuvre. However, from this model we can extrapolate applications to other types of vehicles considering minor modifications.

The codification of the states constitutes a finite automaton, whose entries correspond with the steering levers, the speed selector and the interrupter of the trigger sprayer pump.

The entry alphabet S possesses three subsets: the first one, with respect to the direction $S_d=\{d_{11}, d_{10}, d_{01}, d_{00}, d_{0-1}, d_{-10}, d_{-1-1}, d_{1-1}, d_{-11}\}$ in function of the state of action of the drive state of steering levers. In this way the entry $d_{11}$ indicates the two levers forward, $d_{00}$ stop, $d_{0-1}$ left lever stop and right lever backward, etc; the second one with respect to speed $S_s=\{s_{00}, s_{01}, s_{10}, s_{11}\}$ $s_{00} \rightarrow v_{slow}$, $s_{01} \rightarrow v_{slow}$, $s_{10} \rightarrow v_{medium}$ and $s_{11} \rightarrow v_{high}$ and finally with respect to the actuator $S_a=\{a_0, a_1\}$ $a_0$ -> no action, $a_1$ -> action.

The subset of direction entries produces a subset of states which are dependent on the direction according with the following table:

<table>
<thead>
<tr>
<th>dL dR</th>
<th>state</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1</td>
<td>S1</td>
<td>Straight</td>
</tr>
<tr>
<td>1 0</td>
<td>S2</td>
<td>front-right</td>
</tr>
<tr>
<td>0 1</td>
<td>S3</td>
<td>front-left</td>
</tr>
<tr>
<td>0 0</td>
<td>S0</td>
<td>Stop</td>
</tr>
<tr>
<td>0 -1</td>
<td>S6</td>
<td>reverse-left</td>
</tr>
<tr>
<td>-1 0</td>
<td>S5</td>
<td>reverse-right</td>
</tr>
<tr>
<td>-1 -1</td>
<td>S4</td>
<td>reverse-straight</td>
</tr>
<tr>
<td>1 -1</td>
<td>S7</td>
<td>turn on clockwise</td>
</tr>
<tr>
<td></td>
<td></td>
<td>direction</td>
</tr>
<tr>
<td>-1 1</td>
<td>S8</td>
<td>turn on anti-clockwise</td>
</tr>
<tr>
<td></td>
<td></td>
<td>direction</td>
</tr>
</tbody>
</table>
TELEOPERATION SYSTEM FOR VEHICLES

Not all possible transitions between states are possible for a right functioning. The next diagram defines an automaton with the set of states reduced direction of the movement.

![Diagram of an automaton representing states and transitions]

**Fig. 2 Automaton representing states and transitions**

We have taken into account that we cannot pass from entries 1 to -1 and vice versa without passing through entry 0.

For each of the states of this subset we have as a new subset the speed and the actuator system, which produces a total number of 72 possible states, although not all of them will be considered in practice because of the following exceptions:
- Rotational states on its axis S8 and S7 only admit the lowest speed, ignoring other speed entries.
- In the states which imply a turn S2, S3, S5 and S6, the band corresponding to stop, what it is carried out in practice is to decrease one degree in the speed and it will only be stop when the speed selector is in vslow.
2.2 Vehicle control

The controller of the actuators of the engine of the vehicle has been implemented in a microcontroller of the same type of the console by means of another automaton. This automaton receives as inputs the packets that are sent by the console and jointly the sensorial information about direction, speed and proximity to obstacles of the vehicle, determine its next state that contains the outputs towards the actuators and the state information to be sent back to the console. Proximity detectors in the vehicle generate the entries $Sp = \{p_0, p_1\}$, where $p_0$ indicates free way and $p_1$ that an obstacle has been detected and detention is needed. Communications state generates the entries $Sf = \{f_0, f_1\}$, where $f_0$ indicates that the last two packets have been received with a right checksum and $f_1$ indicates that two consecutive errors of checksum in the packets of orders that have not been received (see Figure 5). In case that the vehicle does not receive two packets of orders consecutively (fail transmission), the automaton goes to an inactivity state. Figure 3 represents transitions between states of speed that are mapped on the states of direction $Sj$, depending on the codified selector on the console $Ss$, the proximity detectors $Sp$ and the state of communications $Sf$.

![Figure 3](image_url)

**Fig. 3** Transition of states in the vehicle corresponding to speed

Each state $S_mn$ is duplicated in function of the estate of the actuator $a_0$ to $a_1$. The diagram of states of the vehicle does not shows differences of speed in each rolling band that is inherent to changes of direction indicated in the console automaton. We are assuming that such information is codified in each state $S_j$.
3. Communication System

We have used a method that allows encoding the actions that at any time the vehicle can carry out using four ASCII characters. Figure 4 shows an example of the encoding used for some states in the case of tracking vehicles with a spraying system. Other vehicles with a more complex functionality can also use this system by adding some characters to the states encoding. This system of states encoding allows notorious saving in band width with respect to classical telecontrol systems and so a bit-rate of 4800 b/s is enough to the bidirectional communication (orders sending/receiving of states). Narrow band communication systems by radio are the most adequate for this type of telecontrol operations by the high ratio distance/power with low consumption, their stability and reliability and a lot of operation channels to be used. We have used a radiomodem with bit-rate 9600 b/s and F.E.C. ¾ in the UHF common used band 433 MHz. The power of 250 mW are enough to a long distance control of the vehicle. Other communication systems such as Bluetooth or Zigbee can be used to implement this system for telecontrol in short distance, substituting the narrowband radiomodem, but with possible collisions with other users given the more extended use of these types of communications. Moreover this system increases the reliability of the control of vehicle. In case of a packet is mismatched in the communication process and F.E.C. does not detect and correct the error, this does not produces any action unless it coincides with some of the expected packets related with the state of the automaton at that time.

One example of chronogram of the interchange of information between the vehicle and the console of control is given in Figure 5. It can be observed the messages transmitted by the console and the corresponding answers by the vehicle. In this case after a series of commands that order the running of the vehicle, all of them answered by the vehicle with its state, two consecutive fails occur due to interference or any other cause, recall that all the radio communication systems are susceptible of loss of information. In this case the vehicle goes to a stop state, restarting the running after receiving another valid command from the console.
3.1 Security of communications

The fact that communication between the vehicle and the console takes place in real time is of great importance. There exists a class of algorithms, known as stream cipher algorithms such that all of them treat the information bit-to-bit, usually binary digits and in real time and are very appropriate when buffering is limited some telecommunications applications as could be a radio modem. They are based in Linear Feedback Shift Registers (LFSR), which give an encryption sequence and are very suitable for hardware implementation (cf. [4] for details).

We use good properties of LFSRs to give an efficient selection key method which allows generating sequences of key identifiers. Source an destination share a list of keys and an easy algorithm to generate sequences of identifiers and therefore, these are not sent, which solves questions relative to possible compromised pairs of key-identifier and only some additional information bits about the initial state of the system that generates the sequence of identifiers is required to encrypt/decrypt a big number of blocks of information.

3.1.1 The key selection method

In this case, the source A (console or vehicle) and the destination B (console or vehicle) use a block cipher and share a list of l keys and an algorithm to generate a sequence of positions (identifiers) of the list of keys. The algorithm that we use consist in a binary LFSR (stages store one bit) with k stages, such that \(2k \geq l\) and a Boolean function whose input is the state vector of the LFSR at some moment and its output is a number in the range \(1\)–\(l\).

Now if A wants to send a message to B then A proceeds as follows:
TELEOPERATION SYSTEM FOR VEHICLES

1. A divides the plain text into packets $P_j$, $j=1,\ldots,n$ of blocks $B_{j,i}$, $i=1,\ldots,r$ of appropriate length.
2. For $j=1,\ldots,n$, A generates, by means of a Real Time Clock, a random number of $k$ digits, $S_j$, which is taken as initial state of the LFSR.
3. Using the LFSR and the Boolean function, A generates a sequence of numbers $j,i$ for $i=1,\ldots,r$ in the range 1-1 and consider the key whose position in the list is $j,i$, $k_{j,i}$.
4. A encrypts every block $B_{j,i}$ of the packet $P_j$, $j=1,\ldots,n$, using the key $k_{j,i}$, obtaining packets of blocks $C_j$, for $j=1,\ldots,n$.
5. A sends $S_j$ and $C_j$ for $j=1,\ldots,n$ to B.

When B receives $S_j$ and $C_j$, he uses $S_j$ to generate the sequence of keys necessary to decipher the message.

In case we do not want to send $S_j$ as plain text, we can use some of the characters of the first encrypted block of the packet $C_j$ to get a new seed for the LFSR and so, generate a pseudorandom number which gives an identifier of a new key $k$ to encrypt $S_j$. In that case, when B receives the message proceeds as follows:

1. B takes selected characters of $B_{j,1}$ to get a seed for the LFSR and gets the identifier of the key $k$.
2. B uses $k$ to get $S_j$.
3. B uses $S_j$ to get the sequence of keys $k_{j,i}$ and decrypts packet $C_{jj}=1,\ldots,n$

![Fig 6. Key selection method](image)

Figure 6 shows a diagram composed by an LFSR whose state vector is taken as input of a logic circuit given by a Boolean function, which produces keys $k_{j,i}$. This method has been also used in [2] and [3] for telecontrol and telemetry applications.

4. Conclusions

We have introduced a novel teleoperation system for vehicles based on a finite automaton and with a secure communication system which allows to handling vehicles for different purposes in an easy and safe way. This system was
implemented on a platform for greenhouses spraying [5]. The functioning given by the designed automaton shows an easily operable vehicle and with an acceptable level of security, in what concerns to possible loss of control and with a high security level of communication in what concerns to possible interferences or outsiders as evidenced after a long testing period [6].

![Vehicle and console](image)

**Fig 7.** Vehicle and console

### 4. Acknowledgements

This paper was supported by TEC2009-13763-C02-02. First and second authors are also supported by TIC019. Third author is supported by FQM0211.

### 5. References


Mutation rate and the maintenance of cooperation: a parsimonious model of somatic evolution and oncogenic transitions

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Background and Objectives: Multicellularity, and biological complexity in general, are ultimately the result of natural selection’s paradoxical tendency to foster cooperation through competition. Cooperating communities ranging from complex societies to somatic tissue are constantly under attack, however, by non-cooperating mutants or transformants, called “cheaters”.

Methods: We employ simulations and analytical game-theoretic models of interactions on networks with an array of different network topologies.

Results: Structure in these communities promotes the formation of cooperating clusters whose competitive superiority can alone be sufficient to thwart outgrowths of cheaters and thereby maintain cooperation. But we find that when cheaters appear too frequently – exceeding a threshold mutation or transformation rate – their scattered outgrowths infiltrate and break up cooperating clusters, resulting in a cascading loss of community integrity, a switch to net positive selection for cheaters, and ultimately in the loss of cooperation.

Discussion and Conclusions: We discuss the possibility that our model may provide a parsimonious framework for understanding the somatic evolutionary processes leading up to transitions from normal to cancerous tissue.

Grant support: NIH (R01 GM079483 to P.J.G; AI28433, RR06555, P20-RR18754 to A.S.P); European Community (FP7 231807 to P.J.G.); FTC-Portugal (J.M.P.).
Model assumptions

Cooperation and multicellularity evolved and are maintained by very complex processes, but a first approximation to these processes may be formulated as a simple evolutionary game:

On average, cooperators "help" others (increasing others' fitness) at their own expense (decreasing their own fitness).

On average, cheaters don't "help" others (don't increase others' fitness or decrease their own fitness).

Interactions are structured on a network (regular, random, or scale free).

Cooperation and cheating are heritable traits, and mutation can toggle between the two.

Main result: critical mutation rate above which cooperation is lost as 2nd order phase transition.

\[ \mu_c = (1 - q_0) \left( e^{-(1+\beta)} \left( \frac{1 + (n-1)q_0\varepsilon}{1 + \beta} \right)^{\alpha} - e^{-((n+m)\varepsilon)} \left( 1 + q_0 \left( \frac{1 + ((n-1)q_0 + 1)\varepsilon}{1 + \beta + \varepsilon} \right)^{\alpha} - 1 \right) \right)^{-1} \]

\[ \mu_c = k \varepsilon^{-1} (\alpha + 1)(\phi\varepsilon - \beta). \]

\( \alpha = \) sampling coefficient
\( \varepsilon = \) average "help" conferred by cooperators
\( \beta = \) average advantage of being a cheater
Figure 1. Equilibrium cooperator frequencies as a function of mutation rate. (a) As determined from simulated populations that were spatially structured on a three-dimensional grid. The population initially consists of all cooperators, and cheaters arise by spontaneous mutation. The intrinsic advantage of being a cheater (or cost of being a cooperator) was 0.01, the advantage conferred by a cooperating neighbor was 0.05, and total population size was 27,000. (b) As predicted by the analytical equilibrium solution of the “pair approximation” model, using the same parameter values but implicitly assuming an infinite population. The analytical curve reveals a sharp transition between the maintenance of cooperation and the complete loss of cooperation; the sharpness of the inflection resembles that of a second-order phase transition.
Transmission coefficient in monolayer graphene

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Abstract

We present a calculation for the transmission coefficient in the monolayer graphene in function of the angle through a barrier and a double barrier.

Key words: transmission, graphene, Klein paradox.

1. Introduction

Graphene is a planar and monoatomic layer of carbon atoms - then is two-dimensional (2D) - arranged on a densely packed honeycomb crystal lattice.

P.R. Wallace wrote the first paper [5] in 1947 to the band structure of graphene and showed the unusual semimetallic behaviour in this material. More time after, in 2004 A. Geim and K. Novoselov has obtained experimentally graphene. They
started with graphite three-dimensional and extracted a single sheet (a monolayer of atoms).

The graphene is a zero-gap semiconductor [2],[3], and for low energies the carriers with proximity to the Dirac points can be described by the Dirac-like Hamiltonian

\[
\hat{H} = \hbar v_F \begin{pmatrix} 0 & k_x - i k_y \\ k_x + i k_y & 0 \end{pmatrix} = \hbar v_F \sigma \cdot \vec{k}
\]

Where \( \vec{k} \) is the momentum, \( \sigma \) the 2D Pauli matrix and \( v_F \) the Fermi velocity that is independent of \( k \), and your value is \( v_F \approx 10^6 \text{ m/s} \). This play the role of speed of light, but is \( v_F \approx c/300 \). Giving rise to the conical sections for \( |E| < 1 \text{ eV} \).

We have a linear spectrum \( E = \hbar v_F k \), leading to the zero effective mass for electrons and holes, and then they are called Dirac fermions. They are like particles relativistic described by the Dirac equation for spin \( \frac{1}{2} \) particles. The electronic states are composed of states belonging to the different sublattices, and then we use two-component wave-functions (spinors).

The graphene is very interesting because it has a exceptional electronic quality. Experimental results from transport measurements show *high electron mobility* \( \mu \) that can exceed 15,000 cm\(^2\)/Vs in the concentrations \( n \) as high as \( 10^{13} \text{ cm}^{-2} \) even under ambient conditions [3].
2. Theory

The differences in the calculus of the transmission coefficient between traditional semiconductors (AlGaAs, ...) and the graphene are:

1. The carriers are governed in the first case by an equation differential of second order and in the second by an equation differential of first order.

\[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(r) \psi(r) = E \psi(r) \quad \text{Ec. Schrödinger} \]

\[ -i v_F \vec{\sigma} \cdot \vec{V} \psi(r) = E \psi(r) \quad \text{Ec. Dirac} \]

2. In the graphene we will have only carbon atoms, not its possible different combinations of elements.

The two components of \( \psi(r) \) close to the Dirac point, obeys the 2 D Dirac equation [4].

\[ -i v_F \vec{\sigma} \cdot \vec{V} \psi(r) = E \psi(r) \]

And we can write

\[ \psi_k(\vec{k}) = \frac{1}{\sqrt{2}} \left( \pm e^{i\theta_k} \right) \text{ when } \theta_k = \arctan \left( \frac{k_x}{k_y} \right). \]

2.1 Square barrier

We begin with a barrier of width D. Then the potential is

\[ V(x) = \begin{cases} 
0, & x < 0 \quad \text{region I} \\
V_0, & 0 \leq x \leq D \quad \text{region II} \\
0, & D < x \quad \text{region III} 
\end{cases} \]

The wavefunctions in the three regions can be write in terms of incident and reflected waves, in principle, but we can consider for the total the condition that the incident amplitude is the unity, the reflected amplitude is \( r \) and the transmitted amplitude is \( t \), and is not reflected amplitude in the final.

In the region I, II and III:
\[ \psi_1(\vec{r}) = \frac{1}{\sqrt{2}} \left( \frac{1}{s e^{i\phi}} \right) e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \left( \frac{1}{s e^{i(\pi - \phi)}} \right) e^{i(-k_x x + k_y y)} \]

\[ \psi_\Pi(\vec{r}) = \frac{a}{\sqrt{2}} \left( \frac{1}{s' e^{i\theta}} \right) e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \left( \frac{1}{s' e^{i(\pi - \theta)}} \right) e^{i(-q_x x + k_y y)} \]

\[ \psi_\text{III}(\vec{r}) = \frac{t}{\sqrt{2}} \left( \frac{1}{s e^{i\phi}} \right) e^{i(k_x x + k_y y)} \]

When \( s = \text{sgn}(E) \), \( s' = \text{sgn}(E-V_0) \), \( \phi = \arctan(k_y/k_x) \), \( k_x = k_F \cos \phi \), \( k_y = k_F \sin \phi \), \( k_F \) the Fermi momentum is \( k_F = \frac{2 \pi}{\lambda} \) and \( q_x = \frac{\sqrt{(V_0 - E)/h \nu F}}{2} - k_y^2 \).

The coefficients are determined only by the continuity of the wavefunction, because it is an equation differential of first order

\[ \psi_1(x = 0, y) = \psi_\Pi(x = 0, y) \]

\[ \psi_\Pi(x = D, y) = \psi_\text{III}(x = D, y) \]

Then we obtain \( t \), after we multiply to the conjugate \( t^* \), and we will have the transmission coefficient \( T(\phi) \)

\[ T_{\text{exc}}(\phi) = \frac{\cos^2 \theta \cos^2 \phi}{[\cos(Dq_x) \cos \phi \cos \theta]^2 + \sin^2(Dq_x)(1 - ss' \sin \phi \sin \theta)^2} \]

We achieve an approximation \( |V_0| >> E \), \( \theta \rightarrow 0 \), and

\[ T_{\text{aprx}}(\phi) \approx \frac{\cos^2 \phi}{1 - \cos^2(Dq_x) \sin^2 \phi} \]

### 2.2 Double barrier

We construct a double barrier because then we will have a well. Then the potential is

\[ V(x) = \begin{cases} 
V_0 & \text{for } |x| > L \\
0 & \text{for } |x| < L 
\end{cases} \]
And the equations are:

\[
\psi_1(\bar{r}) = \frac{1}{\sqrt{2}} \left( 1 \right) e^{i(k_x x + k_y y)} + \frac{r}{\sqrt{2}} \left( 1 \right) e^{-i(k_x x + k_y y)}
\]

\[
\psi_{II}(\bar{r}) = \frac{a}{\sqrt{2}} \left( 1 \right) e^{i(q_x x + k_y y)} + \frac{b}{\sqrt{2}} \left( s e^{i(\pi - \theta)} \right) e^{-i(q_x x + k_y y)}
\]

\[
\psi_{III}(\bar{r}) = \frac{c}{\sqrt{2}} \left( 1 \right) e^{i(k_x x + k_y y)} + \frac{d}{\sqrt{2}} \left( s e^{i(\pi - \theta)} \right) e^{-i(k_x x + k_y y)}
\]

\[
\psi_{IV}(\bar{r}) = \frac{f}{\sqrt{2}} \left( 1 \right) e^{i(q_x x + k_y y)} + \frac{g}{\sqrt{2}} \left( s e^{i(\pi - \theta)} \right) e^{-i(q_x x + k_y y)}
\]

\[
\psi_V(\bar{r}) = \frac{t}{\sqrt{2}} \left( 1 \right) e^{i(k_x x + k_y y)}
\]

We will have only two angles, \( \phi \) when the potential is zero and \( \theta \) when is \( V_0 \).

We impose another the continuity of the wavefunctions in the limits.

\[
\psi_1(x = 0, y) = \psi_{II}(x = 0, y)
\]

\[
\psi_{II}(x = D_1, y) = \psi_{III}(x = D_1, y)
\]

\[
\psi_{III}(x = L, y) = \psi_{IV}(x = L, y)
\]

\[
\psi_{IV}(x = L + D_2, y) = \psi_V(x = L + D_2, y)
\]

3. Results

3.1 Square barrier

\( T_{\text{exac}}(\phi) \) depends on the width of barrier \( D \), the energy \( E \), the high of potential \( V_0 \) and the angle of incidence \( \phi \). The graphic of the transmission coefficient is simetric because \( T_{\text{exac}}(\phi) = T_{\text{exac}}(-\phi) \).

\( T_{\text{exac}}(\phi) \) is the unity:
a/ for the values of $Dq_x$ satisfying $Dq_x = n\pi$

b/ for normal incidence $\phi = 0$

The transmission coefficient unity has the significance the barrier is total transparent, and this is relationated with the Klein paradox [1].

$T_{\text{aprx}}(\phi)$ depends on D, E, $V_0$ and $\phi$. The difference between $T_{\text{exac}}$ and $T_{\text{aprox}}$ is more important in the minimum of the function.

3.1 Double barrier

The function $T(\phi)$ is symmetric in $\phi$. 
When $D_1 = D_2$ we will have a symmetric system, and only the variables are $E$, $V_0$, $D$ and $L$. We will appear three zones with high transmission coefficient even there is some points which arise the unity.

![Graph 1](image1)

**Fig 5.** $T$ for $E = 80$ meV, $V_0 = 200$ meV, $D_1 = D_2 = 110$ nm, $L = 55$ nm

When $D_1 \neq D_2$ it's different the result of to place the barriers in the position first or second. The behaviour of a system with two barriers when $L = D_1$, is the same that a only barrier with width $D_1 + D_2$.

![Graph 2](image2)

**Fig 6.** $T$ for $E = 80$ meV, $V_0 = 200$ meV, $D_1 = 110$ nm, $D_2 = 220$ nm, $L = 110$ nm
Acknowledgment

This research has been supported in part by the DGICYT under project FIS2009-07880 and also by the project FS/7-2009 of the Fundación Samuel Solórzano Barruso.

4. References

Improving sample flow in planar preconcentrator

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Abstract

Preconcentrators are really important to detect gases that are dangerous at very low concentrations. We use Comsol Multiphysics to study their behaviour and improve their design. We are working with a planar device. In such a device most part of the analyte to be detected does not affect the absorbing material. We discover this problem by means of simulation and propose a solution which improves the chamber design forcing a bigger amount of the sample flow to interact with the absorbent material, thus increasing the concentration factor almost twice.

Key words: simulation, fluid flow, preconcentrator

1. Introduction

Several toxic gases such as benzene are dangerous at low concentrations. At present gas sensors are not able to detect so low concentrations. That is why the design and implementation of preconcentrators is an important task. Our aim is to design a microsystem which contains a sensor and a preconcentrator constructed in the same silicon substrate. In this way we obtain a planar device which is technologically and economically more efficient than 3D devices[1]. In such a device most part of the analyte to be detected does not affect the absorbing material. Our proposal improves the chamber design forcing a bigger amount of the sample flow to interact with the absorbent material increasing the concentration factor almost twice.
Improving sample flow in planar preconcentrator

We have simulated the chamber we are using to emulate the microsystem in order to be able to compare our results with experimental ones. It is a cylindrical 6-mm diameter 3.8-mm height chamber. It has input and output 1.27-mm diameter tubes situated at 2 mm above the base (See Fig. 1a). Preconcentrator is located at the base of the chamber (See Fig. 1b).

During the adsorption phase preconcentrator is at ambient temperature and the adsorbent is taking volatiles. During the desorption phase the preconcentrator is heated in order to desorb all the volatiles in a really short time. Adsorption and desorption processes are modelled in the preconcentrator as a simple linear function.

Fig. 1: Preconcentrator Chamber: a) Chamber morphology b) Preconcentrator location
2. Fluid flow simulation

We are coupling different models of Comsol Multiphysics in transient mode: Weakly Compressible Navier-Stokes model for fluid flow and Convection and Diffusion model for concentration. Temperature model has not been used because, at working conditions, temperature changes has no effect in flow dynamics as there are no significant density variation, neither convection effects. Thus simulation time is greatly reduced. We use the Weakly Compressible Navier-Stokes model for fluidic. We introduce laminar velocity as input and constant pressure as output boundaries constrains. With the Convection and Diffusion model we simulate the concentration variations. In the preconcentrator there is a two-way reaction which converts analyte free (Af) to analyte in the wall (AW). This is governed by the velocity of reaction.

\[
A_W \xrightarrow{k_{\text{off}}} A_f \xleftarrow{k_{\text{on}}}
\]

(1)

So, next function must be fulfilled in our preconcentrator[2-4]:

\[
\frac{\partial C_{A_W}}{\partial t} = -k_{\text{off}} \cdot C_{A_W} + k_{\text{on}} \cdot \left( C_{\text{max}} - C_{A_f} \right)_{W}
\]

(2)

In our model, we use this function in the preconcentrator boundary.

First, we simulated the flow in the conventional chamber. We realized that most part of the gas sample crosses the chamber without affecting the preconcentrator because it is at high distance above of it and passes as laminar flow (See Fig. 2). So, we proposed a new design using an “obstacle” which forces the gas sample to go down almost perpendicular to the preconcentrator surface (See Fig. 3). We constructed a “wall” and repeated the measurements in order to see the difference.
Improving sample flow in planar preconcentrator

Fig. 2: Streamline of velocity field simulation in a conventional chamber

Fig. 3: Streamline of velocity field simulation in a chamber with wall
3. Simulation results

In Fig. 4, we compare the amount of benzene adsorbed without wall and with the wall placed in the middle. In Table 1 we can see the concentration of benzene during the adsorption phase. The analyte column represents the amount of analyte going out of the chamber. ∆Analyte input-output column shows the difference between input and output analyte, with this value we extract the percentage adsorbed and the improvement factor related to this percentage. We observe that the wall enhances the retention capability in a 1.78 factor. So, using this wall, the preconcentrator system adsorbs more analyte in the same period of time.

![Fig. 4: Comparison results of input and output analyte without and with wall](image)

Table 1: Comparison of simulation results without and with wall

<table>
<thead>
<tr>
<th></th>
<th>Analyte (u.a.)</th>
<th>∆Analyte input-output (u.a.)</th>
<th>Amount of analyte adsorbed (%)</th>
<th>Retention factor improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input</td>
<td>0.1273</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Output without wall</td>
<td>0.1088</td>
<td>0.0185</td>
<td>14.53 %</td>
<td>1</td>
</tr>
<tr>
<td>Output with wall</td>
<td>0.0944</td>
<td>0.0329</td>
<td>25.84 %</td>
<td>1.78</td>
</tr>
</tbody>
</table>
Improving sample flow in planar preconcentrator

4. Experimental results

Preliminary studies were made on a 4 mm x 4 mm side porous alumina substrate with activated carbon deposited on top as a preconcentrator. However, future implementation will be made on 3 mm x 3 mm preconcentration membranes in silicon technology, already fabricated. We used gas chromatograph mass spectrometry (GCMS) to measure the desorption peak.

A flow of 150 ppb of benzene diluted in CO2 is injected during 10 minutes at ambient temperature, so the preconcentrator is adsorbing the analyte. Then, we introduce helium and heat the preconcentrator to desorb all the benzene.

Experimentally, we have obtained an improvement factor of 1.85, which fits quite well the simulation result.

5. Conclusions

By means of simulations, we detected an inefficiency which was completely unknown and proposed a solution which was substantiated by the experimental measurements.

6. Acknowledgments

This work is financially supported by the CICYT Project TEC2009-07107

7. References

COMPUTATION OF THE RESPONSE TO THE MOVING LOAD OF PERIODICALLY SUPPORTED BEAM

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Abstract

A mathematical model is presented to predict the vibration of a rail excited by a moving load. The track is modeled as an infinitely long beam supported over a finite section by discrete support. The supports represent pad/sleeper/ballast system of railway track, they are spaced regularly. The rail idealizes these periodic structures. A periodic system consists on a number of identical elements; coupled together in identical ways to form a whole system. This paper describes the computation of the wave field induced by a moving load on a periodically supported beam. The work starts by calculate the Green function of the free Euler beam without support by using the direct integration. After woods, it introduces the supports into the model established by using the superposition principle which states that the response from all sleepers points and from the external point force add up linearly to give a total response. The periodicity of supports is described by Bloch’s theorem. The model developed gives the choice of different support types: mass support, spring support, mass/spring systems…The homogeneous system thus obtained represents a linear differential equation which governs rail response. It is initially solved in the homogeneous case, it admits a no null solution if its determinant is null, this permit the establishment the dispersion equation to Bloch waves and wave bands. The Bloch waves and dispersion curves contain all the physics of the dynamic problem and the wave field induced by a dynamic load applied to the system is finally obtained by decomposition into Bloch waves, similarly to the usual decomposition into dynamic modes on a finite structure. The method is applied to obtain the field induced by a load moving at constant velocity on a thin beam supported by periodic elastic supports.

Key words: Bloch wave, Euler beam, Green function, Computation, Moving load
1. **Introduction**

Vibration of infinite periodic structures has been studied extensively in the past 30 years with the focus mainly on free vibration propagation and forced vibration induced by stationary harmonic loads [1]. A mathematical model is presented by Heckl [2] to predict the vibration of a rail excited by a rolling wheel. The track is modeled as an infinitely long beam supported over a finite section by discrete support systems for non-moving load. Vibration of an infinite periodic beam subject to a moving harmonic load has been investigated by Belotserkovskiy [3]. In this study, the author considered a single segment only by using boundary conditions derived according to the Euler beam theory. The rail is modeled as an Euler beam with flexible supports in the work of Nordborg [4]. The supports of the beam represent pad/sleeper/ballast system of the railway track; they are spaced regularly. The exact solution, in the frequency domain, of the linear differential equation is presented.

The method used to obtain the response to dynamic load include the computation of transfer matrices ([5][6][7][8], the use of Bloch waves [9] [10] and finite element solutions[11][12]. For a Timoshenko beam, Heckl ([13]) produced the dispersion curves and showed that different modes appear, related to the coupling between different degrees of freedom of the beam (flexion, torsion, shear...). The response of a Timoshenko beam to a static (non-moving) dynamic load was produced by Hamet [14].

The aim of the paper is to produce the response of a periodically supported thin beam submitted to a moving load, by using the Bloch transform (Allaire [15], Sanchez [16]). Parts of the solution are similar to the one used by (Langley [8]) for 2D structures or Hamet [14] for a Timoshenko beam submitted to a dynamic (non-moving) load.

2. **Green function for Euler beam**

Let us consider a thin beam with an inertia section moment $I$ which is subjected to a moving vertical moving load $F(x,t)$. The vertical beam displacement is the solution of the dynamic beam equation (eq. 1). Euler model is considered:

$$EI\frac{\partial^4 u(x,t)}{\partial x^4} + m\frac{\partial^2 u(x,t)}{\partial t^2} = F(x,t)$$

(1)

Where $m$ is the mass of the beam by unit of length and $E$ the Young’s modulus.
If the harmonic concentrated load is applied at the point \( x_0 \), in the Fourier space, the movement equation becomes:

\[
\mathcal{U} \frac{d^2 \mathcal{U}(x, \omega)}{dx^2} - m \omega^2 \mathcal{U}(x, \omega) - \mathcal{U}(x - x_0) = 0
\]  

(2)

Where \( \mathcal{U} \) is the Fourier transform of \( U \).

The Green function associated to this equation is the response to an unit load applied at the point \( x_0 \). It is the solution of the equation:

\[
\frac{d^2 G(x, x_0)}{dx^2} - k_2^2 G(x, x_0) = \delta(x - x_0)
\]

(3)

With:

\[
k_2 = \sqrt{\frac{m \omega^2}{EI}}
\]

(4)

The Green function \( G(x, x_0) \) can be now determined by direct integration; it is thus the solution of the equation (3) and represents the vertical vibration at the point \( x_0 \), of the beam rail subjected to an harmonic force.

- In any point \( x \neq x_0 \) (in any point other than the excitation point) the system is free and :

\[
\frac{d^2 G(x, x_0)}{dx^2} - k_2^2 G(x, x_0) = 0 \quad x \neq x_0
\]

(5)

At the point \( x = x_0 \), the discontinuity is assumed by the third derivative of \( G(x, x_0) \). The function and its two first derived are continuous at \( x = x_0 \). The integration of the equation (2) on both sides of \( x_0 \) and if we take into account the continuity of the function \( G(x, x_0) \) at \( x_0 \), we obtain :

\[
\frac{d^3 G(x, x_0)}{dx^3} \bigg|_{x_0} = \frac{1}{EI}
\]

(6)

- At \( x = \frac{L}{2} \) the function is limited: \( |G(x, x_0)| < \infty \)
The Green function is then expressed by a combination of elementary solutions of the equation (3). Taking into account the condition at infinity, it can be written:

\[
G(x, x_0) = a_1 e^{\kappa_2 (x-x_0)} + a_2 e^{\kappa_3 (x-x_0)} \quad x < x_0
\]  

\[
G(x, x_0) = b_1 e^{-\kappa_2 (x-x_0)} + b_2 e^{i\kappa_3 (x-x_0)} \quad x > x_0
\]  

The coefficients \(a_1, a_2, b_1, b_2\) are evaluated from the Green function and its first derived must satisfy:

\[
G(x, x_0) \mid_{x_0}^{x_0+} = 0 \quad \frac{d}{dx} G(x, x_0) \mid_{x_0}^{x_0+} = 0 \quad \frac{d^2}{dx^2} G(x, x_0) \mid_{x_0}^{x_0+} = 0
\]

The solution of this problem is exposed by Heckl (Maria A. Heckl, 2001) in the more general case of the Timoshenko beam. The result in this case of the Euler beam is a Green function.

\[
G(x, x_0) = \frac{1}{4\pi R_2} \left[ e^{i\theta} e^{\kappa_2 |x-x_0|} - e^{-\kappa_2 |x-x_0|} \right]
\]  

3. The free motion of the periodically supported beam: Bloch waves

We consider a beam periodically supported with \(N\) supports placed between \(x = 0\) and \(x = L\). The period is given by the regular spacing \(l\). The rigidity of the \(N\) discrete elastic support, corresponding to the deformation of the system (elastic support, mass support...), is \(Z_n\), the force transmitted by the discrete support is:

\[
F_n = -Z_n U(n, l)
\]  

It is considered that all the discrete supports are characterized by the same rigidity \(Z_n = Z\). The global response of the structure can be described by applying the superposition principle, which consists of the linear summation of all the answers due to the various supports. Then, the displacement with the position \(x\) is given by:

\[
\eta(x) = \sum_{n=-\infty}^{+\infty} G(x, x_n) F_n
\]
Where \( G(x_m, x_{m'}) \) is given by the equation (10) for the Euler beam.

The relation (9) is thus valid for any point \( x_m \).

\[
\eta(x_m) + \sum_{m=0}^{\infty} Z \eta(x_m') G(x_m, x_{m'}) = 0
\]

(13)

The application of the Floquet theorem gives the relation between two adjacent supports:

\[
\eta(x_{m+1}) = \eta(x_m) e^{-\gamma}\n\]

(14)

With:

\[
\gamma = \alpha + \mathbf{i} \kappa
\]

(15)

\( \gamma \) is the Bloch constant propagation. It is generally complex. \( \alpha \) is the wave attenuation and \( \kappa \) is the Bloch wave number.

By substituting the expression of the Green function given by the equation (9) in the equation (12) and by multiplying this equation by \( e^{-\gamma m} \), changing the index of summation \( m \rightarrow n \) by \( n \) gives the following equation which defines the relation between \( \gamma \) and the displacement \( \eta_0 \):

\[
\eta_0 + Z \eta_0 \sum_{m=0}^{\infty} \left[ \frac{1}{4EIk_0^2} \left( e^{(2\kappa_0m+i\gamma)m} - e^{-i\gamma m} \right) e^{i\gamma m} \right] = 0
\]

In the following, only the waves not attenuated will be considered, which means that the sum can be evaluated by usual formulas of the geometrical series.

For the Euler model, we can have:

\[
1 + \frac{Z}{4EIk_0^2} \left[ \frac{\sinh(k_0l)}{\cos(k_0l) - \cos(\kappa l)} - \frac{\sinh(k_0l)}{\cosh(k_0l) - \cos(\kappa l)} \right] = 0
\]

(16)

\[
\cos^2(\kappa l) + \cos(\kappa l) \left[ -\cosh(k_0l) + \cosh(k_0l) + \frac{Z}{4EIk_0^2} \left( -\sinh(k_0l) + \sinh(k_0l) \right) \right] + \frac{Z}{4EIk_0^2} \left[ \sinh(k_0l) \cosh(k_0l) - \sinh(k_0l) \cosh(k_0l) \right] + \cos(k_0l) \cosh(k_0l) = 0
\]

This is a second degree polynomial for \( \cos(\kappa l) \). The solution produces the values of the wave number \( k \) which is between 0 and. It is a function of \( k_0^2 \) which depends on the radial frequency (eq.4). It leads therefore to the dispersion equation.
Similar relations were obtained previously by other authors (for example Heckl for a Timoshenko beam).

The shape of the Bloch wave can be obtained by using a similar process. Let us consider the free motion related to a couple $k_1, k_2$ complying to equation (16).

The displacement at position $x$ between two supports is related to the displacements of all supports by using the Green’s function $G$, leading to:

$$\eta(x) = -Z\eta_0 \left[ \sum_{m=-\infty}^{+\infty} G(x, x_m) \eta(x_m) \right]$$

(17)

Introducing the Green’s function and the propagating constant $\gamma$ leads to:

$$\eta(x) = -Z\eta_0 \frac{1}{4k_0^2EI} \left[ \sum_{m=-\infty}^{+\infty} \left( e^{i\gamma R_2|x-x_m|} - e^{-i\gamma R_2|x-x_m|} \right) e^{-\gamma x_m} \right]$$

(18)

Computing the sum of the series leads to:

$$\eta(x) = C \left[ \frac{N_1}{D_1} + \frac{N_2}{D_2} \right]$$

(19)

Where: $C = Z\eta_0 \frac{1}{4k_0^2EI}$ and where the following notations are introduced:

$$N_1(x, k) = e^{ikx} \sinh(k_2 x) - \sinh(k_2 (x - l))$$

(20)

$$N_2(x, k) = -\left( e^{ikx} \sinh(k_2 x) \right) - \sinh(k_2 (x - l))$$

(21)

$$D_1(k) = \cos(k_2 l) - \cos(kl)$$

(22)

$$D_2(k) = \cosh(k_2 l) - \cos(kl)$$

(23)

Due to the Floquet’s theorem, the Bloch wave may be written:

$$\eta(x) = \eta_{1}(x) e^{i\xi}$$

(24)

Where $\eta_{1}$ is a periodic function of $x$.

The value of $\eta_0$ and therefore the value of $C$ must be chosen to build from the Bloch waves an orthonormal basis of $\mathbb{L}^2(Y)$ where $Y$ is the periodic cell obtained after transforming the space variable $x$ into the non dimensional variable $X = \frac{x}{2\pi}$. Through this process, the period $[0, l]$ is transformed into $[0, 2\pi]$.
The constant C is chosen to insure that the $L^2$ norm of $\eta(x^*) \left( \partial_x \eta_k(x^*) \right)$ on $[0,2\pi]$ is equal to 1, leading to:

$$C^{-1} = \left[ \frac{2\pi}{l} \int_0^l \left( \frac{N_2}{\bar{D}_1} + \frac{N_4}{\bar{D}_2} \right) dx \right]^{1/2}$$  

(25)

4. The response of the structure to moving load

As for the space coordinate, it is convenient, to define the Bloch transform, to use a no-dimensional wave-number $K^*$ define by:

$$K^* = \frac{kl}{2\pi}$$  

(26)

The Bloch transform of a function $F(x)$ is then defined by:

$$\hat{F}_n(K^*) = \int_0^{2\pi} F(x^*) \eta_n(x^*,K^*) dx^*$$  

(27)

Where $\eta_n(x^*,K^*)$ is the complex conjugate of the Bloch wave contained in the $r_n^{th}$ band obtained by equation (12).

The Bloch decomposition theorem whose proof and conditions of validity can be found in (Sanchez, Allaire) states that.

$$F(x^*) = \sum_{n=1}^{2\pi} \int_0^1 \hat{F}_n(K^*) \eta_n(x^*,K^*) dK^*$$  

(28)

The Bloch transform of equation (1), considering that the Bloch wave $\eta_n(x,k)$ is the solution of the homogeneous equation for an harmonic equation at radial frequency $\omega_n(k)$, lead to:

$$m \omega_n^2 u_n(K^*,\xi) + m \frac{\partial^2}{\partial \xi^2} u_n(K^*,\xi) = \hat{F}_n(K^*,\xi)$$  

(29)

This equation shows that each Bloch component is solution of the dynamic equation for a ‘1 DOF’ system.

Let us use this result to obtain the response of the beam to a load having a constant intensity $F_0$ which is moving at the velocity $V$. It means that $F$ is given by:

$$F(x,\xi) = \delta(x - V\xi) F_0$$  

(30)

Where $\delta$ is the Dirac distribution.

The Bloch transform of $F(\xi)$ is:
COMPUTATIONAL OF THE RESPONSE TO THE MOVING LOAD

\[ P_n(K^n, t) = \eta_n \left( X^n = Vt \frac{2\pi}{l}, K^n \right) P_0 \frac{2\pi}{l} \]  

(31)

The Bloch components of the displacement induced by the moving load are therefore solution of:

\[ m\omega_n^2 U_n(K^n, t) + m \frac{\partial^2}{\partial t^2} U_n(K^n, t) = \eta_n \left( X^n = Vt \frac{2\pi}{l}, K^n \right) P_0 \frac{2\pi}{l} \]  

(32)

Its solution is given by:

\[ U_n(K^n, t) = \frac{2\pi F_0 C^2}{l} \left[ \frac{e^{-2\pi K^n t} \sin(k_n Vt) - \sin(k_n (Vt - i))}{Y_2 \cosh(2\pi k_n) - \cos(2\pi k_n)t - i} \right] \]  

(33)

Where \( \gamma_1 \) and \( \gamma_2 \) are given by:

\[ \gamma_1 = m(\omega_n^2 - k_n^2 V^2) \]  

(34)

\[ \gamma_2 = m(\omega_n^2 + k_n^2 V^2) \]  

(35)

The displacement induced by the moving force is finally obtained by composition of all the Bloch components, leading to:

\[ U(X^n, t) = \sum_{n=1}^{N} \int_{K^n=0}^{2\pi} U_n(K^n, t) \eta_n(X^n, K^n) dK^n \]  

(36)

Coming back to \( x \), \( k \) and taking into account that \( k \) is involved in \( \eta \) only by \( \cos(kl) \), lead to:

\[ U(x, t) = \sum_{n=1}^{N} \int_{k=0}^{\pi/l} V_n(k, x, t) dk \]  

(37)

The function \( V_n(k, x, t) = \frac{1}{\pi} U_n(k, t) \eta_n(x, k) \) is given by:

\[ V_n(k, x, t) = 2F_0 C^2 \left[ \frac{N_1(Vt, k)}{\gamma_2 D_2} + \frac{N_2(Vt, k)}{\gamma_1 D_1} \right] \left[ \frac{N_1(x, k)}{D_1} + \frac{N_2(x, k)}{D_2} \right] \]  

(38)

This solution can be transformed by using new dimensionless variables \( T, X, B, K \) defined by \( x = XL \), \( t = TL/V \), \( k = K/l \), \( k_b = B/l \).
Computational of the Response to the Moving Load

Using these variables $U$ is given by:

$$U(X,T) = \frac{F_0}{\pi B i} \sum_{n=0}^{N} \int_{N_0}^{N} \frac{P}{\alpha_1 \alpha_2 Q} dK$$

(39)

Where:

$$\alpha_1 = B^4 - B^2 \phi$$

(40)

$$\alpha_2 = B^4 + B^2 \phi$$

(41)

$$\phi = \frac{m v^2 l^2}{EI}$$

(42)

$$\beta = \frac{E I}{h^4}$$

(43)

$$P = \alpha_2 D^2 P_{11} + \alpha_1 D^2 P_{12} + D_1 D_2 (\alpha_1 P_{21} + \alpha_2 P_{22})$$

(44)

$$Q = \int_0^1 \left( D_2^2 [N_2]^2 + D_1^2 [N_1]^2 + D_1 D_2 (N_1 N_2 + N_2 N_1) \right) dZ$$

(45)

All integrals in $Q$ are obtained explicitly:

$$\int_0^1 |N_1|^2 dZ = \frac{1}{B} \left[ \cos(K) \left( \sin(B) - B \cos(B) + B - \sin(B) \cos(B) \right) \right]$$

(46)

$$\int_0^1 |N_2|^2 dZ = \frac{1}{B} \left[ \cos(K) \left( B \cosh(B) - \sinh(B) \right) + \sinh(B) \cosh(B) - B \right]$$

(47)

$$\int_0^1 (N_1 N_2 + N_2 N_1) dZ = \frac{2}{B} \left[ \cos(K) \left( \sin(B) - \sinh(B) \right) + \cos(B) \sinh(B) - \sinh(B) \cosh(B) \right]$$

(48)

The terms appearing in $P$ are given by:

$$P_{11} = -\cos(K) \left[ \sin(BZ) \sin(BZ - 1) \right] + \sinh(BZ) \sinh(B(T - 1))$$

$$+ \sin(B(T - 1)) \sin(BZ - 1) + \sin(BZ) \sin(B(T - 1))$$

(49)

$$P_{22} = -\cos(K) \left[ \sinh(BZ) \sinh(BZ - 1) \right] + \sinh(BZ) \sinh(B(T - 1))$$

$$+ \sinh(B(T - 1)) \sinh(BZ - 1) + \sinh(BZ) \sinh(B(T - 1))$$

(50)

$$P_{21} = \cos(K) \left[ \sinh(BZ) \sinh(BZ - 1) \right] + \sinh(BZ) \sinh(B(T - 1))$$

$$- \sinh(B(T - 1)) \sinh(BZ - 1) - \sinh(BZ) \sinh(B(T - 1))$$

(51)

$$P_{12} = \cos(K) \left[ \sinh(BT) \sinh(BZ - 1) \right] + \sinh(BZ) \sinh(B(T - 1))$$

$$- \sinh(B(T - 1)) \sinh(BZ - 1) - \sinh(BT) \sinh(BZ)$$

(52)
COMPUTATIONAL OF THE RESPONSE TO THE MOVING LOAD

It is convenient to use the dispersion equation with non-dimensional variables

\[ 1 + \frac{\beta}{\beta_0} \left[ \frac{\sinh(\beta)}{\cosh(\beta) - \cos(\beta)} - \frac{\sinh(\beta)}{\cosh(\beta) - \cos(\beta)} \right] = 0 \]  
(53)

Where the non dimensional parameter \( \beta \) is given by:

\[ \beta = \frac{l^2 Z}{4EI} \]  
(54)

From the previous results, it can be seen that the displacement depends of the non dimensional position and time and also of the three following parameters:

The parameter \( \beta_0 \) which is the ratio between the stiffness of the beam and the stiffness of the support and which is involved in the dispersion curve.

The parameter \( \beta_1 \) which is the ratio between the elastic energy and a kinetic energy computed from the moving load velocity.

The parameter \( \beta_2 \) related to the flexure stiffness of the beam.

5. Example of application

Let us consider a rail whose properties are given in table 1.

<table>
<thead>
<tr>
<th>Young's modulus</th>
<th>Section's inertia</th>
<th>Mass per un. length</th>
<th>Support stiffness</th>
<th>Spacing</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 GPa</td>
<td>8.10-5 m^4</td>
<td>158 kg/m</td>
<td>30 and 0.02 GN/m</td>
<td>0.6 m</td>
</tr>
</tbody>
</table>

Table 1. Physical properties of the beam and support

The dispersion curves are show on figure 1 for the first three passing bands for the stiffer support \((Z=30 \text{ GN/m})\). Similar results are obtained for the softer support at lower frequencies.
Computational of the response to the moving load

Figure 1 Dispersion curve for the first band tree bands: case for stiffer support

Figure 2 Displacement vs non-dimensional time for the stiffer case (high speed and low speed)

The displacement induced by a unit moving load at the center of a given period is next computed when the load is moving over that period with two speeds: a low speed 10 m/s and a high speed 140 m/s. Results are given in the case of stiff support in figure 2 and in the case of soft support in figure 3. It appears that the displacement is the same for low speed and high speed, in the case of the stiffer support, while the displacement depends significantly of the speed for the softer support.
This result is due to the fact that the passing bands are at higher frequencies for the stiffer supports. The velocity-dependent term $\varphi$ in (35) is negligible when compared to $B^2$ for any velocity.

![Figure 3. Displacement vs non-dimensional time for the softer case](image)

### 5. Conclusion

The method of Bloch transform was used to study the dynamics of a beam resting on a periodic support. It allows to compute the response of the beam to any dynamic loading by computing the Bloch transform of the displacement induced by the loading. It involves only to solve a (continuous) set of decoupled "1 DOF" dynamic equations. The method is applied to the dynamic response of a thin beam. The authors intend to extend the method to the dynamics of a Timoshenko beam for any loading, implying the coupling between different components of the motion of the beam (torsion, flexion,...).


Electromagnetic Wave Effect On Semiconductor Device :
FDTD Method

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Abstract

The electromagnetic wave effects on the behavior of semiconductor devices are investigated by coupling a TM wave (transverse magnetic wave), solution of Maxwell’s equations to an active device model. In this paper, 2D (Two-dimensional) simulations verify the expect device-wave interaction. The active semiconductor model is based on the drift–diffusion equations. The coupling between the two models is established by using fields obtained from the solution of Maxwell’s equations in a semiconductor device model. Its permit to calculate the current densities witch used to update both the electric and magnetic fields.

The study of an electromagnetic field influence on a semiconductor structure is carried out by MATLAB software. We have developed an efficient and accurate tool to solve the Maxwell’s equations by using FDTD method, and finite differences and Euler’s method to solve the drift-diffusion equations.

Numerical results relative to the study of two-dimensional device are included to valid the effectiveness of the method. We observe that the semiconductor device significantly attenuate the input wave as it propagates along the structure. This is, essentially due to the electromagnetic energy loss by the conducting electrons.
1. Introduction

The evolution of electronic market fosters a continuous quest for small-size and low-cost systems. Propagation and radiative effects become more and more important, most notably, signal reflections due to interconnecting line discontinuities, dispersion, and crosstalk phenomena [1]. So the assessment of potential hazards caused by electromagnetic influence to electronic systems as well as transmission is an essential engineering task. This is essentially due to nearby transmitters and electrically active device.

At high frequencies and reduced circuit sizes, however, such an approach can hardly be pursued, due to the difficulty of properly characterizing (both qualitatively and quantitatively) the coupling phenomena typical of a densely packed circuit.

In these cases, the full-wave solution of Maxwell's equations may provide a more comprehensive investigation tool. To this purpose, different solution techniques can be followed.

In this work, we describe the modeling and the simulation of semiconductor devices were previously achieved by solving various combinations of Poisson and continuity equations conventionally.

The Gummel's method is most commonly used to solve the nonlinear steady-state problem arising from the semiconductor device equations [2], which can be written as sparse nonlinear system of equations. In this approach, the two unknown variables in drift-diffusion model are coupled together through the whole process of computation [3], each equation is solved using Newton’s method. It's more robust, and converges in relatively little iteration.

However, interesting physical phenomena arise from the manner in which charge fluctuations and current responses are coupled to the electromagnetic field, a 2D FDTD model has been developed in order to solve the coupled Maxwell’s and drift-diffusion equations. This model permits to establish a rigorous simulation of the active device.

2. Semiconductor model

The semiconductor model consists of the Poisson equation and continuity one. These equations represent a coupled nonlinear system of partial differential-integral equations (PDE equations).

In our case, we treat the steady-state condition and further neglect the contribution from holes because the we have an N type substrate where the electrons are predominant versus holes[4].

Then the basic equations become the following

\[ \frac{\partial n}{\partial t} \]
1) Poisson’s equation
\[ \nabla^2 V = \frac{q}{\varepsilon_s} (n - N_p) \]  
(1)

2) Continuity equation of electron current:
Current equations for electrons and holes must be solved simultaneously.
In the present case, however, a simplified approach is adopted because the type of the substrate is N (n>>p), so we consider only the electrons equation continuity.
\[ \frac{\partial n}{\partial t} - \frac{1}{q} \text{Div}(j_n) = 0 \]  
(2)

3) Electron current equation
\[ j_n = -q\mu_n \vec{V} + qD_n \vec{n} \]  
(3)

The drift-diffusion approach is known to possibly lack of accuracy if large field changes, either in time and space are encountered.

3. Electromagnetic model
The electromagnetic wave propagation can be completely characterized by solving Maxwell’s equations are first-order linear coupled differential equations. These equations coupled differential equations relating the field vectors and current densities at any point in our structure at any time [5].
Maxwell’s equations are given by:
\[ \vec{\nabla} \times \vec{H} = \vec{j} + \varepsilon_{si} \frac{\partial \vec{E}}{\partial t} \]  
(4)
\[ \vec{\nabla} \times \vec{E} = -\mu_{si} \frac{\partial \vec{H}}{\partial t} \]  
(5)

4. Electromagnetic wave propagation
The excitation is applied as a TM mode (Transverse Magnetic mode). For the electromagnetic-wave analysis, a sinusoidal excitation is applied in the electrode A of the silicon structure. The electric wave excitation becomes:
\[ E = E_0 \sin(\omega t) \]

\[ E_0 \] represent the maximum amplitude and \( \omega = 2\pi f \) the wave pulsation, where 
\[ f = 1000 \text{GHz} \]
The length wave corresponding is \( \lambda = 75 \mu m \)
5. Simulated Structure

The TM wave model is then solved for a few picoseconds, to avoid the effects of the electromagnetic wave interference. The 2D structure used in the simulation is shown in Fig.1. It’s constituted by a silicon semiconductor doped $N_D = 10^{18}$ At/cm$^3$. The distance between the two electrodes A and B is 50 µm. The width of the plate is 40 µm. A constant space step of discretization $\Delta x = \Delta y = h = 1$ µm is considered.

![Fig. 1. A view of the simulated device](image)

6. Simulation technique

1) Drift Diffusion model

The discretization uses a first and second order of equation (1) in 2D-finite difference mesh, and the discretization of equation (2) uses Euler’s implicit method leads to have equations:

$$
H.V'(i, j+1) + B.V'(i, j-1) + G.V'(i-1, j) + D.V'(i+1, j) - (H + B + G + D).V'(i, j) = \frac{q}{\varepsilon_{si}} \left( n'(i, j) - N_D \right)
$$

(6)

$$
a.n^{n+1}(i, j+1) + b.n^{n+1}(i, j-1) + c.n^{n+1}(i-1, j) + d.n^{n+1}(i+1, j) - e.n^{n+1}(i, j)
$$

$$
= \frac{h^2}{\mu_n \Delta t} \left( n^{n+1}(i, j) - n'(i, j) \right)
$$

(7)

Where $H = B = D = G = \frac{1}{h^2}$

$a, b, c, d$ and $e$ are coefficients depending on the electrostatic potential:

$$
a = U_r - \frac{1}{4} \left( V(i+1, j) - V(i-1, j) \right)
$$
In the case of Ohmic contacts, the electron and hole densities are determined by assuming charge neutrality and thermal equilibrium.

At free surfaces, the normal derivatives of current density and electrostatic potential are set to zero.

\[ V = V_{\text{Contact}} + U_T \ln \left( \frac{n}{n_i} \right), \text{where } n_i \text{ is an intrinsic concentration.} \]

Solution of equations (6) and (7) provide the space and time distribution of the unknown functions \( n \) and \( V \) at each point and each time step in the considered structure which leads to have a two matrix systems which depend in time.

\[ A \cdot V_n^{i+1} = V_n^i \] (8)
\[ B \cdot V_n^{i+1} = V_n^i + 1 \] (9)

A and B represent respectively the corresponding matrix coefficient of equations (6) and (7).

\( V_n \) and \( V_n^i \) are respectively the electrostatic potential and electron density vectors.

At each time step Gummel’s method is most commonly used to solve the coupled system arising from equations (8) and (9). Where these equations can be solved in a decoupled manner using Newton’s method [6].

The whole numerical procedure to solve the two system equations can be summarized as:

1. For \( t \) from 0 to final time
2. Select time-step which ensures stability convergence.
3. Solve (8) and (9) using Gummel’s iterations
4. Set \( n' \leftarrow n^{i+1} \)
5. End time iterations

1) Electromagnetic model

The electromagnetic model simulates the evolution of both electric and magnetic fields due to moving free charges [7]

\[ \frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon_{SI}} \left( \nabla \wedge \vec{H}^{ac} + \vec{J}^{dc} - \vec{J}^{tot} \right) \] (10)
\[ \frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu_{si}} \nabla \times \vec{E} \]  

(11)

Where \( \vec{j}^{dc} \) is obtained by solving the drift-diffusion model in conjunction with Poisson’s equation [8].

Equations (10) and (11) can be replaced with an explicit finite difference approximation in its known values at the previous nth time step. Using the first-order upwind scheme for time and spatial derivatives yields the following equations:

\[ E_{ix}^{n+1}(i, j) = E_{ix}^n(i, j) + \frac{\Delta t}{\varepsilon_{si}} \left( \frac{1}{\Delta y} \left( H_{iy}^n(i, j) - H_{iy}^n(i, j - 1) \right) - \frac{1}{\Delta x} \left( H_{ix}^n(i, j) - H_{ix}^n(i, j - 1) \right) \right) \]  

(12)

\[ H_{ix}^{n+1}(i, j) = H_{ix}^n(i, j) - \frac{\Delta t}{\mu_{si}} \frac{1}{\Delta y} \left( E_{iy}^n(i, j) - E_{iy}^n(i, j - 1) \right) \]  

(13)

\[ H_{iy}^{n+1}(i, j) = H_{iy}^n(i, j) + \frac{\Delta t}{\mu_{si}} \frac{1}{\Delta y} \left( E_{ix}^n(i, j) - E_{ix}^n(i, j - 1) \right) \]  

(14)

Notice from equations (10), (11) and figure (2) that the components \( E \) and \( H \) are interlaced within the unit cell and evaluated at alternate half-time steps. Electric and magnetic field components are extracted from two separate sets of equations [9]. At each time step, electromagnetic model and semiconductor equations should be solved sequentially [10], where the equations (12), (13) and (14) gives the electric and magnetic field distributions at each time step, these
latter are used by semiconductor model to update the current density at the same time step, which fed back to electromagnetic model again for the following time step [11]. Figure 3 shows flowchart of the sequence FDTD scheme

![Flowchart](image)

Fig. 3. Flowchart describing the calculate of the total current as a function of electromagnetic wave

In practice, at each time step the iterative process is stopped at the minimum value of iterations such that \( \max \left( \frac{\delta n}{n} \right) \leq \varepsilon \), where \( \varepsilon \) is a fixed tolerance, in our case, we have fixed \( \varepsilon \) at \( 10^{-5} \). However, since the exact solution is obviously not available, it is necessary to introduce suitable stopping criteria to monitor the convergence of the iteration [12].

7. **Results and discussions**

For a polarization \( V_D = 1V \) the results given by the drift-diffusion model using a finite differences method are in agreement with theoretical concepts.
Figure (4) represent the equipotential lines in steps 0.5. The electrons density is almost constant along the semiconductor. Its value takes approximately the doping value.

Fig. 4. Contour plot for the equipotential lines

Fig. 5. Time variation of the electric field at several points in the x-direction

Fig. 6. Time variation of the magnetic field at several points in the x-direction
Figures (5) and (6) depicts the impute wave evolution at different points along the x-direction. The input wave decreases in magnitude as it propagates along the x-direction (along the device). This is mainly due to the electromagnetic energy loss to the conducting electrons. The active device role in attenuating the input wave can be confirmed by the comparison of two waves, one of them propagates on the active device and the other in a semi-insulating one.

8. Conclusion
The effect of electromagnetic wave on electrical characteristics in semiconductor devices is studied, for that we have combined the electromagnetic model with drift-diffusion equations. To this purpose, a FDTD method has been used. An explicit scheme assumption is formulated, which allows for the fully decoupled of the two models, electromagnetic equations and drift-diffusion ones. A “leapfrog” scheme is adopted for the FDTD solution of the Maxwell’s equations and “Gummel” scheme for the finite difference solution of the semiconductor equations [8]. It has been shown that a model consisting of a TM wave time domain solution of Maxwell’s equations coupled to the semiconductor model capable of evaluating the effect of the propagating wave on semiconductor behaviour. The Gummel iterative process is stopped at the exact solution for each time step, where the convergence criterion is fixed for the minimum of \( \frac{\delta n_i}{n_i} \).

We also concluded that the numerical method used help us to explain some physical phenomena like:
- The increasing in the number of electrons in semiconductor cause the increasing of the conductivity, which leads to an attenuation of the electromagnetic wave in the space.
- The electromagnetic wave leads to the change of the electrons velocity in the space, which cause a discontinuity in the current density.
9. Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>QUANTITY</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>Electrostatic potential</td>
<td>v</td>
</tr>
<tr>
<td>n</td>
<td>Electron density</td>
<td>At/Cm$^{-3}$</td>
</tr>
<tr>
<td>$N_D$</td>
<td>Donor doping density</td>
<td>At.Cm$^{-3}$</td>
</tr>
<tr>
<td>q</td>
<td>Electron charge</td>
<td>C</td>
</tr>
<tr>
<td>$U_T$</td>
<td>Thermal voltage</td>
<td>26 mv</td>
</tr>
<tr>
<td>$\mu_n$</td>
<td>Electron mobility</td>
<td>m$^2$/v.s</td>
</tr>
<tr>
<td>$D_n$</td>
<td>Electron diffusion coefficient</td>
<td>m$^2$/s</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
<td>s</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time increment</td>
<td>s</td>
</tr>
<tr>
<td>$\Delta h$</td>
<td>Space increment</td>
<td>m</td>
</tr>
<tr>
<td>$J_n$</td>
<td>Electrons current density</td>
<td>A/m$^2$</td>
</tr>
<tr>
<td>$j_{dc}$</td>
<td>Direct current density</td>
<td>A/m$^2$</td>
</tr>
<tr>
<td>$j_{tot}$</td>
<td>total current density</td>
<td>A/m$^2$</td>
</tr>
<tr>
<td>E</td>
<td>Electric field</td>
<td>V/m</td>
</tr>
<tr>
<td>H</td>
<td>Magnetic field</td>
<td>A/m</td>
</tr>
<tr>
<td>$\varepsilon_Si$</td>
<td>Silicon permittivity</td>
<td>F/m</td>
</tr>
<tr>
<td>$\mu_Si$</td>
<td>Silicon permeability</td>
<td>H/m</td>
</tr>
<tr>
<td>$H_{dc}$</td>
<td>Direct component of magnetic field</td>
<td>A/m</td>
</tr>
<tr>
<td>$H^{ac}$</td>
<td>Alternative component of magnetic field</td>
<td>A/m</td>
</tr>
<tr>
<td>$\omega$</td>
<td>frequency</td>
<td>Rd.s$^{-1}$</td>
</tr>
</tbody>
</table>

TABLE 1: UNITS FOR DIFFERENT PARAMETERS

10. References

FDTD METHOD IN SEMICONDUCTOR DEVICE


Complexes of Free Helical Gold Nanoclusters and Carbon Monoxide: A Density Functional Study

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Abstract

Gold nanoclusters have attracted a surge of interest over the past decade due to their potentially significant applications in heterogeneous catalysis. In particular, when supported on an oxide surface, it has been shown that gold nanoclusters can catalyze the oxidation of carbon monoxide. Free gold nanoclusters often exhibit a variety of stable structural isomers ranging from compact to hollow to helical. The surface gold atoms of these structural isomers have very distinct electronic properties which could result in very different catalytic properties. In this presentation we examine complexes of free helical gold nanoclusters and carbon monoxide.

Key words: Gold nanoclusters, carbon monoxide

1. Introduction

Metal nanoclusters represent a novel organization of matter which is yet to be fully understood. In particular, gold nanoclusters have been shown to exhibit size-related properties that differ significantly from those observed for small clusters or the bulk material [1,2]. It has been established that there exists a close relationship between the properties of nanoclusters and their geometries but it is difficult to elucidate this connection by experimental techniques alone and, in this regard, quantum calculations can be very helpful. Density functional theory (DFT) has become an increasingly important tool in quantum calculations since the effects of electron correlation, which are large for metal nanoclusters, can be included at a moderate computational cost [3]. Relativistic effects, which are
large for gold nanoclusters, can be efficiently included via an effective core (or pseudo) potential [4].

Gold nanoclusters have potentially significant applications in heterogeneous catalysis. This area was initiated by Haruta in 1997 when he showed that gold nanoclusters (when supported on an oxide surface) could catalyze the oxidation of carbon monoxide (CO) [5]. The oxide surface was employed to prevent coalescence of the gold nanoclusters and it was initially believed to be inert. However, it subsequently became clear that the oxide surface plays an important role in the catalysis process. Nonetheless, it is of considerable interest to study the complex of a free gold nanocluster and CO and, in particular, to examine the effect of the free gold nanocluster on CO. In this presentation, we focus on helical gold nanoclusters since the surface gold atoms of these structural isomers exhibit very different electronic properties depending on their location. We have shown that Au_{24}, Au_{32} and Au_{40} all have structural isomers which are helical [6]. Although the lowest energy structural isomer is the compact structure, the helical structure is both stable and robust. In this presentation we focus on Au_{40} and examine the strength of the bonding between the surface gold atom and CO, charge transfer to CO, and changes to the CO bond distance and frequency as a result of complex formation.

2. Method
In our DFT calculations, four generalized gradient approximation (GGA) exchange-correlation functionals are employed: the Becke exchange functional with the Perdew correlation functional (BP86), the Becke hybrid three-parameter exchange functional with the Perdew correlation functional (B3P86), the Becke exchange functional with the Perdew-Wang correlation functional (BPW91), and the Becke hybrid three parameter exchange functional with the Perdew-Wang correlation functional (B3PW91). We used the LANL2DZ effective core potential, although other effective core potentials have been successfully used for gold nanoclusters. We believe that these functionals, and BP86 in particular, are appropriately accurate for the neutral gold nanoclusters considered in this presentation. The harmonic-frequency calculations were performed based on the optimized geometries of the nanoclusters. For simplicity, we employ the commonly used Mulliken charge analysis to examine the electronic properties of the nanoclusters. All calculations were performed with the Gaussian 09 program package [7] and, unless otherwise noted, all results are for the BP86 functional.

3. Results
For helical Au_{40} there are 5 gold core atoms, each of which is surrounded by 7 gold surface atoms which spiral in a helical fashion (see Fig. 1, top row). The
diameter is 0.553 nm and the length is 1.138 nm. The average Au-Au distance in each surface atom row is 2.84 Å. For bare CO, the C-O bond distance is 1.139 Å while the C-O vibrational frequency is 2120 cm$^{-1}$. These results compare favorably with the experimental values of 1.128 Å and 2143 cm$^{-1}$ respectively.

For helical Au$_{40}$ a Mulliken charge analysis (using the calculated wave function of the optimized geometry) shows that, although the total charge is zero, the terminal and central surface gold atoms are negatively charged while the intermediate surface gold atoms are positively charged. This indicates that Au$_{40}$ has strong selective reactivity and that nucleophiles will prefer to attack at the terminal and central gold atoms, while electrophiles will prefer to attack at the intermediate gold atoms. In contrast, the surface gold atoms of compact Au$_{40}$ are all negatively charged. For bare CO, the charge on the C atom is -0.041 and the charge on the O atom is 0.041.

We now consider the complex that is formed when CO bonds to a terminal gold atom of helical Au$_{40}$ (which carries a negative charge). As shown in Fig. 1, bottom row, a bond is formed between a single surface gold atom and the carbon atom of CO. Note that the helical structure is largely preserved and Au$_{40}$ does not collapse to the more stable compact structure. In the complex formation there is charge transfer from Au$_{40}$ to CO. The charge on the C atom is now 0.125 and the charge on the O atom is now -0.329 and the total charge of CO is -0.204. Upon complex formation, the C-O bond distance increases to 1.146 Å while the C-O vibrational frequency decreases to 2065 cm$^{-1}$. This is indicative of a weakening of the C-O bond which means that CO will be more reactive and, in particular, more susceptible to oxidation.

We are currently considering the complex that is formed when CO bonds to an intermediate gold atom of helical Au$_{40}$ (which carries a positive charge). We are also considering the complex that is formed when CO bonds to compact Au$_{40}$.

4. References


Figure 1. Top row: Two views of helical Au$_{40}$. Bottom row: Complex between helical Au$_{40}$ and terminally bonded carbon monoxide.
Isotropic Image Analysis for Case Base Creation in a CBR Forecasting System.

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Abstract

This interdisciplinary study presents a novel Case-Based Reasoning (CBR) system that applies an isotropic buffer operator for case-based creation. Commonly used as an image analysis tool by commercial Geographic Information Systems (GIS), the operator in this particular system calculates the areas of different environmental phenomenon for simulation and visualization tasks. The systems presented in this paper use CBR methodology to generate predictions from data sets that were generated after having applied the isotropic buffer operator to the environmental images.

Keywords: Isotropic image analysis, Case-Based Reasoning, Forecasting.

1. Introduction

All customised Geographical Information Systems (GIS) include a buffer operator, also known as the buffering or influence zone. It is defined as the geometric space of the points that are at a shorter or similar distance to a given object (point, polyline or polygon) [5]. This definition is isotropic or directionally uniform, since the distance of the object to the edge of the buffer is constant in any direction on the plane. Among other fields, this operator is used in the simulated visualization of environmental processes, such as surveys of pesticide and chemical fertilizer contamination in the shallow waters of hydrographic basins; the influence of nitrates and silt levels on the growth of local flora, the
environmental impact of installing new industries in close proximity to urban centers, the determination of areas of high seismic risk.

Case-Based Reasoning (CBR) systems make use of past information in order to generate new solutions to new problems. The quality of the information stored within the case base will determine the quality of the solutions offered by these systems. Thus, the isotropic buffer operator is an important element in image analysis, as it provides the CBR system with accurate information that may be used in future situations.

The following section gives a brief explanation of CBR methodology. The third section develops the concept of isotropic image analysis, after which the fourth section describes the CBR system presented in this study, prior to the conclusions, which are advanced at the end of the paper.

2. **Case-Based Reasoning**

*Case-Based Reasoning* is a technique that has its origin in knowledge-based systems. CBR systems learn from previous situations [1]. The main element of a CBR system is the *case base*; a structure that stores problems, elements (*cases*), and its solutions. So, a case base can be visualized as a database that stores a collection of problems with some sort of relationship to the solutions to every new problem, which gives the system the ability to generalize in order to solve new problems.

The learning capabilities of CBR systems rely on their own structures, which consist of four main phases [2]: retrieval, reuse, revision and retention. The *retrieval* phase consists of finding the cases in the case base that most closely resemble the proposed problem. Once a series of cases have been extracted from the case base, they must then be *reused* by the system. In this second phase, the selected cases are adapted to fit the current problem. After offering a solution to the problem, it is then *revised* to check whether the proposed alternative is in fact a reliable solution to the problem. If the proposal is confirmed, it is *retained* by the system and could eventually serve as a solution to future problems.

CBR is a methodology [16] that has been applied to solve different kind of problems. It is a model that can easily be applied to solve soft-computing problems [15], since the methodology used by CBR is quite easy to assimilate using soft-computing approaches. Further applications are predictive models for the stock market [7], where inputs of different daily values allow a CBR model to assist with stock market investment decisions; construction models, for the generation of functional databases [18] to improve the somewhat chaotic
organization of construction projects, and also [6] to select different methods and materials, using expert system-oriented applications.

In most cases, CBR has not been used by itself, but is combined with various artificial intelligence techniques. Growing Cell Structures (GCS) has been used with CBR to automatically create the intern structure of the case base from existing data. It has been combined with multi-agent applications [4] to improve its results. ART-Kohonen neural networks [17], artificial neural networks and fuzzy logic [8] have also been used to complement the capabilities of the CBR methodology.

3. **Isotropic image analysis**

There are two methods for the generation of influence areas: Voronoi triangulation and the Minkowski Sum [12]. In the latter method, a *secondary polygon or generating polygon* is defined as being located on a point or moving on a polyline or polygon and generating a surface formed by the points that the generating polygon finds on its way. In the isotropic buffer, the generating polygon is a circle, which implies a constant distance between the border of the buffer and the object.

3.1. **Von Misses Distribution**

We can define the *circular variables* [3] as those that represent directions on the plane, which are quantified by angles that range from 0 to \(2\pi\). One of the most important differences with regard to the lineal variables is that, while these can take values of the whole real straight line \((+\infty, -\infty)\), the circular variables take cyclical values and consequently, the sum or difference of observations can surpass 360º and can even result in a negative value, it being possible in such cases to find an equivalent value within the interval 0-360º. This characteristic allows the circular variables to be treated differently from the lineal ones, by means of statistical creation, correlation analysis and specific distributions for these types of variables.

Conceptually, a circular distribution can be considered in the same way as a bivariated lineal distribution where the total probability (or total mass) is dispersed within the circle unit. Therefore, in the same way as in the bivariated lineal statistic, a mean vector \(\vec{m}\) of module \(r\) and mean angle \(\bar{\phi}\) exists in the circular statistic, at the tip of which the mass centre \(C\) of the distribution may be found (*Fig. 1*).
Let \( Z(\Phi) \) be the random variable. If we take a monomodal sample of frequencies \( n_1, n_2, \ldots, n_j \) in the directions \( \Phi_1, \Phi_2, \ldots, \Phi_j \), the mean vector \( \bar{m}(r, \Phi) \) may be defined as

\[
r = \sqrt{\bar{x}^2 + \bar{y}^2}
\]

\[
\Phi = \begin{cases} 
\arctan(\bar{y}/\bar{x}) & \text{si } \bar{x} > 0 \\
180 + \arctan(\bar{y}/\bar{x}) & \text{si } \bar{x} < 0
\end{cases}
\]

(1)

Where, \( \bar{x} \) and \( \bar{y} \) are the projections of \( \bar{m} \) on the \( X \) and \( Y \) axes, respectively:

\[
\bar{x} = \frac{1}{N} \sum_{i=1}^{N} n_i \cos \Phi_i \\
\bar{y} = \frac{1}{N} \sum_{i=1}^{N} n_i \sin \Phi_i \\
N = \sum_{i=1}^{j} n_i
\]

(2)

If the data are contained in intervals of width \( \lambda \), \( r \) should be corrected, the correct module being \( r_c = r \cdot c \), where

\[
c = \frac{\lambda/2}{\sin(\lambda/2)}
\]

(3)

Among the existing circular distributions [14], one of the most widely used for the modelling of circular variables is the Von Mises distribution, whose density function for \( v \)-modal and symmetric samples is

\[
f(\Phi) = \frac{1}{2\pi I_0(k)} \exp[k \cos v(\Phi - \theta)]
\]

(4)

Where \( I_0 \) is the Bessel function of an imaginary pure argument of order 0, \( v \) is the number or modes and \( k \) it is the concentration parameter [14], that indicates to what measure the distribution around the dominant direction \( \theta \) is concentrated. The \( v \)-modal samples should be considered as being extracted from a distribution.
generated by the overlapping \( v \) monomodal distributions. When the distances between modes are arbitrary, standard methods do not exist to decompose a \( v \)-modal sample into \( v \) monomodal samples; in practice, the multimodal samples are usually shown as bimodal and are diametrically opposed. In this case, it is possible to reduce the bimodal sample to a monomodal sample, duplicating the angles. With the new angles, the average vector is calculated \( \mathbf{r}_2(\theta_2, \Phi_2) \) using Eq.(1)(2)(3). To obtain the symmetrical modal angle \( \Theta_1 \) from the original sample, the angle duplication effect must be cancelled, which gives us \( \Theta_1 = \Theta_2/2 \) \( \hat{k} \Theta_1 = \Theta_2/2 + 180^\circ \).

For \( \hat{k} = 0 \), \( f(\Phi) \) degenerates in an uniform distribution. Mardia demonstrated [11] that the maximum likelihood estimation \( \hat{\theta} \) and \( \hat{\rho} \) for parameters \( \theta \) and \( \rho \) of a Von Misses distribution are respectively \( \Theta \) and \( r \). Likewise,

\[
\frac{I_1(\hat{k})}{I_0(\hat{k})} = r
\]

is fulfilled. Hence, the maximum likelihood \( \hat{k} \) is the solution of the Eq.(5).

### 3.2. Minkowski Sum

Given two images, \( A \) and \( B \) in \( \mathbb{R}^2 \), the Minkowski sum is defined as

\[
A \oplus B := \bigcup_{b \in B} A + b
\]

(6)

Where \( A \) is the generating polygon, and \( B \) the skeleton or primary element (point, polyline, or polygon. \( A \oplus B \) is generated by moving \( A \) though each element \( b \in B \), and then by adding the result of all the translations later on. The translation of the generating polygon \( A \) through the element \( b \in B \) is defined as

\[
A + b := \{a + b, a \in A\}
\]

(7)

If we take a circle as generating polygon \( A \), and the group of points \( B = \{(2,3),(3,4),(2,5),(1,5)\} \) as the primary element:

\[
A \oplus B = [(A + (2,3)) \cup (A + (3,4)) \cup (A + (2,5)) \cup (A + (1,5))]
\]

(8)

*Fig. 2* shows the result, as well as \( A \oplus L \) and \( A \oplus P \), additions which have respectively taken polyline \( L \) and polygon \( P \) as primary elements.
Conceptually, the Minkowski sum is a dilation or expansion of the primary image B, whose form is determined by the generating polygon A. In the previous example we have chosen a circle as the generating image. The expansion of the primary image is directionally uniform or isotropic, since the generating image is a symmetrical figure with regard to both axes.

4. Forecasting CBR system

In the CBR system presented here, the images to be analyzed are divided into smaller squares. A squared zone determines the area that will be independently analyzed. The values of the different variables in a square area at a certain moment, which define the problem or the situation that has to be solved, is known as a case.

4.1. Case base creation

In this study, we have applied isotropic image analysis based on the buffer operator using Von Misses distribution and the Minkowski Sum, both previously introduced in Section 3. Owing to its good adaptation capabilities, this system has been applied to calculate the areas of different environmental phenomenon, which enable them to be modelled.

Once the data is structured, it is stored in the case base. Every case has its temporal situation stored, which relates every case with the next situation in the same position. That temporal relationship is what creates the union between problem and solution. The problem is the past case, and the solution is the future case, the future state of the square under analysis.

Growing Cell Structures (GCS) [9] are used when introducing the data into the case base,. GCS can create a model from a situation organizing the different cases
by their similarity. If a 2D representation is chosen to explain this technique, the most similar cells (cases in OSCBR) are near one or the other. If there is a relationship between the cells, they are grouped together, and this grouping characteristic helps the CBR system to retrieve the similar cases in the next phase. When a new cell is introduced in the structure, the closest cells move towards the new one, changing the overall structure of the system as shown in (9) and (10). The weights of the winning cell, \( \omega_x \), and its neighbours, \( \omega_y \), are changed. The new value is represented by \( \omega_x(t+1) \), and \( \omega_y(t+1) \) respectively. The terms \( \epsilon_x \) and \( \epsilon_y \) represent the learning rates for the winner and its neighbours, while \( x \) represents the value of the input vector.

\[
\omega_x(t+1) = \omega_x(t) + \epsilon_x(x - \omega_x) \tag{9}
\]
\[
\omega_y(t+1) = \omega_y(t) + \epsilon_y(x - \omega_y) \tag{10}
\]

4.2. Generating predictions

Once the case base has stored the historical data, and the GCS has been structured according to the original distribution of the variables, the system is ready to receive a new problem. When a new problem is introduced into the system, GCS are used once again. The stored GCS behaves as if the new problem were stored in the structure, and finds the most similar cells (cases in the CBR system) to the problem introduced into the system. In this case, the GCS does not change its structure, because it is being used to retrieve the most similar cases to the introduced problem. Only in the retain phase does the GCS change, introducing the proposed solution once again if it is correct.

The similarity of the new problem to the stored cases is determined by the GCS calculating the distance between them. Every element in the GCS has a series of values (every value corresponds to one of the principal components created after de FIK-PCA analysis) and the distance between the elements is therefore a multi-dimensional distance, where all the elements are considered to establish the distance between cells. Then, after obtaining the most similar cases from the case base, they are used in the next phase. The selected case bases will be used to generate an accurate prediction according to the previous solutions that relate to the problem that was introduced.

Having retrieved the most similar cases to the problem that has to be solved from the case base, they are used to generate the solution. The prediction of the future probability of finding oil slicks in an area was generated by using an artificial neural network, with a hybrid learning system. It was obtained with an adaptation of Radial Basis Functions Networks [10]. The chosen cases are used to train the artificial neural network. Radial Basis Function networks have been chosen
because of the reduction of the training time comparing with other artificial neural network systems, such as Multilayer Perceptrons. In this case, in every analysis the network is trained, using only the cases selected from the case base which are the most similar to the proposed problem.

Growing RBF networks [13] are used to obtain the predicted future values that correspond to the proposed problem. This adaptation of the RBF networks allows the system to grow during training gradually increasing the number of elements (prototypes) which play the role of the centres of the radial basis functions. In this case, the creation of the Growing RBF must be made automatically, which implies an adaptation of the original GRBF system. The pseudocode of the growing process and the definition of the error for every pattern is shown below:

$$e_i = \frac{1}{p} \sum_{k=1}^{p} |t_{ik} - y_{ik}|.$$  \hspace{1cm} (11)

Where $t_{ik}$ is the desired value of the $k^{th}$ output unit of the $i^{th}$ training pattern, and $y_{ik}$ the actual values of the $k^{th}$ output unit of the $i^{th}$ training pattern.

5. Conclusions

We have presented a novel CBR system, by using for the first time a GIS technique based on the use of an isotropic buffer operator.

The areas in our CBR system were calculated by dividing the global images into smaller ones, so that we can apply a different buffer to each one. Changing the size of the buffer will help the system to generate a more accurate analysis, improving the quality of the data in the final case-based solution, resulting in better prediction results.

6. References


Nonlinear Modelling and Forecasting of Intraday Stock Returns

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Abstract
We studied the predictability of intraday stock market returns using both linear and non-linear time series models. For S&P-500 index, we compared simple autoregressive and random walk linear models with a range of nonlinear models that included smooth transition, Markov switching, artificial neural network, nonparametric kernel regression and support vector machine models for horizons of 5, 10, 20, 30 and 60 minutes. The empirical results indicate that nonlinear models outperformed linear models on the basis of both statistical and economic criteria. Specifically, although return serial correlation receded by around ten minutes, return predictability still persisted for up to sixty minutes according to nonlinear models, even though profitability decreases as time elapses. More flexible nonlinear models such as support vector machines and artificial neural network did not clearly outperform other nonlinear models.

Key words Forecasting; Intraday stock returns; Stock price forecasting; High frequency data; smooth transition regression, Markov switching regression, Neural networks, nonparametric kernel regression; support vector machine regressions
1. Introduction

The predictability of stock market returns has long attracted much interest of financial researchers and practitioners alike as it has profound theoretical and practical implications. The cornerstone of predictability is the idea of financial market efficiency that states that stock returns fully adjust to all relevant information, so they cannot be forecastable.

This paper focuses on return predictability at intraday level. Intraday trading data prediction is particularly important as it offers practitioners the opportunity to gain high annual returns from a trading strategy. We should expect such predictability to weaken as traders’ actions to exploit profit opportunities expunge serial return correlation and adjust prices to their new equilibrium levels quickly since the stock market in nowadays is assumed to be highly efficient, so predictability recedes over long horizons. In addition, intraday horizons are important in the management of the risk of a trading desk (see Chew (1994)). Despite its economic and financial importance, the analysis of stock return predictability at very short forecast horizons is scarce in the academic literature. An exception is Clements and Taylor (2003) who analyze interval forecasts of high-frequency data.

We explore intraday nonlinear return predictability for the S&P500 index during the June of 2003 to September of 2003 for different within the day temporal horizons of 5, 10, 20, 30 and 60 minutes. We use a wide set of nonlinear modelling techniques that includes smooth transition autoregressive model, Smooth transition autoregressive model with GARCH errors, Markov switching models, artificial neural networks, non parametric time series regression (NP); and finally, a support vector machines, a technique that comes from the statistical learning theory and whose predictive ability for intraday stock return data was not evaluated as yet to the best of our knowledge. Finally, we compare the forecasting performance of different models in terms of (a) some statistical criteria such as the root mean squared error, proportion of times the signs of returns are correctly forecasted, directional accuracy test of Pesaran and Timmermann (1992), and the popular Diebold and Mariano (1995) test for the equality of accuracy of competing forecasts; and (b) an economic criteria, using a simple trading strategy guide by forecasts in order to test the relative pay-offs generated by different forecasting models.

2. Methodology

To forecast stock returns we used various models for $E[r_t|I_{t-1}]$, where $r_t$ represents the first difference of the logarithmic stock price, and $I_{t-1} = \{r_{t-1}, r_{t-2}, \ldots\}$ is the information set available at time $t-1$. The information set only included lagged returns, given that we only analyzed the dynamic characteristics of returns and nonsynchronous trading effects may result in autocorrelation in returns. Below we briefly describe the different models considered for the conditional mean.
We considered nine forecasting models, the simplest of which were the random walk model (RW) and an autoregressive (AR) specification:

\[ r_{t+1} = \beta_0 + \sum_{j=1}^{k} \beta_j r_{t+1-j} + e_{t+1}, \]  

where \( k \) was selected to minimize the Bayes Information Criterion. To account for the possibility that the conditional mean \( E[r_t|I_{t-1}] \) could be time-varying in a nonlinear form we employed several nonlinear models in addition to the linear models used as a benchmark. We briefly discuss the set of nonlinear specifications below.

Smooth transition autoregressive models (STAR) models account for the existence of different regimes with different dynamic properties and with smooth transition between regimes (Granger and Teräsvirta, 1993, Teräsvirta et al, 1994). A first-order STAR model with two regimes takes the following form:

\[ r_{t+1} = \phi_{10} + \phi_{11} r_t + [\phi_{20} + \phi_{21} r_t] F(z_{t+1}; \gamma, c) + e_{t+1}, \]

where \( F(z_{t+1}; \gamma, c) \) is the smooth transition function that depends on the transition variable \( z_{t+1} \) and the parameters \( \gamma \), which is the transition rate or smoothness parameter; and where \( c \) is the threshold value which represents the change from one regime to another. The transition variable can be defined as a linear combination of the lagged values of \( r_t \): \( z_{t+1} = \sum_{h=1}^{H} \alpha_h r_{t+1-h} \). The most widely used smooth transition functions are the logistic function and the exponential function:

\[ F(z_{t+1}; \gamma, c) = \frac{1}{1 + \exp(-\gamma (z_t - c))} \]  

\[ F(z_{t+1}; \gamma, c) = 1 - \exp(-\gamma (z_t - c^2)), \]

with \( \gamma > 0 \). This model is estimated by quasi-maximum likelihood using the logistic function.

To account for the possible effect of nonlinearities in variance on the mean, we also considered the model in Equation (2) with a GARCH(1,1) errors (STAR-GARCH). Thus, \( e_{t+1} = \eta_{t+1} \sqrt{h_{t+1}} \), where

\[ h_{t+1} = \alpha_0 + \alpha_1 e_t^2 + \alpha_2 h_t, \]

\( \alpha_0 > 0 \), \( \alpha_1, \alpha_2 \geq 0 \), \( \eta_{t+1} \) is a i.i.d. process with zero mean and unit variance.

The main feature of an autoregressive Markov switching (MS) model is the possibility for some of the parameters to switch across different regimes or states according to a Markov process governed by a state variable denoted by \( s_t \) (see Hamilton, 1989). A first-order autoregressive MS model has the following specification:

\[ r_{t+1} = \alpha_{s_t,1} + \beta_{s_t,1} r_t + e_{t+1}, \]

where \( e_{t+1} \) is i.i.d. \( N(0, \sigma^2_{e}) \) and \( s_t \) is an unknown state variable that follows a first-order Markov chain, with a transition probability \( \Pr(s_t = j|s_{t-1} = i) = p_{ij} \) that indicates the probability of switching from state \( i \) at time \( t-1 \) to state \( j \) at time \( t \). For simplicity sake, we assume that there are only two states of the economy, denoted as state one and state two, as in Maheu and McCurdy (2000) and in Perez-Quiros
and Timmerman (2000) (e.g., bull and bear markets (Chen and Shen (2007)) or low and high uncertainty in stock markets (Li (2007)). We can use nonparametric kernel regression (KR) when nonlinearity in the conditional mean cannot be characterized explicitly. In such cases the return conditional mean is specified in a general form as:

$$E(r_{t+1}|I_t) = g(r_t, r_{t-1}, \ldots, r_{t-p+1})$$

(5)

where \( p \) is the number of lagged stock returns and where the function \( g(\cdot) \) can be approximated locally at each point by a linear function.

As an alternative to nonparametric nonlinear conditional mean, we considered artificial neural networks, which have proven to be useful in capturing nonlinearity-in-mean for forecasting financial time series. Artificial neural networks are a universal approximator in a wide variety of nonlinear patterns (see Hornik et al, 1990) and generate good predictions (Swanson and White, 1995, 1997). The basic structure of neural networks combines many basic nonlinear functions via a multilayer structure, where there is at least one hidden layer between inputs and outputs. The idea is that explanatory variables simultaneously activate the units in the hidden layer through some function, and output is produced subsequently from the units in the hidden layer through another function. The specific type of ANN employed in this study is the multilayer perceptron (MLP) model, the most basic but perhaps most widely used neural network in economic and financial applications. Hence, MLP\((p,q)\):

$$f(x;\theta) = \sum_{j=1}^{q} \psi(w_j^x + w_j^\theta) + c_0$$

where \( \psi \) is a sigmoid function (typically, a logistic or hyperbolic tangent function).

The universal approximation properties of MLP (see Leshno, 1993) neural networks permit us to approximate any continuous or integrable function (the universal approximation property). In order to ensure consistency in a stochastic environment, in addition to considering the error associated with the approximation of the regression function via a finite number of parameters, it was necessary to consider the estimation error arising from the use of a limited quantity of data. The consistency of the MLP neural networks for different hypotheses was thus obtained (see Krzyzak, 1996; Fine, 1999), and specifically for dependent observations (Chen, 1999). When the series responds to an autoregressive model, then:

$$y_t = f(x_t;\theta) + \epsilon_t$$

where \( f(x_t;\theta) \) is a neural network and \( \epsilon_t \) is, for example, white noise. Trapletti (2000) demonstrated the stationarity and strongly mixing nature of the series \( \{y_t\} \), as also the consistency and asymptotic normality of the least squares estimator for a hypothesis that ensures the identifiability of the network parameters (Hwang and Ding, 1997).
MLP training, which usually uses the squared loss, is performed through nonlinear optimization algorithms. In this research we used the Bayesian algorithm proposed by Foresee and Hagan (1997) as it is less dependent on expert criteria.

Another alternative to the previous regression models is the support vector machine (SVM) (Vapnik, 1998, Schölkopf and Smola, 2002). The SVMs for regression are linear models obtained in a new feature space $X$ as a result of a transformation $\varphi : \mathbb{R}^d \rightarrow X$ of the input space, in which an inner product is defined through a positive definite function (kernel), $\langle \varphi(x_i), \varphi(x_j) \rangle = k(x_i, x_j)$. SVMs for regression have the following general formulation:

$$y_i = f(x_i) = \langle w, \varphi(x_i) \rangle + b.$$

Given a sample, the parameters $w, b$ in the SVM are estimated as the solution to the following regularization problem:

$$\min_{w,b} \left\{ \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{n} \ell(y_i, f(x_i)) \right\}$$

where $C$ is a regularizing constant and $\ell$ is the $\varepsilon$-insensitive loss:

$$\ell(y, f(x)) = \left| y - f(x) \right|_{\varepsilon} = \max\{0, |y - f(x)| - \varepsilon\}.$$

The only solution to the problem in Equation (12) is a linear combination of key points of the sample (the support vectors), $w = \sum_{i,s} \alpha_i \varphi(x_i)$, in such a way that the SVM results as:

$$f(x) = \sum_{i,s} \alpha_i \langle \varphi(x_i), \varphi(x) \rangle + b = \sum_{i,s} \alpha_i k(x_i, x) + b.$$

SVMs share the general form of radial basis function neural networks, which are universal approximators to continuous or integrable functions (e.g., Park, 1993). Consistency results also exist (see Bousquet and Elisseeff, 2002; Steinwart, 2002).

We obtained in-sample and out-of-sample one-step-ahead forecasts that were composed of the estimated parameters of the model and lagged returns. The market timing ability of forecasting models was also compared with a simple buy and hold (B&H) intraday investment strategy for out-of-sample forecasting. This strategy implements a naïve allocation that consist of maintaining a 100% stock index or cash if the quantity predicted exceeds a threshold given by the transaction costs. Hence, the forecast by each predictor determines the position to be taken for the following time period. Thus, if the share price is expected to fall below a threshold on the basis of a particular predictor, then shares are sold if the agent holds assets or they are not bought if the agent holds cash. In contrast, if the share price is expected to rise above a threshold on the basis of a particular predictor, then shares are bought if the agent holds cash or they are not sold if the agent holds assets. The threshold is determined by transaction costs, which are assumed to be low for intraday transactions, as otherwise commissions would
erode profits. The value of these cost were determined in our training set as the mean value of rises and falls divided by 1000 (around 3 bps.).

3. Results

Our main empirical findings verify the predictability of stock returns beyond the time serial correlation recedes; i.e., although market is weak form efficiency according to linear models and therefore prices are not linearly predictable, predictable nonlinearity-in-mean is possible up to a 60 minutes time interval. Surprisingly, the forecast performance of nonlinear models decreases very slowly, mainly directionally predictability, which has an important implication for market timing and the resulting active intraday asset allocation management.

we show that simple autoregressive and random walk linear models are surpassed by a wide range of nonlinear models, including smooth transition autoregressive, smooth transition autoregressive with GARCH errors, Markov switching, multilayer perceptron, nonparametric kernel regression and support vector machine models, which potentially capture nonlinearity-in-mean in intraday stock returns. Traditional statistical criteria suggest that nonlinearities-in-mean are relevant to forecasting intraday stock returns both in-sample and out-of-sample and for any intraday time return period. Of the nonlinear models, for short time periods of five minutes, the Markov switching model performed best for in-sample forecasting, whereas kernel regression was the best performer for out-of-sample forecasting. Despite return serial correlation receding and returns behaving as a random walk for more than ten minutes, return predictability still persisted for up to sixty minutes according to nonlinear models. For the longer intraday time periods studied, smooth transition and neural network models appeared to be better performers, even though the Diebold-Mariano test was not conclusive on equal predictability among the models. We also evaluated linear and nonlinear models in terms of economic criteria, using a simple trading rule driven by model predictions and transaction cost. On economic grounds, trading rules based on Markov switching and support vector machine models were the most profitable for short time horizon returns, whereas smooth transition and neural networks behaved better for longer periods, even though profitability decreased as time elapsed.

4. References


Screening effect on the convective heat transfer coefficients during vacuum frying of potato cylinders

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Abstract

In this study convective heat transfer coefficients were determined during vacuum frying of potato cylinders (5, 10 mm radius) in sunflower oil at 100, 120 and 140 °C. These parameters were evaluated with indirect method based on the adjustment of experimental temperatures, obtained with a teflon probe, and a thermal model implemented with the finite elements software COMSOL.

The results obtained shown higher values for the vacuum frying than for atmospheric frying. Geometry and use of vacuum conditions played an important role in the convective heat transfer, being more importants than the oil temperature. A screening effect, originated for bubble collapsing due to high evaporation rate, was also observed in the case of vacuum fried thinner cylinders and was incorporated into the model, with the use of an effective temperature, T_{ef}.

Key words: Vacuum frying, convective heat transfer, bubble screening, finite element method, COMSOL.

1. Introduction

Frying is an extensively process used both in the food industry and domestically. It basically consists of cooking foodstuffs in oil or fat at temperatures well above the boiling point of water. This fast and easy preparation results in products with organoleptic qualities (colour, texture, flavour) much appreciated by consumers. However, these products end up with a high fat content that in some cases reaches a third of their total weight. In recent decades, therefore, numerous complementary processes have been proposed to reduce fat content while retaining sensorial qualities [1].
One of these alternative processes is frying at reduced pressure, used for many years in the snacks industry especially in South-East Asia. Working in vacuum conditions reduces the boiling point of water in the foodstuffs which can therefore be eliminated at lower temperatures, allowing frying with oil at a lower temperature. Numerous studies have evaluated the adaptation of this technique with different vegetables, comparing it with frying at atmospheric pressure. It has been found that as well as reducing the final fat content [2,3], vacuum fried products have several other advantages such as a lower acrylamide content [4] and improved organoleptic and nutritional qualities [5,6,7,8]

Coupled heat and mass transfer with bubbling make those processes difficult for modeling and further optimization purposes. This is especially important in the case of vacuum frying as lower pressure increases the evaporation rate and the size of the bubbles. Across the solid surface, there becomes a vigorous movement of evaporation causing a considerable mixing in the oil affecting convective heat transfer coefficient. The knowledge of this coefficient is expected to allow accurate determination of temperature distribution and hence the calculations to lead to development of an optimum frying process.

It was therefore decided to evaluate the convective heat transfer during moderate vacuum frying of potato cylinders.

2. Material and methods

The experimental material was potato (Solanum Tuberosum, cv. Agria) obtained from local distributors. Each sample consisted of cylinders of different radii (1 and 0.5 cm respectively) and 5 cm in length extracted from the middle of the potato, using a metal punch. Sunflower oil with a high oleic acid content specially prepared for frying was used (Titan, Koipe, Spain).

A pressure cooker (Gastrovac ICC, Spain) with a nominal pressure of up to 20 kPa was used for the reduced pressure frying, sufficient for the pressure levels required. The changes in pressure and temperature were recorded with a piezoresistive pressure transducer (Picovacq PT, Digitem, France) placed inside the system. In order to obtain suitable working conditions and keep them constant throughout the process, a ratio of 3.5 L of oil for every 100 g of potato was used. Each frying operation consisted of an initial depressurization step with the potatoes and the probe outside the oil, an immersion step with the oil already hot and subsequent removal and
draining during 1 min and vacuum breaking during 1 min. Under these conditions the absolute pressures recorded were between 20 and 35 kPa depending on the working temperature and the exact moment of frying, given that the vigorous initial vaporization causes a certain degree of oscillation in the pressure of the system. Before each experiment, the oil was kept at the working temperature and the maximum vacuum level for one hour, and discarded after a maximum of five hours of use. Frying was carried out at temperatures of 100, 120 and 140 ºC.

Similar experiments were carried out at atmospheric pressure and 140 ºC using the same equipment but without applying the vacuum conditions. Three replications were made for each of the conditions.

To determine the heat transfer coefficient during atmospheric and pressure frying conditions an indirect method was used [9, 10]. A cylindrical teflon probe was placed inside the frying oil with potato cylinders, three big or four small, at different conditions to simulate the bubbling of a normal frying process as can be observed in Fig 1. K-type thermocouples were used to determine the time history of sample temperatures during frying. One thermocouple was placed in the oil to determine the process temperature while the other thermocouple was put across the cylinder radius and fixed near the geometric center of the sample. To determine the convective coefficients the obtained thermal values were adjusted to a mathematical two-dimensional axialymmetric model.

Heat transfer from the oil to the teflon probe was simulated using a commercial simulation package COMSOL Multiphysics 3.4 with the heat transfer module (Comsol, Swedish), that makes use of finite element method. General solution form and Direct (UMFPACK) linear system
solver were used in simulations. For the probe a heat transfer scheme was adopted as convective at the exterior and conductive in the interior of the cylinder according the following expressions:

\[ \rho C_p \frac{\partial T}{\partial t} + \nabla (-k \nabla T) = 0 \]  

For the teflon probe

The boundary conditions are:

\[ k \nabla T = h A (T_\infty - T_s) \]  

For the external boundaries

\[ k \nabla T = 0 \]  

For the axes of symmetry

where \( \rho \) is the density, \( C_p \) is the specific heat, \( k \) is thermal conductivity, \( A \) is the area, \( h \) is the convective heat transfer coefficient, \( T_\infty \) is the oil temperature and \( T_s \) is the surface temperature.

These equations were implemented using a mesh of 362 nodes with triangular elements. The input data were the thermal and physical properties of the teflon: \( k, 0.35 \text{ W m}^{-1} \text{ K}^{-1} \); \( C_p, 1,050 \text{ J kg}^{-1} \text{ K}^{-1} \); and \( \rho, 2,200 \text{ kg m}^{-3} \) [11]. The convective heat coefficient was adjusted appropriately until the best fit (minimum mean squared error, MMSE) was obtained between the experimental data of temperature at the central point and those predicted from simulation. The parametric optimization was achieved using the Nelder-Mead method through MATLAB 7.0 (Mathworks, USA), specifically the “FMINSEARCH” utility.

3. Results and discussion

Fig. 2 presents changes in the values of the experimental data for the central temperature in the teflon probe for the studied conditions. There are big differences between the different geometries and studied conditions. In the case of the thick cylinders the temperature rises up faster ending close to the set point. For the small ones the temperature remains between 18 and 20 °C under the oil values and increases slowly. This could be explained attending to the different evaporation rates, just after the vapour escapes from the potatoes the bubbles start collapsing isolating the surface of the probe. This screening effect is more important in the case of vacuum frying, because the bigger bubbles, and for the thinner cylinder, because its ratio surface/volume is higher and their water lose is faster.
As the convective conditions in the oil depends of the moisture transport the base convective coefficient was supposed to follow an exponential form in parallel to water loss in vacuum frying [2]. This form is also used for other authors in atmospheric frying [12] and is expressed as:

\[ h = A + B \cdot e^{(-C \cdot t)} \]

To include the screening effect, the effective temperature parameter, \( T_{ef} \), was introduced into the boundary convective condition instead of set temperature, \( T_x \). With this additional value it is considered that the oil surrounding the surface of the probe is at a lower temperature that the rest due to the bubble screening. The adjusted values for the \( A, B, C \) and \( T_{ef} \) parameters and the corresponding MMSE are shown in Table 1. This also presents the corrected MMSE, calculated as the results of multiply the MMSE by the numbers of adjust parameters, used in each case to represent the global efficiency of each method.

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rest due to the bubble screening. The adjusted values for the $A, B, C$ and $T_{ef}$ parameters and the corresponding MMSE are shown in Table 1, which presents as well the corrected MMSE, calculated by multiplying the MMSE by the fitted parameters, used in each case to represent the global efficiency of each method.

Table 1. Convective heat transfer coefficient $h$ values determined with the indirect method.

<table>
<thead>
<tr>
<th>Heat coefficient</th>
<th>Potato cylinder size</th>
<th>Parameter</th>
<th>Vacuum 120 ºC</th>
<th>Vacuum 140 ºC</th>
<th>Atm. 140 ºC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exponential</td>
<td></td>
<td>$A$ (W m$^2$ K$^{-1}$)</td>
<td>155.34</td>
<td>165.00</td>
<td>177.80</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$B$ (W m$^2$ K$^{-1}$)</td>
<td>1903.64</td>
<td>3684.50</td>
<td>13627.00</td>
</tr>
<tr>
<td></td>
<td>Thick</td>
<td>$C$ (s$^{-1}$)</td>
<td>0.204</td>
<td>0.160</td>
<td>0.332</td>
</tr>
<tr>
<td></td>
<td>MMSE</td>
<td>0.91</td>
<td>1.76</td>
<td>1.58</td>
<td>1.18</td>
</tr>
<tr>
<td></td>
<td>MMSE*n</td>
<td>2.73</td>
<td>5.28</td>
<td>4.74</td>
<td>3.54</td>
</tr>
<tr>
<td></td>
<td>$h=A+B e^{-Ct}$</td>
<td>$A$ (W m$^2$ K$^{-1}$)</td>
<td>56.75</td>
<td>57.34</td>
<td>60.78</td>
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<tr>
<td></td>
<td></td>
<td>$B$ (W m$^2$ K$^{-1}$)</td>
<td>429.12</td>
<td>406.91</td>
<td>407.54</td>
</tr>
<tr>
<td></td>
<td>Thin</td>
<td>$C$ (s$^{-1}$)</td>
<td>0.066</td>
<td>0.059</td>
<td>0.066</td>
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<tr>
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<td>0.81</td>
<td>1.29</td>
<td>1.36</td>
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<td>MMSE*n</td>
<td>3.21</td>
<td>2.43</td>
<td>3.87</td>
<td>4.08</td>
</tr>
<tr>
<td>Exponential with screen effect</td>
<td></td>
<td>$A$ (W m$^2$ K$^{-1}$)</td>
<td>128.71</td>
<td>125.00</td>
<td>177.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$B$ (W m$^2$ K$^{-1}$)</td>
<td>2194.46</td>
<td>2684.99</td>
<td>13311.00</td>
</tr>
<tr>
<td></td>
<td>Thick</td>
<td>$C$ (s$^{-1}$)</td>
<td>0.214</td>
<td>0.131</td>
<td>0.340</td>
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<td></td>
<td>$T_{ef}$ (ºC)</td>
<td>102.4</td>
<td>123.5</td>
<td>140.1</td>
<td>141.7</td>
</tr>
<tr>
<td></td>
<td>MMSE</td>
<td>0.71</td>
<td>1.63</td>
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<tr>
<td></td>
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<td>2.84</td>
<td>6.52</td>
<td>6.20</td>
<td>4.60</td>
</tr>
<tr>
<td></td>
<td>$h=A+B e^{-Ct}$</td>
<td>$A$ (W m$^2$ K$^{-1}$)</td>
<td>75.80</td>
<td>83.18</td>
<td>87.58</td>
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<tr>
<td></td>
<td></td>
<td>$B$ (W m$^2$ K$^{-1}$)</td>
<td>492.11</td>
<td>528.34</td>
<td>500.31</td>
</tr>
<tr>
<td></td>
<td>Thin</td>
<td>$C$ (s$^{-1}$)</td>
<td>0.067</td>
<td>0.078</td>
<td>0.089</td>
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<tr>
<td></td>
<td>$T_{ef}$ (ºC)</td>
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<td>112.3</td>
<td>131.5</td>
<td>132.9</td>
</tr>
<tr>
<td></td>
<td>MMSE</td>
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<td>0.56</td>
<td>0.86</td>
<td>1.07</td>
</tr>
<tr>
<td></td>
<td>MMSE*n</td>
<td>3.08</td>
<td>2.24</td>
<td>3.44</td>
<td>4.28</td>
</tr>
</tbody>
</table>

For the first model the MMSE are below 2 so could be considered a good adjust. The parameter ‘$A$’, that represents the heat transfer at high times, increases with temperature in both geometries. The use of vacuum conditions increases this value in the case of thick cylinders while slightly decreases the coefficients for the small ones. There are frying studies that found convective coefficients being proportional [12] or inverse proportional [13] to temperature, depending of the operating conditions. In our case the differences are small comparing with the geometry or the use of vacuum conditions, so we can ignore the effect of temperature for the
conditions used. The sum ‘$A+B$’, that represents heat transfer at initial times, show high values for the vacuum frying comparing with atmospheric frying due to the lower agitation observed in this case. The high values that can be registered with this model are similar to the values registered for other authors using similar experimental conditions [9].

The second model shows lower MMSE in all cases. The $T_{ef}$ calculated for the thick cylinders is higher than set temperature, $T_\infty$, being indicative of this modification only affects the adjustment due to the use of an extra parameter. As the corrected MMSE is also high for the thin cylinders fried at atmospheric pressure the same conclusion can be added for these working conditions. In the case of thin cylinders and vacuum conditions $T_{ef}$ is lower than $T_\infty$ in all cases; the difference from the set temperature is between 5.5 and 8.5 °C showing that the screening is an important effect that has to be considered during frying, specially while using vacuum conditions in products with high evaporation rates. In addition, the introduction of the $T_{ef}$ parameter is mathematically justified by the MMSE*n values, which are lower than the obtained with the first model.

The second model shows lower MMSE in all cases. The $T_{ef}$ calculated for the thick cylinders is higher than the set temperature, $T_\infty$, indicating that this modification only affects the fit due to the use of an extra parameter. As the corrected MMSE is also high for the thin cylinders fried at atmospheric pressure the same conclusion can be added for these working conditions. In the case of thin cylinders and vacuum conditions $T_{ef}$ is lower than $T_\infty$ in all cases; the difference from the set temperature is between 5.5 and 8.5 °C showing that screening during frying is an important effect that has to be considered, especially while using vacuum conditions in products with high evaporation rates. In addition, the introduction of the $T_{ef}$ parameter is mathematically justified by the MMSE*n values, which are lower than those obtained with the first model.

4. Acknowledgements

The authors express their gratitude to the ‘Ministerio de Educación y Ciencia’ (Spain) (Project: AGL2007-64252/ALI) and to the ‘Diputación General de Aragón’ (Project: ALCOTEC 2009/0196) for providing the financial support for the study.

5. References


Comparison of GPS observations made in a forestry setting using functional data analysis

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Abstract

GPS receiver observations made in forestry settings are affected by data distortion and signal losses and this negatively affects precision and accuracy measurements. Using a technique for identifying functional outliers, we determine whether there are differences between errors for coordinates obtained at 10 different points of a forest characterized by a set of dasometric data. Our results indicate that the 2 points with highest error correspond to areas with dasometric values that would indicate these areas to have a more dense forest canopy than the remaining areas.

Key words: GPS, forest canopy, functional data, outlier, depth

1. Introduction

Geographic positioning system (GPS) receivers are frequently used in forestry settings for, among other applications [7], the monitoring of harvesting machinery [9] and cadastral forest surveys [19]. In forestry settings, however, measurement precision and accuracy are affected by forest canopy interference in the satellite signals. Tree trunks, branches and leaves distort or break up satellite signals and
negatively affect the accuracy and precision of receiver-measured coordinates in these conditions [6], [16]. For a forest of lodgepole pines (Pinus contorta Douglas, Gerlach (1989) found that radio signal losses from a satellite could be attributed to tree trunks, branches and foliage 23%, 28% and 36% of the time, respectively.

The typical approach to studying the effect of the forest canopy on GPS positional accuracy is to seek associations between accuracy and dasometric variables characterizing the forest canopy, such as basal area, stand density and the Hart-Becking index [11], [12], [16], [18]. In these cases, tests for comparing statistical distributions (parametric or non-parametric) are generally used to determine whether or not precision values obtained in zones with different forestry variable values can be considered to come from the same population. Analysis of variance (ANOVA) is also frequently used to identify the variables that significantly affect GPS positional accuracy [1]. However, this kind of test is not appropriate when working with a dense set of data collected over time (such as GPS data), as such data is more suitably handled as observations made at discrete points of a smooth stochastic process.

Data mining techniques have advanced to the point where the exploitation of vectorial data has proven to be inadequate; this has led to the emergence of functional data analysis (FDA) [17]. FDA applications are very varied and include environmental research [10], [15], sensors [21], industrial methods [8], [13] and medical research [2], [20].

In the functional approach, comparisons are made overall and take into account the time correlation structure of the data. This is the focus we give to our forest canopy problem. The method used to compare curves is based on the concept of functional depth, which is a measure of the centrality of a given curve within a group of curves [5].

The article is structured on the basis of a description of our methodology, a description of our results and the most relevant conclusions to be drawn from the results.

2. Methodology

We identified outliers using a functional approach, in such a way that the sample of observations was considered to be composed of a series of curves rather than a discrete set of point observations. First the curves were fitted to the discrete data by means of a process called smoothing and then outliers were identified using the concept of functional depth. In this section we explain the basic concepts
underlying the methodology for detecting outliers in the initial sample, namely, smoothing, functional depth and outlier identification.

2.1. Smoothing

One of the first studies in the FDA fields [17] considered functional data to be observations at discrete points of continuous random processes. Assume a set of observations \( f(t_j) \) in a set of \( n_p \) points \( t_j \in \mathbb{R} \), where \( t_j \) represents each instant of time. These observations can be considered as discrete observations of the function, where is a functional space.

In order to estimate the function \( f(t) \), it is considered that \( F = \text{span}\{\phi_1, \ldots, \phi_n\} \), where \( \{\phi_k\} \ k = 1, ..., n \) is a set of basis functions. In other words, for each function \( f(t) \in \chi \subset F \), we have:

\[
f(t) = \sum_{k=1}^{n} c_k \phi_k(t)
\]

(0.1)

The smoothing problem now consists of determining the solution to the following regularization problem [17]:

\[
\min_{f \in F} \sum_{j=1}^{n_p} \left( z_j - f(t_j) \right)^2 + \lambda \Gamma(f)
\]

(0.2)

where \( z_j = f(t_j) + \varepsilon_j \) (\( \varepsilon_j \) is random noise with zero mean) represents each of the observations of the function \( f \) in the instant \( t_j \), \( \Gamma \) is a differential operator that controls the complexity of the function and \( \lambda \) is a regularization parameter.

Bearing in mind (1.1), the problem (1.2) may be written as:

\[
\epsilon \left\{ (z - \Phi c)^T (z - \Phi c) + \lambda c^T R c \right\}
\]

where \( z = (z_1, ..., z_{n_p})^T \) is the vector of observations, \( c = (c_1, ..., c_n)^T \) is the vector of coefficients expressed in (0.1), \( \Phi \) is the \( n_p \times n_b \) matrix with elements \( \Phi_{jk} = \phi_k(t_j) \) and \( R \) is the \( n_b \times n_b \) matrix with elements:

\[
R_{ll} = \left\{ D^2 \phi_l, D^2 \phi_l \right\}_{L_2(\tau)} = \int_\tau D^2 \phi_l(t) D^2 \phi_l(t) dt
\]
2.2. Functional depth

Depth measurement was originally introduced in the context of multivariate analysis to measure the centrality of a point with respect to a sample. Depth provides a way of ordering a sample from its centre in such a way that the points closest to the centre have greater depth. Like most vectorial concepts, the concept of depth has been generalized to the functional case [5]. Functional depth measures the centrality of a curve within a set of curves.

In this study we focus on 2 of the most widely used depth measurements:

- Fraiman-Muniz depth (FMD): Let the empirical distribution function

\[ F_{n,i}(f_i(t)) = \frac{1}{n} \sum_{k=1}^{n} I(f_k(t) \leq f_i(t)) \]

where \( I(\cdot) \) is the indicator function. The FMD for a curve \( f_i \) is given by:

\[ \text{FMD}_n(f_i(t)) = \int_a^b D_n(f_i(t)) dt \]

where \( D_n(f_i(t)) \) is the point depth of \( f_i(t), \forall t \in [a,b] \) given by:

\[ D_n(f_i(t)) = 1 - \frac{1}{2} \left[ 1 - F_{n,i}(f_i(t)) \right] \]

- H-modal depth (HMD): The functional mode (based on the mode concept) is defined as the curve most densely surrounded by the other curves in a sample. HMD is expressed as:

\[ \text{MD}_n(f_i,h) = \sum_{k=1}^{s} K \left( \left\| f_i - f_k \right\| \right) \]

where \( K : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \) is a kernel function, \( \left\| \right\| \) is a norm in a functional space and \( h \) is the bandwidth parameter. One of the most widely used norms for a functional space is \( L^2 \), expressed as:

\[ \left\| f_i(t) - f_j(t) \right\|_2 = \left( \int_a^b (f_i(t) - f_j(t))^2 dt \right)^{1/2} \]

The infinite norm \( L^\infty \) is sometimes used:

\[ \left\| f_i(t) - f_j(t) \right\|_\infty = \sup_{t \in [a,b]} \left| f_i(t) - f_j(t) \right| \]
Different kernel functions $K(\cdot)$ can also be defined, among them the truncated Gaussian kernel:

$$K(t) = \frac{2}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right), t > 0$$

### 2.3. The functional outlier concept

A functional sample may include elements that, although they do not constitute error in themselves, may feature patterns different from the rest of the sample. Depth measurement, as described above, is used to identify outliers in functional samples.

Depth and outlier are inverse concepts: outliers in functional samples have considerably less depth than non-outliers.

For this study we used the HMD to measure depth. The cutoff $C$ was obtained so that type 1 error—the percentage of correct observations wrongly identified as outliers—was approximately 1%:

$$\Pr(MD_n(x_i(t)) \leq C) = 0.01, \quad i = 1, \ldots, n$$

In practice, the distribution of the functional depths for which the value for $C$ needs to be estimated is unknown. Of the different estimation methods available [4], we selected the bootstrapping approach [14].

### 3. Application. Forest canopy impact on GPS accuracy

#### 3.1. GPS measurements

The sample used in this research $\{(t_1, t_2, \ldots, t_{3600})\}_{j=1}^{10}$ consists of a set of GPS observations measured, for a set of 10 points, second by second over 1 hour, where $t_j$ represents measurement in instant $i$ (in seconds) over the period of 1 hour at point $j$.

The data were collected using a double-frequency GPS receiver (HiperPlus, Topcon Positioning Systems, Inc., Livermore, CA, USA) while observing GPS pseudorange and carrier phase.

The GPS experimental data were collected during 2 days over periods of 5-6 hours between 18 and 21 July 2008. Antenna heights ranged from 1.35 to 1.70 m and the logging rate was 1 second. The collection of observations lasted for at
least 1.5 hours and the process was repeated 3 times a day. GPS data were revised to ensure continuity and were cut to obtain 10 datasets representing 1 hour.

The observation point was located at latitude 42°41'08.79872''N and longitude 6°38'03.210587'' W (WGS84) and at an ellipsoidal height of 933.829 metres (considered the \( Z_{\text{true}} \) coordinate). These coordinates were calculated by differential correction in static surveying. Post-processing correction was carried out using the PONF base station as the nearest reference station in the regional GNSS network (http://gnss.itacyl.es/). This point was projected and the position set up as the ‘true’ position for calculating horizontal and vertical accuracy. The UTM coordinates were \( X_{\text{true}}=693814.623 \) and \( Y_{\text{true}}=4728635.531 \) (Datum ETRS89; zone 29N).

The planimetric error in each instant of time \( i \) was calculated using the expression:

\[
E_{XY} = \sqrt{(X_i - X_{\text{true}})^2 + (Y_i - Y_{\text{true}})^2}
\]

The altimetric error in each instant was calculated using the formula:

\[
E_z = |Z_i - Z_{\text{true}}|
\]

3.2. Forest environment characterization

With a view to characterizing the forest lots studied, we calculated the parameters associated with the forestry characteristics of each. The parameters were determined by measuring the trees in a radius of 10 metres around the point where the GPS observations were made.

The parameters studied were the following:

- \( D_m \): Normal diameter (measured at a height of 1.3 metres).
- \( H_m \): Mean height.
- \( H_0 \): Dominant height (mean height of the 4 thickest trees).
- \( H_t \): Treetop height (total height less the height to the first branch).
- \( N \): Number of feet/hectares.
- \( G \): Basal area (cross-section at normal tree height).
- \( D_g \): Mean squared diameter (\( D_g = \frac{4G}{\pi n} \); \( n \) = number of trees).
- \( \text{HBI} \): Hart-Becking index (relationship between mean spacing between trees \( a \) and dominant height \( H_0 \) (\( IH = \frac{a}{H_0} \times 100 \))
FUNCTIONAL STATISTICS FOR GPS DATA COMPARISON

- V: Wood volume.
- W: Biomass.
- SC: slenderness coefficient (relationship between mean height and mean diameter of the biomass)

Table 1 shows the parameter values for the 10 studied plots and also minimum, maximum and mean values and standard deviation for the entire set.

<table>
<thead>
<tr>
<th>Lot</th>
<th>$D_m$ (cm)</th>
<th>$H_m$ (m)</th>
<th>$H_s$ (m)</th>
<th>HBI (%)</th>
<th>$V$ (m$^3$/ha)</th>
<th>$W$ (kg/ha)</th>
<th>SC</th>
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<tr>
<td>1</td>
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<tr>
<td>9</td>
<td>13.46</td>
<td>21.41</td>
<td>22.23</td>
<td>12.48</td>
<td>2960.08</td>
<td>53.96</td>
<td>16.01</td>
</tr>
<tr>
<td>10</td>
<td>12.73</td>
<td>23.26</td>
<td>22.85</td>
<td>13.06</td>
<td>2992.34</td>
<td>46.35</td>
<td>14.23</td>
</tr>
</tbody>
</table>

| Min | 12.73      | 15.34     | 15.02     | 9.85     | 605.82        | 24.47       | 14.23 |
| Max | 29.68      | 27.69     | 28.01     | 19.21    | 3056.36       | 60.18       | 29.79 |
| Mean| 20.12      | 21.38     | 21.66     | 13.62    | 1811.63       | 42.72       | 20.94 |
| STD | 6.70       | 4.33      | 4.48      | 3.33     | 1044.93       | 11.91       | 6.05  |

4. Results

The first step in identifying possible outliers in the data was to fit curves to the set of values for the planimetric and altimetric errors. The smoothing method described in Section 2.1 was used for this purpose, resulting in a set of 10 curves for each error type. Figure 1 shows the 10 planimetric error curves. The great functional complexity of the sample is evident in the irregularity of the functions.
Figure 1. Functional sample for planimetric errors, with 2 outliers depicted in black.

Given the complexity of the sample, it was necessary to select a set of 1000 basis functions in order to obtain the most information possible. The outcome was a fit defined by an R-squared value (RSQ) of 0.99.

In order to study the functional outliers the HMD function was selected considering the norm $L^2$ of a functional space. The analysis identified 2 functional outliers (depicted in black in Figure 1) in the sample for the specific case of the planimetric errors; these outliers corresponded to Lots 5 and 8 in Table 1. No functional outliers for the error in Z were detected.

This result differs from that obtained using the Kruskal-Wallis test for all the positions except numbers 5 and 8 (the fact that the errors do not follow a normal distribution was first checked and was the reason a non-parametric test was used). This test rejected the null hypothesis, for a 99% significance level, that the 8 error observations (all except numbers 5 and 8) came from the same population. Recall that, since the Kruskal-Wallis test compares the medians of the groups, it is possible to have a tiny $p$ value—clear evidence that the population medians are different—even if the distributions overlap considerably.
FUNCTIONAL STATISTICS FOR GPS DATA COMPARISON

The 2 points corresponding to the outliers are characterized by high values for tree density (N), volume (V) and biomass (W), low values for the Hart-Becking index and the largest basal areas. Our result corroborates the results obtained by other authors, such as Naesset (1999, 2001)—who found that the basal area is a parameter that has a significant bearing on GPS measurement accuracy—and Rodríguez-Pérez et al. (2007)—who detected an association between the Hart-Becking index and precision.

5. Conclusions

We have analysed the application potential of functional data analysis to the evaluation of the impact of the forest canopy on the accuracy of GPS receiver measurements. Adopting a functional approach means that error measurements over the period of an hour can be considered as a continuous function. In other words, we can work with all the information rather than just with mean values, which is the basis for the traditional statistical approach.

Outliers were detected using functional depth measurement (a generalization of the vectorial case), which provides information on the distance of a function from the centre of a sample. In contrast with conventional vectorial techniques, this methodology does not require a normality hypothesis for the sample (whether this hypothesis would be valid was, nonetheless, checked) and also takes into account the time correlation structure of the data.

The 2 outliers detected in our study can be explained by the fact that they correspond to points located in lots with the highest basal areas and also high tree density, volume and biomass values and a low Hart-Becking index.

References


Mathematical Modeling of Forest Fire Front Spread

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Abstract

In this paper the assignment and theoretical investigations of the problems of crown forest fire spread in windy condition were carried out. Mathematical model of forest fire was based on an analysis of known experimental data and using concept and methods from reactive media mechanics. In this context, a study - mathematical modeling - of the conditions of forest fire spreading that would make it possible to obtain a detailed picture of the change in the velocity, temperature and component concentration fields with time, and determine as well as the limiting conditions of forest fire propagation is of interest.

Key words: mathematical, forest fire, ignition, discrete analogue, control volume.

1. Introduction

A great deal of work has been done on the theoretical problem of crown forest fire initiation. Crown fires are initiated by convective and radiative heat transfer from surface fires. However, convection is the main heat transfer mechanism (Van Wagner [1]). The proposed in [1] theory depends on three simple crown properties: crown base height, bulk density of forest combustible materials and moisture content of forest fuel. Also, crown fire initiation and hazard have been studied and modeled in details later (Alexander [2]; Van Wagner [3]; Xanthopoulos [4]; Rothermel [5]; Cruz and others [6]; Albini and others [7]; Scott and Reinhardt [8]). The more complete discussion of the problem of crown forest fires is provided by coworkers at Tomsk University (Grishin [9]; Grishin and Perminov [10]; Perminov [11,12]). In particular, a mathematical model of forest fires was obtained by Grishin [9] based on an analysis of known and original experimental data (Grishin [9]; Konev [13], and using concepts and methods from reactive media mechanics. The physical two-phase models used by Morvan and
Dupuy [14,15] may be considered as a continuation and extension of the formulation proposed in [9]. This study gives a two dimensional averaged mathematical setting and method of numerical solution of a problem of a forest fire spread. The boundary-value problem is solved numerically using the method of splitting according to physical processes. It was based on numerical solution of two dimensional Reynolds equations for the description of turbulent flow taking into account for diffusion equations chemical components and equations of energy conservation for gaseous and condensed phases, volume of fraction of condensed phase (dry organic substance, moisture, condensed pyrolysis products, mineral part of forest fuel).

2. Physical and mathematical model

It is assumed that the forest during a forest fire can be modeled as 1) a multi-phase, multistoried, spatially heterogeneous medium; 2) in the fire zone the forest is a porous-dispersed, two-temperature, single-velocity, reactive medium; 3) the forest canopy is supposed to be non-deformed medium (trunks, large branches, small twigs and needles), which affects only the magnitude of the force of resistance in the equation of conservation of momentum in the gas phase, i.e., the medium is assumed to be quasi-solid (almost non-deformable during wind gusts); 4) let there be a so-called “ventilated” forest massif, in which the volume of fractions of condensed forest fuel phases, consisting of dry organic matter, water in liquid state, solid pyrolysis products, and ash, can be neglected compared to the volume fraction of gas phase (components of air and gaseous pyrolysis products); 5) the flow has a developed turbulent nature and molecular transfer is neglected; 6) gaseous phase density doesn’t depend on the pressure because of the low velocities of the flow in comparison with the velocity of the sound. Let the point \(x_1, x_2, x_3 = 0\) is situated at the centre of the surface forest fire source at the height of the roughness level, axis \(0x_1\) directed parallel to the Earth’s surface to the right in the direction of the unperturbed wind speed, axis \(0x_2\) directed perpendicular to \(0x_1\) and axis \(0x_3\) directed upward (Fig. 1).

![Figure 1.](image-url)
Because of the horizontal sizes of forest massif more than height of forest \(- h\), system of equations of general mathematical model of forest fire \([9]\) was integrated between the limits from height of the roughness level - 0 to \(h\). Besides, suppose that

\[
\int_0^h \phi \ dx = \bar{\phi} h
\]

\(\bar{\phi}\) - average value of \(\phi\). The problem formulated above is reduced to a solution of the following system of equations:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho v_j) = Q - (\dot{m}^- - \dot{m}^+) / h, \ j = 1, 2, 3; \quad (1)
\]

\[
\rho \frac{dv_j}{dt} = -\frac{\partial}{\partial x_j} (\rho v_j v'_j) - \rho c_d v_i | \vec{v} | - \rho g_i - Q v_i + (\tau_i^+ - \tau_i^-) / h, \ i = 1, 2, 3; \quad (2)
\]

\[
\rho c_p \frac{dT}{dt} = \frac{\partial}{\partial x_j} (\rho c_p v_j T') + q_5 R_s - \alpha_i (T - T_s) - (q_T^- - q_T^+) / h; \quad (3)
\]

\[
\rho \frac{dc_{\alpha}}{dt} = \frac{\partial}{\partial x_j} (-\rho v_j c'_{\alpha}) + R_{5\alpha} - Q c_{\alpha} + (J_{\alpha}^- - J_{\alpha}^+) / h, \ \alpha = 1, 3; \quad (4)
\]

\[
\frac{\partial}{\partial x_j} \left( \frac{c}{3k} \frac{\partial U_R}{\partial x_j} \right) - k (c U_R - 4\sigma T_S^4) + (q_R^- - q_R^+) / h = 0; \quad (5)
\]

\[
\sum_{i=1}^4 \rho_i c_{pi} \phi_i \frac{dT_S}{dt} = q_3 R_3 - q_2 R_2 + k (c U_R - 4\sigma T_S^4) + \alpha_i (T - T_S); \quad (6)
\]

\[
\rho_1 \frac{\partial \phi_1}{\partial t} = -R_1, \ \rho_2 \frac{\partial \phi_2}{\partial t} = -R_2, \quad (7)
\]

\[
\rho_3 \frac{\partial \phi_3}{\partial t} = \alpha_i R_1 - \frac{M_c}{M_1} R_3, \ \rho_4 \frac{\partial \phi_4}{\partial t} = 0;
\]

\[
\sum_{a=1}^5 c_a = 1, \ p_c = \rho R T \sum_{a=1}^5 \frac{c_a}{M_a}, \ \vec{v} = (v_1, v_2, v_3), \ \vec{g} = (0, 0, g).
\]

The system of equations (1)–(7) must be solved taking into account the initial and boundary conditions

\[
t = 0: \ v_1 = 0, \ v_2 = 0, \ v_3 = 0, \ T = T_e, \ c_a = c_{ae}, \ T_i = T_e, \ \phi_i = \phi_{ie};
\]

\[
t = 0: \ v_1 = 0, \ v_2 = 0, \ v_3 = 0, \ T = T_e, \ T_S = T_e, \ c_a = c_{ae}, \ \phi_i = \phi_{ie}; \quad (8)
\]
\[ x_i = -x_{i_0} : v_1 = V_c, v_2 = 0, \frac{\partial v_3}{\partial x_i} = 0, T = T_e, c_\alpha = c_{\alpha_0}, -\frac{c}{3k} \frac{\partial U_R}{\partial x_i} + cU_R/2 = 0 ; (9) \]

\[ x_i = x_{i_0} : \frac{\partial v_1}{\partial x_i} = 0, \frac{\partial v_2}{\partial x_i} = 0, \frac{\partial v_3}{\partial x_i} = 0, \frac{\partial c_\alpha}{\partial x_i} = 0, \frac{\partial T}{\partial x_i} = 0, -\frac{c}{3k} \frac{\partial U_R}{\partial x_i} + cU_R = 0 ; (10) \]

\[ x_2 = x_{2_0} : \frac{\partial v_1}{\partial x_2} = 0, \frac{\partial v_2}{\partial x_2} = 0, \frac{\partial v_3}{\partial x_2} = 0, \frac{\partial c_\alpha}{\partial x_2} = 0, \frac{\partial T}{\partial x_2} = 0, -\frac{c}{3k} \frac{\partial U_R}{\partial x_2} + cU_R = 0 ; (11) \]

\[ x_2 = x_{2_0} : \frac{\partial v_1}{\partial x_2} = 0, \frac{\partial v_2}{\partial x_2} = 0, \frac{\partial v_3}{\partial x_2} = 0, \frac{\partial c_\alpha}{\partial x_2} = 0, \frac{\partial T}{\partial x_2} = 0, -\frac{c}{3k} \frac{\partial U_R}{\partial x_2} + cU_R = 0 . (12) \]

\[ x_3 = 0 : v_1 = 0, v_2 = 0, \frac{\partial c_\alpha}{\partial x_3} = 0, -\frac{c}{3k} \frac{\partial U_R}{\partial x_3} + cU_R = 0 , \]

\[ v_3 = v_{3_0}, T = T_e \text{ при } |x_1| \leq \Delta, |x_2| \leq \Delta \text{ и } v_3 = 0, T = T_e \text{ при } |x_1| > \Delta, |x_2| > \Delta ; \]

\[ x_3 = x_{3_0} : \frac{\partial v_1}{\partial x_3} = 0, \frac{\partial v_2}{\partial x_3} = 0, \frac{\partial v_3}{\partial x_3} = 0, \frac{\partial c_\alpha}{\partial x_3} = 0, \frac{\partial T}{\partial x_3} = 0, -\frac{c}{3k} \frac{\partial U_R}{\partial x_3} + cU_R = 0 . (14) \]

Here and above \( \frac{d}{dt} \) is the symbol of the total (substantial) derivative; \( \alpha_\psi \) is the coefficient of phase exchange; \( \rho \) - density of gas – dispersed phase, \( t \) - time; \( v_i \) - the velocity components; \( T, T_S \) - temperatures of gas and solid phases, \( U_R \) - density of radiation energy, \( k \) - coefficient of radiation attenuation, \( P \) - pressure; \( c_p \) - constant pressure specific heat of the gas phase, \( \rho_\psi, \rho_i, \varphi_i \) - specific heat, density and volume of fraction of condensed phase (1 – dry organic substance, 2 – moisture, 3 – condensed pyrolysis products, 4 – mineral part of forest fuel), \( R_i \) - the mass rates of chemical reactions, \( q_i \) - thermal effects of chemical reactions; \( k_g, k_S \) - radiation absorption coefficients for gas and condensed phases; \( T_e \) - the ambient temperature; \( c_{\alpha} \) - mass concentrations of \( \alpha \) - component of gas - dispersed medium, index \( \alpha=1,2,3 \), where 1 corresponds to the density of oxygen, 2 - to carbon monoxide \( CO \), 3 - to carbon dioxide and inert components of air; \( R \) - universal gas constant; \( M_\alpha, M_C \) and \( M \) molecular mass of \( \alpha \)-components of the gas phase, carbon and air mixture; \( g \) is the gravity acceleration; \( c_g \) is an empirical coefficient of the resistance of the vegetation, \( s \) is the specific surface of the forest.
fuel in the given forest stratum. In system of equations (1)-(7) are introduced the next designations:

\[
\dot{m} = \rho v_3, \tau_i = -\rho v_i'v_i', J_a = -\rho v_i'c'_a', J_T = -\rho v_i'T'.
\]

Upper indexes “+” and “-” designate values of functions at \( x_3=h \) and \( x_3=0 \) correspondingly. It is assumed that heat and mass exchange of fire front and boundary layer of atmosphere are governed by Newton law and written using the formulas:

\[
(q^- - q^+) / h = -\alpha(T - T_e) / h, \quad (J_a^- - J_a^+) / h = -\alpha(c - c_{ae}) / h c_p.
\]

To define source terms which characterize inflow (outflow of mass) in a volume unit of the gas-dispersed phase, the following formulae were used for the rate of formulation of the gas-dispersed mixture \( m \), outflow of oxygen \( R_{51} \), changing carbon monoxide \( R_{52} \).

\[
Q = (1 - \alpha_e)R_1 + R_2 + \frac{M_c}{M_1}R_3, R_{51} = -R_3 - \frac{M_1}{2M_2}R_5, \quad R_{52} = \nu_g (1 - \alpha_e)R_1 - R_3, R_{53} = 0.
\]

Here \( \nu_g \) – mass fraction of gas combustible products of pyrolysis, \( \alpha_e \) and \( \alpha_5 \) – empirical constants. Reaction rates of these various contributions (pyrolysis, evaporation, combustion of coke and volatile combustible products of pyrolysis) are approximated by Arrhenius laws whose parameters (pre-exponential constant \( k_i \) and activation energy \( E_i \)) are evaluated using data for mathematical models [9,11].

\[
R_1 = k_1\rho\varphi_1 \exp \left(-\frac{E_1}{RT_i}\right), R_2 = k_2\rho\varphi_2 T_i^{-0.5} \exp \left(-\frac{E_2}{RT_i}\right), R_3 = k_3 M_2 \exp \left(-\frac{E_3}{RT_i}\right).
\]

The initial values for volume of fractions of condensed phases are determined using the expressions:

\[
\varphi_{1e} = \frac{d(1-\nu_c)}{\rho_1}, \varphi_{2e} = \frac{Wd}{\rho_2}, \varphi_{3e} = \frac{\alpha_e \varphi_{1e} \rho_1}{\rho_3}
\]

where \( d \) – bulk density for surface layer, \( \nu_c \) – coefficient of ashes of forest fuel, \( W \) – forest fuel moisture content.
It is supposed that the optical properties of a medium are independent of radiation wavelength (the assumption that the medium is “grey”), and the so-called diffusion approximation for radiation flux density were used for a mathematical description of radiation transport during forest fires.

To close the system (1)–(7), the components of the tensor of turbulent stresses, and the turbulent heat and mass fluxes are determined using the local-equilibrium model of turbulence (Grishin, [9]). The system of equations (1)–(7) contains terms associated with turbulent diffusion, thermal conduction, and convection, and needs to be closed. The components of the tensor of turbulent stresses \( \rho \nu_j \nu'_j \), as well as the turbulent fluxes of heat and mass \( \rho \nu_j c_p T' \), \( \rho \nu'_j c'_a \) are written in terms of the gradients of the average flow properties using the formulas

\[
- \rho \nu'_j \nu_j = \mu_t \left( \frac{\partial \nu_j}{\partial x_j} + \frac{\partial \nu_j}{\partial x_i} \right) - \frac{2}{3} K \delta_{ij},
\]

\[
- \rho \nu'_j c_p T' = \lambda_t \frac{\partial T}{\partial x_j},
\]

\[
- \rho \nu'_j c'_a = \rho D_t \frac{\partial c'_a}{\partial x_j},
\]

\[
\lambda_t = \mu_t c_p / Pr_t, \quad \rho D_t = \mu_t / Sc_t, \quad \mu_t = c_\mu \rho K^2 / \varepsilon,
\]

where \( \mu_t, \lambda_t, D_t \) are the coefficients of turbulent viscosity, thermal conductivity, and diffusion, respectively; \( Pr_t, Sc_t \) are the turbulent Prandtl and Schmidt numbers, which were assumed to be equal to 1. In dimensional form, the coefficient of dynamic turbulent viscosity is determined using local equilibrium model of turbulence [9]. The thermodynamic, thermophysical and structural characteristics correspond to the forest fuels in the canopy of a different (for example pine [9,11,13]) type of forest. The system of equations (1)–(7) must be solved taking into account the initial and boundary conditions. The thermodynamic, thermophysical and structural characteristics correspond to the forest fuels in the canopy of a different type of forest; for example, pine forest (Grishin, Perminov [11]).

3. Numerical methods and results

The boundary-value problem (1)–(13) is solved numerically using the method of splitting according to physical processes (Perminov [11]). In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions was calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting was then integrated. A discrete analog was obtained by means of the control volume method using the SIMPLE like algorithm (Patankar [16]). The accuracy of the program was checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions were substituted in (1)–(7) and the closure of the equations were calculated. This was then treated as the source in each equation. Next, with the aid of the algorithm described above,
the values of the functions used were inferred with an accuracy of not less than 1%. The effect of the dimensions of the control volumes on the solution was studied by diminishing them. The time step was selected automatically. Fields of temperature, velocity, component mass fractions, and volume fractions of phases were obtained numerically. The distribution of basic functions shows that the process of crown forest fire initiation goes through the next stages. The first stage is related to increasing maximum temperature in the ground cover with the result that a surface fire source appears. At this process stage over the fire source a thermal wind is formed a zone of heated forest fire pyrolysis products which are mixed with air, float up and penetrate into the crowns of trees. As a result, forest fuels in the tree crowns are heated, moisture evaporates and gaseous and dispersed pyrolysis products are generated. Ignition of gaseous pyrolysis products of the ground cover occurs at the next stage, and that of gaseous pyrolysis products in the forest canopy occurs at the last stage. As a result of heating of forest fuel elements of crown, moisture evaporates, and pyrolysis occurs accompanied by the release of gaseous products, which then ignite and burn away in the forest canopy. At the moment of ignition the gas combustible products of pyrolysis burns away, and the concentration of oxygen is rapidly reduced. The temperatures of both phases reach a maximum value at the point of ignition. The ignition processes is of a gas-phase nature. Note also that the transfer of energy from the fire source takes place due to radiation; the value of radiation heat flux density is small compared to that of the convective heat flux. In the vicinity of the source of heat and mass release, heated air masses and products of pyrolysis and combustion float up. At $V_e \neq 0$, the wind field in the forest canopy interacts with the gas-jet obstacle that forms from the surface forest fire source and from the ignited forest canopy base and burn away in the forest canopy. In the vicinity of the source of heat and mass release, heated air masses and products of pyrolysis and combustion float up. At $V_e \neq 0$, the wind field in the forest canopy interacts with the gas-jet obstacle that forms from the surface forest fire source and from the ignited forest canopy base. On the windward side the movement of the air flowing past the ignition region accelerates. Figures 2, 3 present the distribution of temperature $\bar{T} (\bar{T} = T / T_e, T_e = 300 \, K)$ (1 - 5., 2 - 4.5, 3 - 4, 4 - 3.5) for gas phase. Figures 4-5 present mass concentrations of oxygen $\bar{c}_1 (1 - 0.5, 2 - 0.7, 3 - 0.8)$ and volatile combustible products of pyrolysis $\bar{c}_2$ concentrations (1 - 0.05, 2- 0.1, 3 - 0.5) ($\bar{c}_a = c_a / c_{le}, c_{le} = 0.23$ ) for wind velocity $V_e = 10 \, m/s$: and a) $t=3 \, sec.$, b) $t=5 \, sec$. We can note that the isotherms is moved in the forest canopy and deformed by the action of wind. Similarly, the fields of component concentrations are deformed. It is concluded that the forest fire begins to spread.
4. Conclusion

The results of calculation give an opportunity to evaluate critical condition of the forest fire spread, which allows applying the given model for preventing fires. It overestimates the velocity of crown forest fire spread that depends on crown properties: bulk density, moisture content of forest fuel and etc. The model proposed there give a detailed picture of the change in the velocity, temperature and component concentration fields with time, and determine as well as the influence of different conditions on the crown forest fire initiation. The results obtained agree with the laws of physics and experimental data (Grishin [9]; Konev [13]). From an analysis of calculations and experimental data it was found that for the cases in question the minimum total incendiary heat pulse is 2600 kJ/m² (Grishin [9]). Calculations demonstrated that the value of the radiant heat flux for both problems is considerably less than the convective one, therefore radiation has a weak effect on local and integral characteristics of the problem discussed above. The results obtained agree with the laws of physics and experimental data.

5. References


Methods for Accurate Motion Tracking and Motion Analysis of the Beating Heart Wall

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Key words: Cardiac motion tracking, surface mesh generation, Gordon surface, registration, thin-plate spline transformation, radial basis function

Extended Abstract

1. Introduction

During the past decades, much effort has been devoted to achieving an improved understanding of the contractions of the heart. Numerous methods have been developed and applied to capture specific data from medical images which are then used to describe the motion of the heart. However, the accuracy of these methods is somewhat restricted. Thus, we aimed at an improved method of motion tracking. The pivotal point of our development efforts is the full exploitation of the synergy of the two imaging modalities, viz. cardiac CT and biplane cineangiography, for an accurate quantitative assessment of the regional variations of ventricular motility and to monitor the improvements during therapy. The extraordinarily high spatial and temporal resolution of biplane cineangiography facilitates accurate investigations of the ventricular
motility, which, however, are restricted to the regions of the left ventricular surface that are covered by the coronary arteries. Several methods to extend the tracking of the ventricular motion to the entire epicardial surface have been described in the literature. However, the shape of the epicardial surface was only an assumed one and thus not patient-specific. Our multimodal imaging approach to motion analysis is based on a retrospectively ECG-gated cardiac CT data set at the end of the diastole and a biplane cineangiogram of a particular patient. The utilization of an efficient combination of both imaging modalities enables us to exploit their specific favorable characteristics of both of them and to overcome their respective limitations. In particular, we fully take advantage of

- the capacity of cardiac CT to retrospectively reconstruct a highly-accurate 3D image of the epicardial surface at the end of the diastole and
- the excellent motion tracking capability of biplane angiography, in which there is no significant motion blur.

Our techniques comprise several image processing steps, such as segmentation, registration. In these techniques, the realization of specific transformations. moreover, mesh generation procedures are carried out. This paper is confined to the generation of a deformable mesh to represent the geometry of the outer surface of the myocardium of the left ventricle and its deformations during the cardiac cycle which are highly complex and difficult to describe quantitatively. Our long-term goal, however, is to exploit our mesh generation approach to develop methods to elucidate the spatial and temporal changes of strain and stress within the myocardium of the rapidly moving heart.

2. Image Processing and Mesh Generation Tasks

In the CT imagery for the end-diastolic position, we carry out a segmentation of the surface of the myocardium (cf. Figure 1). In each transaxial slice, we define manually an appropriate number of vertices and a spline (NURBS) curve which approximates these vertices. These splines are subdivided into equal increments. The subdivision points of all transaxial slices are regarded as nodes of a surface mesh. The nodes belonging to each transaxial slice are connected to each other with an interpolating spline (NURBS curve) which is called transversal contour curve. We thus obtain an array of NURBS curves as transversal
Analysis of the Beating Heart Wall

contour curves of the outer surface of the myocardium. We also compute an array of longitudinal interpolating NURBS curves, each of which passes through corresponding points in all slices. These two arrays of NURBS curves constitute a surface mesh which enables us to achieve a preliminary visual representation of the heart wall (myocardium, left ventricle) for the end-diastolic position in the form of a wireframe model.

3. Fig. 1. Medical imagery relating to end-diastolic phase: (a) transaxial slice of CT with manually segmented ventricular wall; (b)+(c) biplane angiograms relating to end-diastolic frame of cineangiography

The points corresponding to the entire surface together with well chosen landmarks, constitute the domains of landmark-based thin-plate spline registration. Thin plate spline transformations are not only instrumental for the accomplishment of our image-registration but also for our motion tracking tasks. In the subsequent description of our mathematical concepts and techniques for the analysis of the heart wall motion, we assume the availability of the following for each patient:

• the above-described surface mesh calculated from three-dimensional CT describing the morphology at the end of the diastole, and
• A series of SEATs (skeletonised epicardial artery trees) which have been derived from biplane cineangiograms with the methods which will be described in the full paper. We have developed a method to achieve a largely automatic segmentation of the epicardial arteries in angiograms. In the first stage of our approach: we use a multi-scale Hessian filter to separate the tubular structure of the arteries from the other structures in the image, then we carry out a conversion of these tubular structures into a binary mask, and finally we apply a thinning filter to obtain an initial
representation of a skeletonised arterial tree. The second stage of our efforts comprises a scan-line-based border detection procedure for an accurate segmentation of the arteries, the calculation of the centre lines in the angiograms, and the three-dimensional reconstruction of these centre lines resulting in space curves which show a tree-like structure. This tree-like arrangement of space curves is regarded as the final version of the skeletonised epicardial artery tree. It will serve as the basis for our registration and motion-tracking tasks. For further details of our segmentation method, please refer to [1].

**Registration Tasks.** As mentioned above, we carry out a landmark-based image registration with the help of our two imaging modalities, cardiac CT and biplane cineangiography. In particular, our end-diastolic three-dimensional CT data set is correlated with the end-diastolic representation of the heart in biplane cineangiography, our reference image modality. The cineangiographic imagery comprises a relatively large number of frames. One frame refers to the end-diastolic position of the heart. In handling the registration task, we refer to this frame and carry out a landmark-based thin-plate spline transformation.

**Motion Tracking Tasks.** Our motion-tracking analyses are also based on a number of thin-plate spline transformations (ca. 60). In the following, we assume that the SEATs are three-dimensionally reconstructed for all frames which are linearly ordered in time). The individual transformations thereby relate to two consecutive frames. The tracking procedure starts with the end-diastolic frame and thus comprises about 60 individual TPS transformations. Some results of our registration and motion-tracking procedures can be seen in Figures 2 and 3.
Analysis of the Beating Heart Wall

Fig. 2. Image Registration: (a) ventricular surface after segmentation in CT, point landmarks are indicated in magenta; (b) ventricular surface after registration to the SEAT belonging to the end-diastolic phase, point landmarks are indicated in cyan.

Fig. 3. Comparison between ventricular surface during end-diastolic phase and at the end of the systole: (a) end-diastolic phase, point landmarks are indicated in cyan; (b) end-systolic phase, point landmarks are indicated in cyan.
3. Analysis and Visualization Aspects

At present, we are elaborating new visualisation and analysis techniques for an accurate quantitative assessment of the regional variations of heart wall motility. From each and every pint of the heart surface, we will be able to draw trajectories which refer to the entire contraction phase of the myocardium. The aforementioned corresponding nodes subdivide the trajectory into equal time intervals. For each and every subdivision point which follows the selected node (material point) in the end-diastolic frame, we plan to compute and to visualize the velocity and acceleration vectors and their variations. What is even more important, several characteristic quantities of surface deformation kinematics, such as displacement tensors describing surface deformations, surface strain tensors, surface strain rate tensors, surface curvature tensors, and, moreover, tensors of changes of curvature. The underlying concepts of the above tensor quantities are based on differential geometry and thus permit a local analysis of the deformation behaviour. For this reason, these tensor quantities are well suited to reveal the regional variations of the deformation behavior of the heart wall. We plan to derive parameters of diagnosis from these tensors. Moreover, we aim at a visualization of the tensor quantities by using standard methods which we will adapt to our problem area.

4. References


Acknowledgements

The work described in this paper is partially supported by the "Austrian GRID" project, funded by the Austrian BMBWK (Federal Ministry for Education, Science and Culture) under contract GZ 4003/2-VI/4c/2004.
Mathematical Modelling of the Biological Pest Control of the Sugarcane Borer

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Abstract

In this paper, we propose a simple mathematical model of interaction between the sugarcane borer \textit{(Diatraea saccharalis)} and its egg parasitoid \textit{Trichogramma galloi}. In this model the sugarcane borer is represented by the egg e larval stages, and the parasitoid is considered in term of the parasitized eggs. Linear feedback control strategy is proposed to indicate how the natural enemies should be introduced in the environment.

\textit{Key words: mathematical modelling, biological control, sugarcane borer, egg parasitoid}

\textit{MSC2000: AMS 92D25, 34H05, 49N90}

1. Introduction

The increase in world demand for ethanol brings an increase of the sugarcane planted in Brazil. The sugarcane borer \textit{Diatraea saccharalis} is reported to be the most important sugarcane pest in south-east region of Brazil [1]. The sugarcane borer builds internal galleries in the sugarcane plants causing direct damages that result in apical bud death, weight loss and atrophy. Indirect damages occur when there is contamination by yeasts that cause red rot in the stalks, either causing contamination or inverting the sugar, increasing yield loss in both sugar and alcohol [2]. It is known that for each 1\% of plant infestation by pests the industries lose 0.2\% of the ethanol production, that is, in average 25 liters per ha.

One of challenges of the improvements in the farming and harvesting of cane is the biological pest control. A good strategy of biological pest control can increase the ethanol production. Biological control is the use of living organisms
to suppress pest populations, making them less abundant and thus less damaging
than they would otherwise be [3]. Pests are species that interfere with human
activity or cause injury, loss, or irritation to a crop, stored product, animal, or
people. One of the main goals of the pest control is to maintain the density of the
pest population in an equilibrium level below economic damages. Natural
enemies play an important role in limiting potential pest populations. Flooding
agroecosystems with parasitoid insects is very effective in lowering the
abundance of crop pests. Thus, parasitoids are commonly reared in
laboratories and periodically liberated in high-density populations as biological
control agents of crop pests [4]. Cotesia flavipes is important wasp parasitoid of
the sugarcane borer larvae in Brazil [1]. In spite of the biological control of Diatraea saccharalis by Cotesia flavipes is considered successful in Brazil, there
are some areas where Cotesia flavipes has not the good control. The using of the
egg parasitoid Trichogramma galloi is considered an interesting option in this
case [5].

Thomas and Willis [6] state that introduction of biological agents against weeds
and insects is a substantially effective control is less than 40% of the cases. In
order for biological control to succeed, the dynamics of the pest and its enemy
populations have to be understood. Mathematical modeling is an important tool
used in studying agricultural problems. Mathematical modeling applied to the
problems of biological pest control allows a qualitative and quantitative
evaluation of the impact between the pest and its natural enemy populations. The
application of host-parasitoid models for biological control were reviewed in [7].

In this paper, we propose a simple mathematical model of interaction between the
sugarcane borer (Diatraea saccharalis) and its egg parasitoid Trichogramma galloi. In this model the sugarcane borer is represented by the egg e larval stages,
and the parasitoid is considered in term of the parasitized eggs. Linear feedback
control strategy is proposed to indicate how the natural enemies should be
introduced in the environment.

2. Mathematical model of interactions between the sugarcane
borer and its parasitoid

Consider two of main stages of development of the sugarcane borer Diatraea
saccharalis – the egg e larval stages. We assume that there exists only an egg
parasitoid (Trichogramma galloi) in a common environment. Assuming
furthermore logistic growth for the egg population we can propose the following
mathematical model that describes interactions between the sugarcane borer and
its parasitoid:
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\[
\frac{dx_1}{dt} = \beta (1 - \frac{x_1}{K}) x_1 - m_1 x_1 - n_1 x_1 - \alpha x_1 x_2
\]
\[
\frac{dx_2}{dt} = \alpha x_1 x_2 - m_2 x_2 - n_2 x_2
\]
\[
\frac{dx_3}{dt} = n_1 x_1 - m_3 x_3 - n_3 x_3
\]

were \(x_1\) is the egg density of the sugarcane borer, \(x_2\) is the density of eggs parasitized by Trichogramma galloi and \(x_3\) is the larvae density of the sugarcane borer; \(\beta\) is the net reproduction rate; \(K\) is the carrying capacity the environment; \(m_1\), \(m_2\) and \(m_3\) are mortality rates of the egg, parasitized egg and larvae populations; \(n_1\) is the fraction of the eggs from which the larvae emerge at time \(t\); \(n_2\) is the fraction of the parasitized eggs from which the adult parasitoids emerge at time \(t\); \(n_3\) is the fraction of the larvae population which moults into pupal stage at time \(t\); \(\alpha\) is the rate of parasitism.

3. Equilibrium points and stability

The equilibrium points can be obtained by setting to zero the right hand sides of (1):

\[
x_1^* (\beta - \frac{\beta}{K} x_1^* - m_1 - n_1 - \alpha x_2^*) = 0
\]
\[
x_2^* (\alpha x_1^* - m_2 - n_2) = 0
\]
\[
n_1 x_1^* - x_3^* (m_3 + n_3) = 0
\]

We obtain therefore the following points:

\[
P_1 = (0,0,0)
\]
\[
P_2 = \left( \frac{K}{\beta} (\beta - m_1 - n_1), 0, \frac{n_1 K (\beta - m_1 - n_1)}{\beta (m_3 + n_3)} \right)
\]
\[
P_3 = \left( \frac{m_2 + n_2}{\alpha}, \frac{\alpha - \frac{\beta}{\alpha^2 K} (m_2 + n_2) - m_1 + n_1}{\alpha}, \frac{n_1 (m_2 + n_2)}{\alpha (m_3 + n_3)} \right)
\]

For \(P_2\) the condition

\[
\beta > m_1 + n_1
\]
ensures the nonnegativity of the larvae population.

For $P_3$ the condition of the nonnegativity of the parasitized egg population is

$$\beta > m_i + n_i + \frac{\beta}{\alpha K}(m_2 + n_2)$$

(5)

Let us consider the Jacobian matrix of the system (1)

$$J = \begin{bmatrix}
\beta - \frac{2\beta}{K} x_1 - m_i - n_i - \alpha x_2 - \alpha x_i^* & -\alpha x_i^* & 0 \\
\alpha x_2 & \alpha x_1 - m_2 - n_2 & 0 \\
n_1 & 0 & -m_3 - n_3
\end{bmatrix}$$

(6)

**Stability analysis of the equilibrium point $P_1$**

In this case the Jacobian matrix assumes the form

$$J = \begin{bmatrix}
\beta - m_i - n_i & 0 & 0 \\
0 & -m_2 - n_2 & 0 \\
n_1 & 0 & -m_3 - n_3
\end{bmatrix}$$

(7)

from which the eigenvalues are easily found to be

$$\lambda_1 = \beta - m_i - n_i, \ \lambda_2 = -m_2 - n_2, \ \lambda_3 = -m_3 - n_3.$$  

It follows then that equilibrium point $P_1$ is stable if

$$\beta < m_i + n_i.$$  

(8)

**Stability analysis of the equilibrium point $P_2$**

In this case the Jacobian matrix assumes the form

$$J = \begin{bmatrix}
-\frac{\beta}{K} x_1 - \alpha x_i^* & -\alpha x_i^* & 0 \\
0 & \alpha x_1^* - m_2 - n_2 & 0 \\
n_1 & 0 & -m_3 - n_3
\end{bmatrix}$$

and the eigenvalues are
\[ \lambda_1 = -(\beta - m_1 - n_1), \quad \lambda_2 = \frac{\alpha K}{\beta} (\beta - m_1 - n_1) - m_2 - n_2, \quad \lambda_3 = -m_3 - n_3. \]

It follows then that equilibrium point \( P_2 \) is stable if

\[ m_1 + n_1 < \beta < m_1 + n_1 + \frac{\beta}{\alpha K} (m_2 + n_2). \] (9)

**Stability analysis of the equilibrium point \( P_3 \)**

In this case the Jacobian matrix has the following form

\[
J = \begin{bmatrix}
-\frac{\beta}{K} x_1^* & -\alpha x_1^* & 0 \\
\frac{\alpha x_2^*}{K} & \alpha x_1^* - m_2 - n_2 & 0 \\
0 & 0 & -m_3 - n_3
\end{bmatrix}
\] (10)

with the characteristic equation

\[
(\lambda^2 + a_1 \lambda + a_2)(\lambda + a_3) = 0
\] (11)

where the coefficients are given by

\[
a_1 = \frac{\beta(m_2 + n_2)}{\alpha K} > 0
\]

\[
a_2 = \alpha x_1^* x_2^*
\]

\[
a_3 = m_3 + n_3 > 0
\]

According to Routh-Hurwitz condition the eigenvalues of the equation \( \lambda^2 + a_1 \lambda + a_2 = 0 \) have negative real parts if \( a_1 > 0 \) and \( a_2 > 0 \). The coefficient \( a_2 > 0 \) if \( x_1^* > 0 \), i.e. if the condition (5) is satisfied. It follows then that equilibrium point \( P_3 \) is stable if

\[
\beta > m_1 + n_1 + \frac{\beta}{\alpha K} (m_2 + n_2)
\] (12)
4. Numerical simulations of the host-parasitoid interactions without control

For numerical simulations of interactions between the sugarcane borer and its parasitoid were used the following values of model coefficients: \( n_1 = 0.1, \quad n_2 = 0.1, \quad n_3 = 0.02439, \quad m_1 = 0.03566, \quad m_2 = 0.03566, \quad m_3 = 0.00256, \quad K = 25000 \). These values were obtained based on data published about the use of the egg parasitoid *Trichogramma galli* against the sugarcane borer *Diatraea saccharalis* these [1], [5], [8].

The value of the parameter \( \beta \) is important for determination the stability of the equilibrium points. When \( \beta \) satisfies the condition \( \beta < m_1 + n_1 \), the equilibrium \( P^* \) is stable and other points are unstable. Fig.1 shows that for \( \beta = 0.13 \) and \( \alpha = 0.0001723 \) all populations go to extinction in this case.

![Fig. 1. Evolution of the egg, parasitized egg and larvae populations for \( \beta = 0.13 \) and \( \alpha = 0.0001723 \)](image-url)

When \( \beta \) satisfies the condition (9):
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\[ m_i + n_i < \beta < m_i + n_i + \frac{\beta}{\alpha K}(m_i + n_i) \]

the equilibrium \( P_2 \) is stable and other points are unstable. In this case, the parasitized egg population goes to extinction, and the egg and larvae populations go to positive equilibrium levels. This case is shown in Fig. 2 for \( \beta = 0.139 \) and \( \alpha = 0.0001723 \)

![Graph showing population evolution](image)

**Fig. 2.** Evolution of the egg, parasitized egg and larvae populations for \( \beta = 0.139 \) and \( \alpha = 0.0001723 \)

When \( \beta \) satisfies the condition (12):

\[ \beta > m_i + n_i + \frac{\beta}{\alpha K}(m_i + n_i) \]

the positive equilibrium point \( P_3 \) is stable and the populations coexist in a common environment. Fig. 3 shows the population oscillations for \( \beta = 0.1908 \) and \( \alpha = 0.0001723 \).
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One can see from Fig. 3 that the sugarcane borer larvae density $x_i$ takes on values more than the pest density threshold level $x_d = 2500$ numbers/ha [1]. Densities above this level cause economic damages the sugarcane crops. In this case, it is necessary to apply the biological control.

![Figure 3: Evolution of the egg, parasitized egg and larvae populations for $\beta = 0.1908$ and $\alpha = 0.0001723$](image)

5. **Numerical simulations of the inundative biological control**

The main objective of the biological pest control is to maintain the pest population in an equilibrium level below the economic injury level. Thus, parasitoids and predators are commonly reared in laboratories and periodically liberated in high-density populations (inundative biological control) when the pest population reaches a control level [4]. Mathematically, the inundative control can be interpreted by impulsive control function $U$ that produces the discontinuous augmentation of the natural enemy population (parasitized egg). The Fig. 4 shows the inundative control applied in initial moment by introduction 20000 parasitoids/ha. From Fig. 4 one can see that the inundative biological control,
applied in initial moment by introduction 2000 parasitized egg /ha, maintain the pest population below the value \( x_i = 2500 \) pests/ha only 88 days. After this period, it is necessary to apply the control again. Another negative factor of the inundative biological control is the high amplitudes of oscillation.

![Graph showing the control application](image)

**Fig.4. Inundative control application by introduction 2000 parasitoids/ha**

### 6. Optimization of the biological control

We hope to formulate the pest control strategy of the sugarcane borer through the parasitized egg introduction in a common environment. This control must move the controlled system to the steady state in that the larvae density is stabilized without causing economic damages, and that the parasitized egg population is stabilized at the level enough to control the pests.

The dynamic system (1) with control has the following form:
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\[ \frac{dx_i}{dt} = \beta (1 - \frac{x_i}{K}) x_i - m_i x_i - n_i x_i - \alpha x_i x_2 \]
\[ \frac{dx_2}{dt} = \alpha x_1 x_2 - m_2 x_2 - n_2 x_2 + U \]
\[ \frac{dx_3}{dt} = n_i x_i - m_3 x_3 - n_i x_3 \]  

(13)

The goal of the pest control strategy maintains the larvae population at level \( x^*_3 = x^*_d < x^*_c \) by control \( u^* \), where \( x^*_d \) is a designed pest population density below economic injury level. The desired positive steady state with control satisfies the following equations

\[ x^*_1 (\beta - \frac{\beta x^*_1}{K} - m_i - n_i - \alpha x^*_2) = 0 \]
\[ x^*_2 (\alpha x^*_1 - m_2 - n_2) + u^* = 0 \]
\[ n_i x^*_1 - x^*_3 (m_3 + n_3) = 0 \]  

(14)

From the third equation of the system (14) we obtain the egg density value which is necessary to maintain the larvae population at level \( x^*_3 = x^*_d \):

\[ x^*_1 = \frac{(m_i + n_i) x^*_1}{n_i} \]  

(15)

From the first equation of the system (14) we obtain the parasitized egg density value which is necessary to maintain the larvae population at level \( x^*_3 = x^*_d \):

\[ x^*_2 = \frac{\beta (1 - x^*_1 / K) - m_i - n_i}{\alpha} \]  

(16)

From the second equation of the system (14) we obtain the value of the control \( u^* \):

\[ u^* = -x^*_2 (\alpha x^*_1 - m_2 - n_2) \]  

(17)

In the general case, the desired steady-state \( (x^*_1, x^*_2, x^*_3) \) of the system (13) controlled by \( u^* \) can be unstable. In this case the feedback control \( u \) can be made so that the desired state becomes asymptotically stable.

Defining the following new variables
and substituting (18) into (13) and admitting (14), we get the following error system:

\[ \dot{y} = Ay + h(y) + Bu \]  

(19)

where the matrices \( A \) and \( B \) are

\[
A = \begin{bmatrix}
\beta \frac{2\beta x_i^*}{K} - m_i - n_i - \alpha x_2^* & -\alpha x_i^* & 0 \\
\alpha x_2^* & \alpha x_i^* - m_2 - n_2 & 0 \\
n_1 & 0 & -m_3 - n_3
\end{bmatrix}, 
B = \begin{bmatrix}
0 \\
1 \\
0
\end{bmatrix}
\]  

(20)

and the vector \( h(y) \) has a form:

\[
h(y) = \begin{bmatrix}
-\beta y_i^* - \alpha y_1 y_2 \\
\alpha y_1 y_2 \\
0
\end{bmatrix}
\]  

(21)

The feedback control \( u \) can be determinate applying the following theorem.

**Theorem** [9]. If there exist constant matrices \( Q \) and \( R \), positive definite, being \( Q \) symmetric, such as that the function

\[
l(y) = y^T Q y - h^T (y) P y - y^T Ph(y),
\]  

(22)

is positive definite then the linear feedback control

\[
u = -R^{-1} B^T P(t) y
\]  

(23)

is optimal, in order to transfer the nonlinear system (19) from an initial to final state

\[
y(\infty) = 0
\]  

(24)

minimizing the functional
MATHEMATICAL MODELLING OF THE BIOLOGICAL PEST CONTROL

\[ J = \int_0^\infty [l(y) + u^T R u] dt \]  \hspace{1cm} (25)

where \( P \) the symmetric, positive definite matrix, is the solution of the matrix algebraic Riccati equation

\[ PA + A^T P - PB R^{-1} B^T P + Q = 0 \]  \hspace{1cm} (26)

In addition, with the feedback control (23), there exists a neighborhood \( \Gamma_0 \subset \Gamma \), \( \Gamma \subset \mathbb{R}^n \), of the origin such that if \( y_0 \in \Gamma_0 \), the solution \( y(t) = 0, \ t \geq 0, \) of the controlled system (19) is locally asymptotically stable, and \( J_{\min} = y_0^T P(0) y_0. \)

Finally, if \( \Gamma = \mathbb{R}^n \) then the solution \( y(t) = 0, \ t \geq 0, \) of the controlled system (19) is globally asymptotically stable.

From theorem one can conclude that if the function (22) is positive definite then the error dynamical system (19) controlled by linear feedback control \( u \) is asymptotically stable, and hence, the system (13), controlled by

\[ U = u^* + u, \]  \hspace{1cm} (27)

tends to the desired steady state \((x_1^*, x_2^*, x_3^*).\)

We illustrate the application of the optimal pest control strategy (27) on the agroecosystem which consisting of sugarcane borer and its parasitoid. We will stabilize the ecosystem (13) at the desired steady state \( x_1^* = 549.2 \) egg/ha, \( x_2^* = 293.67 \) parasitized egg/ha, \( x_3^* = x_4 = 2000 \) larvae/ha. The values of \( x_1^* \) and \( x_2^* \) were calculated from (15) and (16), respectively. In this case, \( u^* = 12.15 \) parasitized egg/day, and the matrices \( A \) and \( B \) have the following form

\[
A = \begin{bmatrix}
-0.0042 & -0.0946 & 0 \\
0.0506 & -0.0414 & 0 \\
0.1 & 0 & -0.0275
\end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}
\]

Choosing

\[
Q = \begin{bmatrix}
0.01 & 0 & 0 \\
0 & 0.01 & 0 \\
0 & 0 & 0.01
\end{bmatrix}, \quad R = [1]
\]

we obtain
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\[ P = \begin{bmatrix} 0.3045 & -0.134 & 0.1202 \\ -0.134 & 0.1511 & -0.0517 \\ 0.1202 & -0.0517 & 0.1334 \end{bmatrix} \]

from the solution of the Riccati equation (26).

Finally, we can conclude that the optimal strategy has the following form:

\[ U = 12.15 + 0.134 y_1 - 0.1511 y_2 + 0.0517 y_3 \]  \hspace{1cm} (28)

The optimal control (28) is designed to drive the trajectory of the system (13) to desired steady state \((x_1^*, x_2^*, x_3^*)\), as shown in Fig. 5. Dynamics of the optimal control function (28) is presented in Fig. 6.

![Fig. 5. Evolution of the dynamic system (13) with optimal control](image-url)
Numerical simulations showed that the function \( l(y) \), defined by (22), was positive for all considered initial condition values, but it is necessary more investigations to prove if this function is positive definite at a positive space.

Fig. 6 shows that the great amount of parasitoid have to be introduced in initial days. This fact suggests that the proposed feedback control strategy can be integrated into existing biological control technologies, combining the feedback control with the traditional inundative pest control. This control strategy directs the ecosystem to the stable equilibrium point which is reached at 40 days. After this period, according above proposed control strategy, it is necessary to apply the constant control \( u^* = 12.15 \) parasitized egg/day. It is not economically advantageous to use this constant control. In agricultural practice this control can be substituted by periodic releases of a small population of natural enemies. It is necessary more studies to justify this substitution.
Acknowledgments
The authors thank Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) and Conselho Nacional de Pesquisas (CNPq) for the financial supports on this research.

References
Modeling of neutron activation process with Americium Beryllium source. Application to the activation of fluorspar samples

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Abstract

This paper shows the mathematical models which represent the phenomena that occur in a neutron activation process. These phenomena are, on the one hand, the neutron flux decreases with the distance between the neutron source and the sample, and on the other hand, the attenuation of the gamma rays originating from the sample activated on its way to the detector position. The development of the mathematical model has been divided into two parts. Firstly, the phenomena are shown separately. Secondly, the phenomena are shown together. Finally, this model is fitted to the neutron activation of a fluorspar sample, and the influence of the two phenomena as defined above can be seen.

Keywords: nuclear activation, deferred gamma rays, mathematical model, fluorspar.

1 Introduction

Neutron activation is a process in which an atom emits a characteristic radiation when it is excited by a neutron. This system can be used to determine the presence of certain elements in a sample.

Neutron activation analysis (NAA) was discovered in 1936 by Hevesy and Levi, who found that samples containing certain rare earth elements became highly radioactive after exposure to a source of neutrons. This observation led to the use of induced radioactivity for the identification of elements.

In the last several decades, this technique has been applied to determine a great variety of elements in many disciplines. These include environmental science as well as, biological, geological, and material science.

The basic elements used in neutron activation are:
an radioactive source that allows the irradiation of a sample by neutrons and,

a radiation detector that reads gamma radiation emitted by a sample during the decaying of the radioactive products. This radiation is produced in a given time and is characterized by the energy and time during which it occurs, and is characteristic of each element.

A neutron activation process is characterized by two phenomena that occur:

- the one during radiation which supposes that the neutron flux decreases with the distance between the neutron source and the sample [1].

- with the radiation reading, that implies the attenuation of the gamma rays originated in the decay of $^{16}$N traversing the sample to the detector position. This attenuation is exponentially dependent on a characteristic attenuation coefficient of the sample [2].

2 Definition mathematical models

In the procedure used, the base of the container sample is located at a distance “a” of the irradiation position (source), and a distance “b” of the reading position (detector), Figure 1.

On the one hand, neutrons emerging from the source after they traverse the space “a” (air) arrive at the sample where they do or do not interact with the sample, resulting in the activation of the fluorine atom. Neutron flux is reduced with the distance from the source.

On the other hand, the produced gamma rays traverse the sample to the detector position, and are attenuated as they travel.
2.1 First model

In the first model, we refer specifically to the phenomenon of the reduction of the neutron flux with distance from the source. It is supposed that the activation of a differential element $dx$ of the sample only depends on the distance $(x+a)$ in the direction $x$ to the source, and that the dependency ratio is inversely proportional to the square of the distance of the differential element at the center of the source. Consequently, it is assumed that gamma rays are not attenuated by distance.

In this process, we have observed the following proportionalities (Figure 2):

- Counts from the sample and reading at the detector $C_m$ are proportional to the counts $C_p$ produced by the sample. The proportionality constant depends on the efficiency of the detector.

- Counts produced in the sample $C_p$ are the integral from $x=0$ to $x=l$ of the differential counts $dC_{px}$ in an element of base $S$ and height $dx$.

- The differential of counts produced $dC_{px}$ at the differential element of height $dx$ is proportional to the number of excited atoms in the differential element ($dN_{ax}$).

- The number of excited atoms $dN_{ax}$ depends on neutron flux and the number of fluorine atoms $dN_{fx}$ at that point.

- The neutron flux $\Phi_{nx}$ is inversely proportional to the square of the distance between the point and the source $(x+a)$.
The number of fluorine atoms in a sample point $dN_{fx}$ is directly proportional to the product of the grade $y$ and the mass $dm$ of differential element.

The mass $dm$ depends on the volume of differential element $dV$ and the density $\rho_m$.

The volume $dV$ is defined by the section of the sample $S$ and by the height of differential element $dx$.

The density of the sample $\rho_m$ is in relation to the density of the fluorspar $\rho_1$, the sterile $\rho_2$, and the sample grade in per unit.

$$dN_{fx} = k_2 \times y \times dm$$

$$dm = dV \times \rho_m$$

$$dV = S \times dx$$

$$\rho_m = \rho_1 \times y + \rho_2 \times (1 - y)$$

Figure 2. Expressions used in the proportionalities
Substituting these terms:
\[ C_m = k_1 \times k_2 \times k_3 \times k_4 \times k_5 \times (P \times y + Q \times y^2) \times \int_0^l \frac{dx}{(x + a)^2} \]

Where,
\[ Q = S \times (\rho_1 - \rho_2) \]

And,
\[ P = S \times \rho_2 \]

The parameters \( Q \) and \( P \) are constants, greater than 0 and have dimensions of mass per unit length.

Making,
\[ K = k_1 \times k_2 \times k_3 \times k_4 \times k_5 \]

and integrating leads to the equation,
\[ C_m = K \times (Q \times y^2 + P \times y) \times \frac{l}{l + a} \]

We can express the value of the height of the sample \( l \) (in cm) in function of the mass \( m \) (in grams), of the cross section of a container sample \( S \) (in cm²), of the grade, of the fluorspar density \( \rho_1 \) and of the sterile density \( \rho_2 \),
\[ l = \frac{m}{(\rho_1 \times y + \rho_2 \times (1 - y)) \times S} \]

Then, in this model the relationship between counts, mass and grade is the following:
\[ C_m = \frac{K \times m \times (Q \times y^2 + P \times y)}{a \times (m + Q \times a + y + P \times a)} + F \]

Where,
- \( Cm \) is the integral of the counts from the sample in a certain range of channels for this first model,
- \( P \ y \ Q \) are constants and their values are greater than 0,
- \( a \) is the distance between the source and the base of the sample,
- \( y \) is fluorspar grade constant in the sample expressed per unit,
- \( l \) is the height of the sample.
- \( F \) counts from detector background without sample.

This equation is a surface in three dimensions whose X and Y axes are mass and grade and the Z axis is the counts (Figure 3).

![Figure 3. Representation of the equation in the study carried out with MATLAB](image)

### 2.2 Second model

In the first model, we refer specifically to the phenomenon suffered by gamma rays produced from an irradiated sample before being detected. In the radiation reading position, the detector is at a distance \( b \) from the sample, as shown in Figure 1. The value \( b \) is very small, negligible compared with the height \( l \) of the sample. This fact together with the attenuation of gamma rays in the air being lower than in the sample, leads to the observation that attenuation takes place only in the mass of the sample.

In this process, we have observed the following proportionality, some of them identical to previous case:

- The counts from the sample and reading in the detector \( C_m \) have an exponential relation to the counts \( dC_{px} \) produced by the sample. The proportionality constant depends on the efficiency and the coefficient of radiation attenuation:
As in the previous case, the count differential \( dC_{px} \) produced in the differential element of height \( dx \) is proportional to the number of excited atoms in the differential element \( dN_{ax} \). The number of excited atoms \( dN_{ax} \) depends on neutron flux \( \Phi_n \) (constant in this hypothesis) and of the number of fluorine atoms \( dN_{fx} \) at that point. The number of fluorine atoms at a sample point \( dN_{fx} \) is directly proportional to the product of the grade \( y \) and of the mass \( dm \) of the differential element, and as in the previous case, the mass \( dm \) depends on the volume of the differential element \( dV \) and on the density \( \rho_m \).

Proceeding as previously, we obtain the equation for this second model, which includes the background, as follows:

\[
C_m = k_1 \cdot \int_0^1 e^{-\mu*y} \cdot d \cdot C_{px}
\]

The parameters \( Q \) and \( P \) are the same as in the previous case, while the factor that includes all proportionality constants \( K' \) is different.

### 2.3 Third model

In this third model, it is supposed that the activation of a differential element sample depends on the distance \((x+a)\) in the direction \( x \) to the source, and that gamma rays are attenuated on their way to the detector following an exponential \( = ae^{-bx} \).

In this case, the number of counts \( C \) in the energy range considered that come to the detector by the neutron activation effect can be expressed as:

\[
\alpha y \beta \text{ being the weight coefficients of each phenomenon individually in the final model, which fulfill the condition of being positive and their sum is equal to 1.}
\]

\[
Solution \text{ of the model 3} = \alpha \ast \text{solution of the model 1} + \beta \ast \text{solution of the model 2}
\]

3 Checking the models

In order to determine which phenomena have greater impact on neutron activation, and therefore, the best model that fits to reality, each model is applied to neutron activation of a fluorspar sample from a concentration plant. Equipment used
NEUTRON ACTIVATION MODELS

consists of an Americium Beryllium source of 1 Ci of activity and a gamma ray
detector of the type NaI. A prototype has been designed [3].

The reason for using fluorspar samples for testing the models is that the radiation
of fluorspar with neutrons from Americium Beryllium source emits a characteristic
high energy (6.13 MeV) which comes, according to previous studies [4], from the
fluorine present in CaF$_2$. This radiation comes from $^{16}$N originated, only and
exclusively, from the nuclear reaction $^{19}$F(n,α)$^{16}$N. Due to the characteristics of the
detector, the energy spectrum of the sample, does not give a single peak at 6.13
MeV, but has a certain width, and has some ‘echoes’ called ‘escape peaks’ at 5.11
and 5.62 [5]. For this reason, the counts used in the study are in a range and are not
in this exact value (6.13MeV). The authors know the reactions produced in this
mineral using the activation for analyzing fluorine in a fluorspar samples. An
activation procedure and a mathematical method that increases the sensitivity were
designed [6].

The fluorspar samples with variable fluorite grades $[\gamma]$ from 4 to 97% and variable
masses $[m]$ from 50 to 450 g (taken at intervals of 50 to 50) have been used.
Samples are found in the same state of humidity and particle size.

3.1 Adjusting the first approach to the experimental data

Equipment was designed specifically to irradiate with neutrons and read the
gamma rays emitted from fluorspar samples with the grades and masses specified
above. Irradiation and reading times were adjusted according to the reaction
sought and the coefficients $K$, $a$, $Q$, $P$, and $F$ were determined. Nonlinear
regression was used to determine the coefficients. The statistical program SPSS [7]
was used. In this work only the coefficients obtained from taking the average
values of the counts detected in the different tests, with an energy range between
4.5 and 6 are shown.

Algorithms used by statistical programs for nonlinear regressions are iterative
processes which require the assignment of initial values for the coefficients. Table
1 shows the initial values for the parameters of the above equation.

<table>
<thead>
<tr>
<th>Density ranges</th>
<th>Parameters</th>
<th>Initial values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_1=1.1-1.9$ g/cm$^3$</td>
<td>$P=3\times p_2$ between 20-50</td>
<td>$K=1$</td>
</tr>
<tr>
<td></td>
<td>$Q=2\times (p_1-p_2)$ between 3 and 16</td>
<td>$P_0=4.5$</td>
</tr>
<tr>
<td></td>
<td>$a$ between 0.5 and 8 cm</td>
<td>$Q_0=2.6$</td>
</tr>
<tr>
<td>$p_2=1.1-1.4$ g/cm$^3$</td>
<td>$F$ between 10 and 25 counts</td>
<td>$a=2$ cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$F_0=13$ counts=1</td>
</tr>
</tbody>
</table>

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Under these initial conditions the program was put into action and the parameters obtained are shown in Table 2.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Energy 4.5-6 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>9.798</td>
</tr>
<tr>
<td>a</td>
<td>1.832</td>
</tr>
<tr>
<td>Q</td>
<td>7.515</td>
</tr>
<tr>
<td>P</td>
<td>38.978</td>
</tr>
<tr>
<td>F</td>
<td>13.598</td>
</tr>
<tr>
<td>R2</td>
<td>0.994</td>
</tr>
</tbody>
</table>

### 3.2 Adjustment of the second approach to the experimental data

Regression was carried out using the experimental results with a sample group. The procedure was repeated with the energy and value types. The parameters of the resulting equation are reflected in Table 3.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Energy 4.5-6 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>K’</td>
<td>1.992</td>
</tr>
<tr>
<td>μ</td>
<td>0.505</td>
</tr>
<tr>
<td>Q</td>
<td>10.122</td>
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<tr>
<td>P</td>
<td>43.464</td>
</tr>
<tr>
<td>F</td>
<td>13.6</td>
</tr>
<tr>
<td>R2</td>
<td>0.991</td>
</tr>
</tbody>
</table>

### 3.3 Adjustment of the third approach to the experimental data

Establishing restrictions of attenuation coefficient $\mu$ in the processing of the third model with the program SPSS, we are found that the correlation coefficient in this third model is lower than in previous models, so it follows that the phenomenon of gamma rays attenuation (expressed by $\beta$) is negligible.
4 Comparison between models

In the first model a very high attenuation coefficient $\mu$ is obtained and the parameters $a$, $K$, $P$, $Q$, $y$, $F$ are consistent with the real values. However, the attenuation coefficient $\mu$ obtained in the second model is about 0.5, which is 10 times higher than expected given the composition of the sample. It therefore follows that the first model is the closest to reality.

5 Validity of the first model

Fluorite grades are compared with grades obtained from the first model for activated fluorspar samples with the parameters identified above. These parameters are $K=9.798$; $a=1.832$; $Q=7.515$; $P=38.978$; $F=13.598$.

The sample grade of mass known $m$ after activation with a count number $C$ emitted is obtained by:

$$y = \frac{(C-F)*Q*a^2-K*m*P+\sqrt{K*m*P-(C-F)*Q*a^2}}{2*K*m*Q} + 4*(K*m*Q)/(C-F)*(P*a^2+m*a)$$

This equation is illustrated in Figure 3, and the comparison is shown in Figure 4. Note the linearity of the response and the validity of the model for all range of grades.

![Figure 4. Comparison between chemical analysis and neutron activation with samples used in the deduction of the model](image-url)
6 Conclusions

A neutron activation process from two basic and simultaneous phenomena has been modeled. The phenomena are the reduction of the neutron flux that activates the sample and the attenuation of gamma rays produced during the activation that reach the detector.

The phenomenon of the reduction of the neutron flux is controlled by the inverse of the square of the distance between the sample and the source.

The phenomenon of the attenuation of gamma rays is controlled by an exponential law that depends on the attenuation coefficient $\mu$, characteristic of sample.

The model was assayed by way of irradiation from a fluorspar sample whose fluorine content is reflected by the emission of high-energy gamma radiation (6.13 MeV).

From the correlation of the results with the models and the experiments, it follows that only the effect of reduction of the neutron flux with the distance can be considered as the effect of the other effect is low.

A high correlation coefficient (~1) has been obtained from the model. In addition the parameter values $a, K, P, Q$ and $F$ are consistent with the real values.

After comparison between the values obtained from chemical analysis and those from neutron activation, the model was considered suitable.

7 Acknowledgements

This work has been supported by Mineral Products and Derivatives Company, SA (Minersa), Government of the Principality of Asturias, Research grant scheme of the University of Oviedo. The authors would like to thank the above-mentioned bodies for their collaboration and financial support during this study.

8 References


Ultrasonic Sensors with Mechanical Couplers:
Simulation and Validation

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Abstract

This paper presents the results obtained in a study of the behaviour of mechanical elements coupled to an ultrasonic sensor using finite element techniques, which can modify the radiation pattern of the original sensor. These results have been obtained using Comsol multiphysics modelling. The effect caused by the sensor size on the radiation acoustic pressure has also been evaluated. In this paper we also present the experimental validation of these simulations.

Key words: ultrasonic, sensors, horns, pattern

1. Introduction

The use of ultrasonic sensors has varied applications including basic ones such as object detection or measurement of distances. For some production process tasks we find that, although the applications are not very difficulty, they involve a great time cost in processes, such as the detection of defects. Some of the more complex applications include recognition and identification of objects.

A common factor in all these applications is that the operating frequency of ultrasounds limit the operating distance of the ultrasonic sensor, due to the already known fact that increasing the operating frequency also increases the attenuation of ultrasonic waves. In contrast, an increase in the frequency of the ultrasound provokes a narrowing in the radiation lobe. Given these facts, it follows that by increasing the operating frequency the directional behaviour of the sensor can be improved, but at the expense of reducing the working distance. In applications
needing a broader or a narrower lobe than that obtained by the sensor itself, there are several options, ranging from the use of sensors of different frequency, appropriate for the application, or increasing the sensor diameter to obtain more power, using arrays of sensors to obtain the radiation pattern. This last option intrinsically leads to an increase in hardware and software complexity. An alternative solution is to couple a mechanical element, commonly called horn. As would be expected, physical and geometrical characteristics of the coupled element influence the new ultrasonic radiation pattern. This is where the need arises to find a simulation model, to find the relation between the coupler parameters and the desired characteristics of the radiation lobe.

To characterize this technique, it is necessary to use software tools to be able to analyse the simulated models. Among the different techniques for simulation, such as boundary element, finite difference, finite element, we choose the latter because of its availability and versatility. The use of finite elements and Comsol software has already provided good results in previous works.

In this paper, we present the results obtained in the radiation pattern using an ultrasonic sensor in two different cases. The first one is the ultrasonic sensor in free radiation and the second one is when a straight horn is linked to the sensor. We also present the variation in sound pressure on the radiation axes when the size of the sensor changes.

2. Simulations descriptions

Taking into account the results already obtained in previous work [1] [2] in the Comsol simulations to study the modifications produced in the ultrasonic radiation patterns using couplers, we have tried to obtain a simulation that describes the real problem more faithfully. This was the reason for simulating the system using the multiphysics modelling that Comsol makes possible.

Simulations have been divided into different parts. The first one is to obtain the ultrasonic radiation lobe in free radiation. The second explores the effect produced when the sensor is provided with a horn with zero opening angle, that is, a tube of a certain length but with no opening (straight horn). Finally, the effects produced on the sound pressure at on the axis of radiation has been simulated as function of the sensor size.

For a description of the model using Comsol multiphysics, the division of the problem into three distinct domains as shown in Figure 1 has to be taken into account. The first one refers to the sensor itself, while the second refers to acoustic wave propagation in air. In the last of the domains we have defined a far-field zone, which provides the attenuation of the wave for longer distances. In this work, the y axis (radiation axis) has been fixed as the axis of symmetry, in order to reduce the large computational cost involved in simulation using the finite
element technique. In this way, the decrease in the numbers of equations is used to increase the extent of the simulations, optimizing the computational resources.

For the first of the domains, which refers to the sensor itself, and taking into account the Comsol enhancement, which enables the different kinds of physics to be combined, the piezoelectric crystal part has been used. In our case, it was established that the sensor was a piezoelectric crystal of PZT5-H (Lead Zirconate Titanate), which is a material commonly used in transducers. Then a voltage difference was applied between its upper and lower surfaces.

The second and third domains refer to ultrasonic propagation in air and therefore must fulfill the Helmholtz equation, which is shown in equation (1).

\[ \Delta p(\vec{r}) + k^2 p(\vec{r}) = 0 \]  

where \( \Delta \) is the Laplace operator, \( p \) is the acoustic pressure, \( \vec{r} \) is the position, \( k \) is the wave number, which is valid in the working domain established. Having established the domain, you must define its boundary conditions. For the piezoelectric crystal the condition of symmetry in the y-axis is established, and a voltage difference between the upper and lower surfaces of the sensor is applied. For the second and third domains, the axis of symmetry is defined as the y-axis and in the other contours, except the interface between domains 1 and 2, as the condition of wave propagation in the air, equation (2).

\[ \frac{\partial p}{\partial n} = ikp \]  

where \( i \) is the imaginary unit.

For the interface between domains 1 and 2, that is, between the upper surface of the sensor and air, the boundary condition is given by equation (3).

\[ n(\nabla p) = a_n \]  

where \( n \) is the outward normal and \( a_n \) is the normal acceleration. Thereby getting the sound pressure produced by the voltage difference applied to two surfaces of the piezoelectric crystal to pass the domain in which the acoustic wave propagates. Note that between the second and third domains, this condition is not produced because the domain characteristics are the same.
Under these conditions, the radiation pattern obtained for the case of an ultrasonic sensor operating at a frequency of 25KHz. and a 7mm. sensor radius is shown in Figure 2.

![Figure 2: Radiation pattern for multi-physical modelling using a sensor in free radiation](image)

It is important to note that the workspace of the simulation is small, only reaching up to 0.6m. This is because the computational cost required by the software is very high, this being one of the main drawbacks and problems encountered in the work.

The second objective of this study was to obtain an ultrasonic radiation lobe when the sensor is attached to a mechanical horn-type element. In addition, this paper presents the case when the horn used was a straight tube, that is, without opening angle and a given length, such as occurs in case in pieces of couplers types. In the case of multi-physical modelling, the introduction of this new element does not increase the complexity excessively, it is only to add a fourth domain, with the same characteristics as domains 2 and 3 defined above, that is, a domain in which the acoustic wave propagates. Figure 3 shows the new situation.

![Figure 3: Representation of the domains in the case of couplers](image)

It should be noted that right now the boundary condition between the upper surface of the sensor and the air is between domains 1 and 4, while for the surface binding domains 4 and 2 we do not have to establish any special status as both possess the same characteristics. In addition, the boundary condition established at the wall of the horn is total reflection as shown in equation (4).
\[
\frac{\partial p}{\partial n} = 0 \quad (4)
\]

Figure 4 shows the radiation pattern obtained for a sensor operating at a frequency of 25Khz. and with a straight coupled horn of length 3cm. and a sensor radius of a 7mm.

![Figure 4: Radiation pattern of a 25KHz. sensor with a 3cm straight horn attached](image)

In the final part of the work, the influence of the size of the ultrasonic sensor on the acoustic pressure on the radiation axis is studied for the case of free radiation. Figure 5 shows that increasing the size of the sensor, the acoustic pressure on the shaft also increases.

![Figure 5: Acoustic pressure on the radiation axis when the sensor size is changed](image)

3. **Measurement system description**

To perform the experimental evaluation of the simulations we used a robotic positioning system inside an environmental chamber.

For the ultrasonic system, two Hexamite long-range sensors (up to 30m.) were chosen. They work with an excitation frequency of 25 KHz. One of the sensors will be used as a transmitter, it being necessary to use a conditioner for sensor excitation, provided by the same manufacturer. For the reception stage, the corresponding conditioner of the ultrasonic sensor has not been used because for the working distances of the measurements, i.e. up to 3m, it is not necessary.
For the sound pressure at all points in an XY plane, we chose to use a Yamaha robot, model BX SBX RCX40 with a RCX40 controller that allows us to vary both the distance and the angle between the transmitter and receiver. The distance between transmitter and receiver varies from 0 to 3m. with a 1cm step, while the scan angle will be between 0º and 90º with a step of 1º, due to the symmetry. However, it is important to project the large number of points obtained for each register, more than 27,000 echoes.

Both systems are situated inside an environmental chamber, which can vary both the temperature and humidity. In Figure 6, a view from inside the climatic chamber of the measuring system is shown.

![Transmitter positioned on the robot inside the climatic chamber](image6.png)

**Figure 6: Transmitter positioned on the robot inside the climatic chamber**

A closed-circuit television/video camera was also placed inside the climatic chamber in order to continue to capture and process of ultrasonic echoes from the outside the chamber. All this is handled by a data acquisition card, supplied by National Instruments and both data acquisition and the further processing is done with Matlab. It has been taken into account that the simulation process which is performed with Comsol can also work in Matlab, which is a very important point for a later comparison of simulations and measurements.

Figure 7 shows the ultrasonic radiation lobe in free radiation obtained in the measurements and represented in Cartesian coordinates.

![Ultrasonic radiation lobe in free radiation](image7.png)

**Figure 7: Ultrasonic radiation lobe in free radiation**

In the case of coupling to the sensor of a straight horn of 3cm. length, we used the piece shown in Figure 8. Notice that the inside of the coupler is a straight pipe.
with the same diameter as the sensor, while on the outside the coupler is threaded to be able to connect horns with different geometry.

![Image of straight horn in measurements used](image1)

**Figure 8:** Straight horn in the measurements used

Figure 9 shows the radiation lobe of the ultrasonic sensor with the coupler in the previous figure, also in Cartesian coordinates.

![Image of ultrasonic radiation lobe with coupler](image2)

**Figure 9:** Ultrasonic radiation lobe of the ultrasonic sensor with the coupler

Figure 10 shows the couplers used to obtain the sound pressures in the radiation axis for the same ultrasonic sensor but with a different internal diameter.

![Image of couplers used](image3)

**Figure 10:** Couplers used

## 4. Experimental validation

Figure 11 shows the simulated sound pressure on the radiation axis in the case of the free radiation sensor and in the case of the horn attached to the sensor.

If in Figure 11 the graph corresponding to the acoustic pressure of the sensor in free radiation is displaced an identical distance from the straight horn, that is, 3cm. then Figure 12 is obtained, in which the two acoustic pressures in the radiation axis match.
Figure 11: Simulated acoustic pressure on the radiation axis for sensor in free radiation and with coupler

Figure 12: Simulated acoustic pressure on the radiation axis for the sensor both with and without being displaced the length of the horn.

If a cut is made in the y-axis to observe how the sound pressure on the x-axis varies, taking into account the shift that occurs when you the horn coupling is done, Figure 13 can be obtained.

Figure 13: Acoustic pressure simulated on the x-axis for free sensor and with the horn coupled, taking into account the shift of the length of the horn.

From the above, and the radiation patterns obtained in Figures 2 and 4, we can conclude that the radiation pattern has not been modified by the coupling of the straight horn, that is, the effect of the straight coupler is the same as situating the ultrasonic sensor at the top of the horn.
Viewing the simulations made varying the size of the sensor at the acoustic pressure on the axis of radiation; it appears that the sound pressure increases with the diameter. The known relation expressed in equation (5) is verified, which provides the sound pressure at a distance $d$ from the oscillator.

$$P = P_o \cdot 2 \cdot \text{sen} \left( \frac{\pi}{2} \sqrt{\frac{D^2}{4} + d^2 - d} \right)$$

where $D$ is the diameter of the oscillator and $\lambda$ the wavelength.

For large distances, $d >> D^2/4\lambda$, the above equation can be approximated by equation (6), that is, the pressure is proportional to the square of the diameter of the sensor. Table 1 shows the proportional constants obtained in each case.

$$P = P_o \cdot \frac{\pi \cdot D^2}{4\lambda}$$

<table>
<thead>
<tr>
<th>Sensor Size (mm.)</th>
<th>Proportionality constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>4.2</td>
</tr>
<tr>
<td>10</td>
<td>4.5</td>
</tr>
<tr>
<td>6</td>
<td>3.6</td>
</tr>
</tbody>
</table>

Table 1: Simulated proportionality constant depending on the size of the sensor

If we analyze the acoustic pressure along the axis of radiation to the measures, both for the case of free radiation is coupled as when you get Figure 14, which shows that there is little difference between the case of free radiation horn coupled radiation increases with distance.

Figure 14: Acoustic pressure measured on the axis of radiation, radiation free and coupled horn

Based on this result, the main conclusion is that by using a coupler in the form of a straight horn with different diameter, change the size of the sensor while maintaining the same intrinsic features of the sensor.
Figure 15 shows the sound pressure measured on the radiation axis when the couplers shown in Figure 10 are used. In this figure, the inner diameter of the coupler is varied from 3mm. to 7mm. in radius with a step of 2mm. These results agree with those predicted in the simulations and expressed in the equation (5), that is, increasing the sensor size increases the pressure on the axis of radiation.

![Figure 15: Acoustic pressure on the radiation axis for different sizes of sensors.](image)

Table 2 shows the proportionality constants of the measurements obtained in each case.

<table>
<thead>
<tr>
<th>Sensor Size (mm.)</th>
<th>Proportionality constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>0.9</td>
</tr>
<tr>
<td>10</td>
<td>1.3</td>
</tr>
<tr>
<td>6</td>
<td>2.6</td>
</tr>
</tbody>
</table>

Table 2: Constant of proportionality of measures according to the size of the sensor

If a comparison is made between the acoustic pressure on the radiation axis for simulations and measurements, both with coupler, Figure 16 is obtained, in which you can see that the sound pressures correspond quite faithfully, after a scale adjustment.

![Figure 16: Acoustic pressure on the axis of radiation, measured and simulated, with a straight horn](image)

In addition comparisons can be made between the simulations and measurements, for different sensor sizes, producing the graph shown in Figure 17, in which the scales have been adjusted.
Figure 17: Acoustic pressure on the radiation axis, simulated and measured, for different sensor sizes

5. Conclusions

Analyzing the simulations, it can be concluded that the use of a coupling element with the shape of a straight horn does not affect the radiation pattern of the sensor. This has been corroborated by the laboratory measurement of the radiation pattern in the case of a free radiation sensor and for a sensor coupled to a horn. This implies that when using a single sensor, different sizes can be used and different horns with different lengths and apertures can be attached to find the most suitable radiation lobe for a given application.

Furthermore, it has also been shown that sensor size affects acoustic pressure, and the mathematical dependence on sensor diameter has been demonstrated.

As noted before, the main problem is the large computational cost entailed when performing the simulations. This is so high that it is not possible to simulate long distances, comparable to the measurement distances.

Acknowledgments

This work has been carried out under the sponsorship of the Spanish Ministry of Science and Innovation (MICINN) in the CICYT with reference DPI2007-640 295.

6. References


Detection of Imperfections within Historic Walls Using Ground-Penetrating Radar

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Abstract

This paper presents a novel application of Ground Penetrating Radar (GPR) to the evaluation of ashlar masonry walls. Several experiments were made on a scale replica of a historic ashlar masonry wall. These models were loaded with different weights, and the corresponding B-Scans (radargrams) were obtained. Several kinds of flaws and inhomogeneities were detected from the analysis of the radargrams.

Key words: GPR, NDT, flaw detection, historic walls

1. Introduction

We here present the results obtained applying auscultation of scaled ashlar masonry walls using Ground Penetrating Radar [1]-[4]. We analyzed two masonry walls, one being homogeneous in structure and the other with many imperfections drilled in it. We intend to detect inhomogeneities inside the wall and characterize the propagation of electromagnetic waves inside the masonry when under different loads.

Equipment employed consisted of a GPR, a SIR 3000 from Geophysical Survey Systems, Inc. We used a 1.6 GHz (Figure 1.b) mounted on an encoder. The receiving antenna has a size of 3.8 x 10 x 16.5 cm and was adequate for both
vertical and horizontal measures.

The configuration parameters used for data capture were: distance mode, 156 scans per meter, range of 10 ns (20 ns in round-trip-time) and 1024 samples per scan.

Measures were taken along the surface of the wall, following 7 columns (2.2 m high each) and four rows (2.87 m long each). The resulting sampling grid is shown in Figure 2. It must be noted that measures were taken from side A, while on the opposite side of the wall there were different sensors and devices (from other NDT) that served as reflectors.

![Figure 1. Photograph of a GPR system: a) conditioning, recording and processing system SIR 3000; b) 1.6 GHz antenna (model 5100) with encoder.](image)

We will try to obtain the dielectric constant to use in our work. We know each A-scan has 1024 time samples and so the time sampling is:

\[
dt = \frac{10 \text{ ns}}{1024 \text{ samples}} = 9.76 \text{ ps/sample}
\]

Using the first trace of horizontal line 2, we find there is a distance of 426 samples between the start and the end of the wall, see Figure 4. Given the distance the signal travelled during that time (20.4 cm, as measured on site) we get a relative dielectric constant:

\[
\varepsilon_r = \left( \frac{c \cdot dt \cdot \# \text{ samples}}{\Delta z} \right)^2
\]

From here on we will use this value in our calculations.
2. GPR System Application Interface

A GUI (Graphic User Interface) was made for simple and visual processing of GPR-captured data. It has two parts: a main program (see Figure 3) and a secondary window used for the selection of the excitation signal.

The main window links to three common processing steps of B-scan data: background signal removal, depth resolution enhancing and Kirchoff migration. We used different ICA algorithms for background signal removal [5]-[8]. The results of each of these steps are shown on screen, with the most recent result being shown of the central, biggest figure. There are also three buttons not related to this processing: an export data button (including parameters used and the most
recent result), an AGC (Automatic Gain Control) button to enhance contrast and an envelope button, which shows the time envelope of the most recent result (sometimes used for data interpretation). The last two apply to the most recent result (the one shown on the central figure) and are discarded if any further processing is attempted. Exported data values, on the other hand, do include AGC and envelope calculation if they have been applied. In addition we used methods of depth resolution enhancement and cepstral deconvolution [9].

2. General Analysis of the Wall

Figure 4 shows a detail of the background corresponding to the opposite side of the background signal for the wall. The left part of the figure corresponds to row 6, while the right part belongs to column 6.

![Figure 4](image)

Figure 4. Background at the opposite side of the wall for different values of the load. a) row 6, no load; b) column 6, no load; c) row 6, 50 mt load; d) column 6, 50 mt load; e) row 6, 80 mt load; f) column 6, 80 mt load.
Row number 6 has a greater variation of its propagation conditions. This is noticeable from the way the opposite side of the wall seems to move away (see Figure 4), indicating a loss in velocity of propagation inside the material. This is due to a worsening of transmission properties due to the load. We noticed that the difference between 0 and 50 mt (metric tons) is greater than the one between 50 and 80 mt.

The column shown (number 6) also shows a difference in depth between 0 and 50 mt loads. The difference is stronger on both ends of the wall and matches with what shown of row 6 (the right parts of the representations for row 6 and for column 6 correspond to the same area of the wall).

Generally speaking, other representations of the background of other rows and columns follow these same tendencies (that is, they show a stronger effect at the start and end of the B-scan). Nevertheless, they keep the same values in the central area of the wall. This behavior seems consistent with in situ measurements of the wall’s distortions.

Figure 5. Steps in the processing of radargrams for flaw detection: a) original map; b) background removal; c) migration; d) contrast enhancing. Wall, column 1, 80 mt load.
3. Analysis of Flaws Within the Wall

For the purpose of flaw detection, some algorithms were implemented to emphasize the discontinuities (typically due to changes in the material) in the radargrams. These methods, as seen on previous sections, were: background removal, depth resolution enhancing, Kirchoff migration and improvement of the contrast in the B-scan.

Because it is a homogeneous wall, there are no important flaws within the ashlars that compose the wall. This means discontinuities found in the radargrams are due only to mortar interfaces with the ashlars. These interfaces are the less dense material in the structure and thus are the most susceptible to strains because of a compression load. We can check the compression suffered under a load of 80 mt in Figure 6. This Figure also includes the unloaded radargram for comparison.

As a matter of fact, we can notice the greatest effect takes place over the central area of the wall, where the compression forces are bigger. This means that the mortar interfaces between ashlars in the wall under study are no longer visible.

![Figure 6. Effect of the load on the detected discontinuities. First column; a) no load; b) 80 mt load.](image)

4. Conclusion

The proposed approach for the auscultation of historical masonry walls with ground-penetrating radar (GPR) has proved to be effective for the detection of flaws and the characterization of walls under load. It was possible to detect flaws with a size of millimeters and variations in the interfaces between ashlars and mortar caused by effect of the compression suffered under load.

Radargrams are techniques that allow representing the internal structure of walls. Nevertheless, one must take into account that inhomogeneities inside the walls will be more or less visible due to their geometry and their physical properties (especially their contrast with the surrounding medium). Because of this, adaptive processing techniques are required to successfully show the different flaws.
In addition, we would like to point out that the proposed approach is a low-cost operation with no required previous preparation of the material or a complex and extensive setup. Even more, one can capture data continuously along the surface of the wall (and its interior) in a short amount of time.

5. Acknowledgments

This work has been supported by the Generalitat Valenciana under grant PROMETEO/2010/040; the Spanish Administration and the FEDER Programme of the European Union under grant TEC 2008-02975/TEC; and the Generalitat Valenciana under grant GV/2009/003 within the research and development programme for Emergent Research Groups.

6. References


Estimation of Missing Seismic Data based on Non-linear Systems

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Abstract

This paper presents a new method for the reconstruction of missing data in seismic signals. The method is based on non-linear (NL) systems considering non-Gaussian statistics in the probability density function of the seismic data. We propose different NL structures by combining different techniques for the linear and non-linear stages. The linearity in the data is recovered using kriging and cross correlation, and the data non-linearity is reconstructed using direct sample estimation and a third order polynomial approximation. The results by linear and NL structures are compared with the results of Multi-Layer Perceptron and Radial Basis Function neural networks.

Key words: kriging, non-linear systems, seismic signals, missing data

Introduction

In seismic analysis, the wavefield generated by seismic sources is captured by a number of sensors located over a large area. Reconstruction of missing data and data interpolation are important issues in the processing of seismic signals. Incomplete data happen due to problems, such as disconnection of sensors during signal acquisition or need for resampling of data at particular non-measured locations. Several techniques have been proposed to deal with these issues, for instance: matching pursuit [1], wave equation-based interpolation [2],
autoregressive spectral extrapolation [3], prediction error filtering interpolation [4], and Fourier reconstruction [5]-[7]. The problem of seismic signal reconstruction can be posed as an inverse problem, where from incomplete data a recovering of the complete seismic wavefield is attempted.

In this paper, we propose a new method for seismic trace reconstruction based on Wiener structures that are composed of a linear processor followed by a non-linear processor. Wiener, Hammerstein, and Wiener-Hammerstein structures represent simple methods to build non-linear predictors capable of prediction for non-Gaussian data [8]-[10].

Several examples of seismic data reconstruction are included using real seismic data from a public dataset of BP Amoco [12]. In order to evaluate the proposed method, maps with simulated missing data were generated by subtracting zones of 4 contiguous A-scans from the complete data set. The quality of the data reconstruction was assessed using mean squared error (MSE), Kullback-Leibler distance (KLD), and absolute values of the differences in variance and kurtosis between the original and the reconstructed data [13].

**Prediction Based on Wiener Systems**

Wiener structures have been used to model non-linear systems in quite different applications, such as blind deconvolution in digital communications [14] and prediction applied to infrared signals [15]. The structure consists of a linear stage followed by a zero-memory non-linear stage (see Figure 1).

From Figure 1, \( x_p(n + l) \) is the output of the linear predictor (i.e. \( x_p(n + l) \) is the linear prediction of \( x(n + l) \) from the past samples \( x(n), x(n - 1), \ldots, x(n - N + 1) \)). \( N \) is the order of the linear predictor and \( l \) the prediction time lag. Thus, the output of the Wiener system is the conditional mean defined as

\[
G(x_p(n + l)) = E[x(n + l)/x_p(n + l)]
\]

(1)

Assuming stationarity, a sample estimate of \( G(\cdot) \) can be made. In this paper we implement Wiener structures with kriging or cross correlation for the linear stage and direct sample estimation or a third order polynomial approximation for the non-linear stage. Let us review the techniques applied in the two stages of the Wiener structure.
**Linear Stage**

Cross correlation

This method consists of assigning a weight to each point involved in the prediction. The weights are obtained from the linear transform that minimizes the mean squared error $E \left[ \| \mathbf{w} - \mathbf{w}_{pd} \|^2 \right]$, where $\mathbf{w}$ are the original signal values $\mathbf{w} = [w(n+1), ..., w(n+D)]^T$ and $\mathbf{w}_{pd} = \mathbf{H} \ast [w(n+1), ..., w(n+D)]^T$ are the predicted values. This problem is a particular case of the Wiener-Hopf equation, and the optimum weight matrix $\mathbf{H}$ is obtained by means of

$$\mathbf{H} = \mathbf{R}_{xw} \ast \mathbf{R}_{ww}^{-1}$$  \hspace{1cm} (2)

The generic elements of these matrixes are: $R_{ww}(i,j) = R_w(i-j), i = 1, ..., N, j = 1, ..., N$; and $R_{xw}(i,j) = R_w(i+j-1), i = 1, ..., D, j = 1, ..., N$, being $R_w(m)$ the autocorrelation function of the signal, $N$ the number of samples used and $D$ the number of values to be predicted.

**Kriging**

This algorithm estimates the weights $\lambda_i(\mathbf{r})$ such that the estimator for the interpolated value $\hat{Z}$ has an optimal relationship with a given set of data values $Z(\mathbf{r}_i), i = 1, ..., N$. Thus,

$$\hat{Z}(\mathbf{r}) = \sum_{i=1}^{N} \lambda_i(\mathbf{r}) Z(\mathbf{r}_i)$$  \hspace{1cm} (3)

where $\mathbf{r}$ is the position vector.
The restrictions, minimum residual variance \( \sigma_e^2 = E\left[ (Z(\mathbf{r}) - Z(\mathbf{r}))^2 \right] \) and \( E[\hat{Z}(\mathbf{r}) - Z(\mathbf{r})] = 0 \), impose the condition that the estimator is both unbiased and gives the least dispersion.

Kriging established the concept of structural analysis. The variogram indicates the degree of correlation between values of the variable as a function of distance. The definitions that are relevant to kriging are the covariance (\( C \)) and the semivariogram (\( \gamma \)). They are defined by

\[
\gamma(\mathbf{r}_1, \mathbf{r}_2) = \text{var}\{Z(\mathbf{r}_1) - Z(\mathbf{r}_2)\}/2
\]
\[
C(Z(\mathbf{r}_1), Z(\mathbf{r}_2)) = E[(Z(\mathbf{r}_1) - E[Z(\mathbf{r}_1)])(Z(\mathbf{r}_2) - E[Z(\mathbf{r}_2)])]
\]

with \( \text{var}\{\cdot\} \) being the variance. We used two different methods. Simple kriging obtains the weights by solving the system of equations (5):

\[
\begin{bmatrix}
C(Z(\mathbf{r}_1), Z(\mathbf{r}_1)) & \cdots & C(Z(\mathbf{r}_1), Z(\mathbf{r}_N)) \\
\vdots & \ddots & \vdots \\
C(Z(\mathbf{r}_N), Z(\mathbf{r}_1)) & \cdots & C(Z(\mathbf{r}_N), Z(\mathbf{r}_N))
\end{bmatrix}
\begin{bmatrix}
\lambda_1(\mathbf{r}) \\
\vdots \\
\lambda_N(\mathbf{r})
\end{bmatrix} =
\begin{bmatrix}
C(Z(\mathbf{r}_1), Z(\mathbf{r})) \\
\vdots \\
C(Z(\mathbf{r}_N), Z(\mathbf{r}))
\end{bmatrix}
\]

On the other hand, ordinary kriging assumes an unknown, constant trend \( \mu \). The system of equations to be solved changes to (6):

\[
\begin{bmatrix}
\gamma(\mathbf{r}_1, \mathbf{r}_1) & \cdots & \gamma(\mathbf{r}_1, \mathbf{r}_N) & 1 \\
\vdots & \ddots & \vdots & \vdots \\
\gamma(\mathbf{r}_N, \mathbf{r}_1) & \cdots & \gamma(\mathbf{r}_N, \mathbf{r}_N) & 1 \\
1 & 1 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
\lambda_1(\mathbf{r}) \\
\vdots \\
\lambda_N(\mathbf{r}) \\
\mu
\end{bmatrix} =
\begin{bmatrix}
\gamma(\mathbf{r}_1, \mathbf{r}) \\
\vdots \\
\gamma(\mathbf{r}_N, \mathbf{r}) \\
\gamma(\mathbf{r}_N, \mathbf{r})
\end{bmatrix}
\]

Non-linear Stage

Direct sample estimation

The non-linear function that relates known to predicted data is estimated by a sliding window,

\[
G(x_{pl}(i)) = \frac{1}{\Delta} \sum_{i}^{i+\Delta-1} x_{l}(i)
\]

where \( x_{pl} \) is a vector with the predicted data sorted from highest to lowest, and \( x_{l} \) is a vector with the known values corresponding to each of the predicted values. The window defined in (7) is rectangular, but any kind of window can be used.
Polynomial approximation

In [15] we developed the following one-dimensional polynomial approximation for the non-linearity of the Wiener system. Assuming that $x \equiv x_l(n + l)$ and $x_p \equiv x_{pl}(n + l)$,

$$G(x_p) = \sum_{m=1}^{\infty} \frac{1}{m!} C_m(x, x_{pl}) H_m(x_{pl})$$

(8)

where $C_m(x, x_p)$ is the cross-cumulant defined as $C_m(x, x_p) = \text{cum} \left( x, x_p, \ldots, x_p \right)$ and $H_m$ is the Hermite polynomial of order $m$.

For the previous application ([15]) $m \geq 3$ was found to be enough to obtain approximate Gaussian predictions.

Results and Discussion

We used a dataset created by BP Amoco corresponding to Carpathians thrusting over the North Sea [12]. From this dataset, a single 2D cut of the whole data model was used (see Figure 2.a). This 2D model has 252 scans, located at intervals of 25 m, and 314 time samples per scan. Time sample rate is 9.9 ms starting at time $t = 0$. For data reconstruction purposes, we considered that four consecutive scans had failed and no data could be recovered from them. These four scans were located for offsets between 1525 and 1600 m (see Figure 2.b) for a total of 1256 missing values, 1.6% of the available data. Some acronyms were used for the different methods applied for the sake of simplicity. They are shown in Table 1.

Figure 2. Complete dataset (a) and dataset after for scans were removed (b).
For a better estimation, we divided the missing traces to be reconstructed in small zones. The size of these zones was adjusted depending on the applied method, see Table 1. The zones were estimated using training data blocks from zones directly adjacent to them.

Figure 3 shows the nonlinearity present in one of the training data blocks and the estimated curves for the different methods. As we can see, the RBF neural network yields the better result in this particular case, with direct sample estimation being a close second. The polynomial fitting was not able to approximate the nonlinearity. MLP was able to model some of it but negative values were incorrectly modeled. That points to an over-fitting of the positive values in the training set.

Table 1. Acronyms used for the different methods and sizes of zones to be reconstructed. Training data blocks and zones are the same size. These sizes are in number of samples.

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Linear predictor</th>
<th>Nonlinear estimator</th>
<th>Zone size</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>Cross-correlation</td>
<td>Direct sample estimation</td>
<td>1 x 5</td>
</tr>
<tr>
<td>CC+SE</td>
<td>Cross-correlation</td>
<td>Direct sample estimation</td>
<td>1 x 5</td>
</tr>
<tr>
<td>CC+Poly</td>
<td>Cross-correlation</td>
<td>Polynomial fit</td>
<td>1 x 40</td>
</tr>
<tr>
<td>SK</td>
<td>Simple kriging</td>
<td>Direct sample estimation</td>
<td>1 x 5</td>
</tr>
<tr>
<td>SK+SE</td>
<td>Simple kriging</td>
<td>Direct sample estimation</td>
<td>20 x 10</td>
</tr>
<tr>
<td>SK+Poly</td>
<td>Simple kriging</td>
<td>Polynomial fit</td>
<td>30 x 10</td>
</tr>
<tr>
<td>OK</td>
<td>Ordinary kriging</td>
<td>Direct sample estimation</td>
<td>10 x 5</td>
</tr>
<tr>
<td>OK+SE</td>
<td>Ordinary kriging</td>
<td>Direct sample estimation</td>
<td>10 x 5</td>
</tr>
<tr>
<td>OK+Poly</td>
<td>Ordinary kriging</td>
<td>Polynomial fit</td>
<td>20 x 5</td>
</tr>
<tr>
<td>MLP</td>
<td>Multi-Layer Perceptron neural network</td>
<td>Polynomial fit</td>
<td>65 x 12</td>
</tr>
<tr>
<td>RBF</td>
<td>Radial Basis Function neural network</td>
<td>15 x 5</td>
<td></td>
</tr>
</tbody>
</table>

Figure 4.a and Figure 4.b show four different error measurements for the whole reconstructed data: Mean Squared Error (MSE), Kullback-Leibler distance (KLD), absolute difference in variance (ΔVAR) and absolute difference in kurtosis (ΔKUR). There is an abnormality in Figure 4.a for OK+Poly. This was caused by a problem in the polynomial fitting: a few of the predicted data were outside the values given in their training set, and so the resulting polynomial fit was bad and yielded values out of range. This can be further confirmed in Figure 4.b.
Figure 3. Estimate of the nonlinearity of a given training data block for all considered methods. x are the data to be fitted.

Figure 4. Error estimators for the different methods: a) Mean Squared Error (left) and Kullback-Leibler distance (right) for all considered methods; b) absolute difference in variance (left) and kurtosis (right) between predicted data and real values. Best predictions are marked with circles.

In Figure 4.b, variance and kurtosis for methods using polynomial approximations of the nonlinearities are further from the desired values. This is especially true in the case of kurtosis, which is a measure of the amount of outliers for a given data distribution. Real data had a kurtosis of 31.90 and a variance of 2.2·10⁻³.

Figure 5 shows zoom-ins of two different reconstructed maps of missing data. The map given in Figure 5.a was obtained with CC+SE, while the second map (Figure 5.b) was obtained using a MLP neural network. The CC+SE results are better that those obtained with the MLP neural network Comparing them we appreciate CC+SE obtains results similar to the desired result; as a matter of fact, reconstructed values are hardly distinguishable from neighboring values.
It is worth noting that while CC+SE does not achieve the best possible MSE, it has a low Kullback-Leibler distance and higher-order statistics very close to those of the real data. Part of the reason for its comparatively high mean squared error is that its values are more attenuated than those obtained with other methods.

Conclusion

We demonstrated the feasibility of a procedure based on Wiener systems for recovering realistic estimates of data structures of missing seismic traces. The versatility of the procedure allows linear and non-linear dependencies of the data to be modelled using different techniques. The accuracy of the recovered data was evaluated by the mean squared error, density distance, kurtosis, and variance between the estimate and the real data. The best results were obtained using ordinary kriging in the linear part and direct sample estimation in the non-linear part of the Wiener structure.

There are several research lines open from this work, such as including priors of the data distributions, attempting other linear and non-linear techniques, and processing in the frequency domain.

Figure 5. Wiggle plot showing data predicted using: a) CC+SE; b) MLP.

Acknowledgments

This work has been supported by the Generalitat Valenciana under grant PROMETEO/2010/040; the Spanish Administration and the FEDER Programme of the European Union under grant TEC 2008-02975/TEC; and the Generalitat Valenciana under grant GV/2009/003 within the research and development programme for Emergent Research Groups.
References


Implementing a GPU fuzzy filter for Impulsive Image Noise Correction

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Abstract

The problem of correcting images with noise has been widely studied in the digital image processing literature, and many techniques and algorithms have been suggested for this purpose. However, due to their high computational cost, and in general their application for large sized images, the need exists to develop the same executable files in parallel. The implementation of image correction algorithms on the CUDA platform is a relatively new field. Although the platform is easy to program, it is not easy to optimize the applications due to the number of decisions that have to be made. Thus, it is necessary to perform an analysis in order to identify the best configuration for each problem. This paper reports an optimization study on the use of the CUDA platform with fuzzy metric and the concept of peer group for noise correction in images.

Key words: noise correction in images, GPU, CUDA
1. Introduction

In recent years, the incorporation of GPUs (Graphics Processor Units) in graphic cards has achieved significant improvements in computational speed, offering a high parallel processing level combined with a very competitive price. For this reason, developments based on this hardware have become increasingly widespread, not only for graphic implementations but also for general purpose applications. The most commonly used programming platform for these graphic cards is CUDA (Compute Unified Device Architecture) [10]. Its multiple fields of application include medicine, astrophysics, biology, computational chemistry and signal processing, among many others. For example, [1] provides an illustration of biomedical image processing for color and phenotype analysis. In [13], the performance obtained by processing various algorithms in several classic images was analyzed, whilst in [2], two proposals for accelerating bioinformatics applications used to analyze DNA sequences are presented. [5] reports the implementation of algorithms for hyperspectral image analysis, and another spectral imaging application is described in [3]. Finally, [7] depicts the scope of FFT (Fast Fourier Transform) for filtering images.

Whilst it is relatively easy to use the CUDA platform to program the GPU, and the process is well documented, the problem lies in the difficult task of optimizing application performance, due to several hardware restrictions and the multiple types of memories included, which are organized on several levels and display different storage capacities, different access patterns and other limitations. Thus, it is necessary to carry out a specific study in order to identify the best approach to using the resources offered by CUDA in each case. Such a study is the subject of the present paper, applied in this case to noise correction in images.

The images used in this study were all in RGB format (three color channels: red, green and blue, with values in a range of 0 to 255), with impulsive noise (where several pixels have changed the value of one of their channels to maximum or minimum, white or black respectively). Many algorithms have been proposed for correcting impulsive noise, for instance those mentioned in [4]. In the present study, the process of noise correction was divided into two steps: (1) erroneous pixel detection, also divided into two phases, and (2) the elimination of these pixels. The fuzzy metric is used [11] together with the concept of peer group $P$ previously mentioned in [12]. In this concept, a set is of pixels created similar to one already given and then a decision is made, according to the cardinality of the set, as to whether the pixel should be treated as corrupted or uncorrupted by noise. In this research, we implemented an adaptation of the algorithms 1 and 3 previously proposed in [6], and algorithm 2 is modified so that each thread labels the pixel as corrupted or not.

This paper is organized as follows: In section 2, the GPU is described together with CUDA programming models. Section 3 illustrates the noise correction method employed and its implementation on CUDA. Experimental results are shown in section 4, and lastly, the conclusions are presented in section 5.
2. GPU and CUDA programming models

Recent years have witnessed a spectacular growth in the parallel calculation capacity of Graphic Processing Units (GPU), due to the high demand for video game applications. Although initially these constituted the principle application of this hardware, in November 2006 NVIDIA introduced CUDA, a technology which enables these units to be used to develop programs for other calculation purposes. Such applications have become increasingly popular in the scientific community due to their combination of reasonable costs and good calculation power.

Physically, the GPU, called a device in CUDA terminology, contains a set of multiprocessors. These execute programs following the SIMD (Single Instruction, Multiple Data) model, whereby each of the multiprocessor’s processor clock cycles executes the same instruction applied to different data, taking into account each application if this instruction is performed by a different thread.

A device has a physical memory (the size of which may vary from 384MB to 1GB, in NVIDIA 9 series) that can be used in different ways. The main use is as global shared memory among the GPU multiprocessors. However, this memory also permits its several areas to be used in other modes:

- As local memory. Each thread may make individual use of 16KB of global memory.
- As texture. In this case, an area of the global memory is blocked in order to be used as read-only, in shared mode and optimized to store structures (arrays) of 1, 2 or 3 dimensions.
- As a constant reading area, shared between all the threads.

Internally, each multiprocessor has four kinds of memories [9]:

- A set of 32 bit registers per processor with read or write access.
- A read/write 16KB cache memory for optimizing access to the global memory, shared by all the multiprocessor processors.
- A constant read-only 64KB cache memory, shared by all the processors, which speeds up reading of the constant memory.
- A read-only cache memory called texture cache, which is shared by all the processors and accelerates reading of the texture memory.

The large variety of memories and their different features complicate the task of achieving optimum performance in programs using CUDA. One of the main issues that must be considered in order to obtain efficient programs is the coalescence of accesses to global memory.

Global memory is addressed in 16 or 32 byte displacements. Furthermore, it is possible to read 4, 8 or 16 Bytes of the global memory in a simple instruction. However, if a variable is not stored just after a memory address multiple of 16, or if its size is not a multiple of 4, more than one access must be performed, penalizing performance. In addition, when the GPU contains a large number of threads, this problem intensifies since even two threads may compete for access to the same memory area. When this happens, it is said that the accesses do not have coalescence [8], that is, they are not well aligned, a situation to be avoided at all costs. The most elemental method (although there are others) is for a thread with
value $i$ access to a value $i$ variable (or array index), and the access address to that point to become multiples of 16.

According to the CUDA programming model, it is necessary to distinguish between the code that is executed on the CPU ("host code" following CUDA terminology) and the code that is executed on each GPU core ("device code"). In particular, the function which we propose here for execution on the GPU takes the name of "kernel". A kernel is processed in parallel by a set of threads which will apply the instructions of that function to a different part of the data in the memory. When the GPU has several multiprocessors, the threads must be grouped in "blocks" to clarify assignment of the execution of a block to a specific GPU multiprocessor (nowadays, a block can contain a maximum of 512 threads). This particularity implies that threads can only be synchronized if they belong to the same block. Once a block of threads has finished, new blocks are launched in the empty multiprocessors.

Meanwhile, the CPU code must analyze the following steps in order to launch execution of the GPU kernels:

- Copy data from the host memory to the device memory.
- Run the kernel, deciding on the number of threads (and their organization in blocks) needed for the processing.
- Wait for kernel execution to finish before moving data from the GPU memory to CPU memory.

A kernel has a predefined variable enabling each thread to recognize its ID and, from this value, identify data to be processed. Initially, data are available in the GPU global memory but if coalescence problems arise, it becomes necessary to consider whether it would be advisable to copy data from the global memory to the cache memories of each multiprocessor in order to process them (returning them later to the global memory). Another option is to use textures, if part of the information is read-only and the information contained is organized dimensionally (in arrays).

As can be seen, the design problems of a CUDA program are:

- Deciding the number of threads and their organization in blocks.
- Deciding at each moment the best location (among the different available memories) for the input and output data, and how to access to them, performing the necessary copies at the appropriate time.

### 3. Image noise correction and implementation strategies with CUDA

In the present study, the process of image noise correction was divided into two steps. The first step was to detect erroneous pixels and the second, to eliminate them. The process was divided into two steps so that in the elimination step, the condition of neighboring pixels could be taken into account (whether previously evaluated as corrupted or not) when defining the new values for corrupted pixels.

For the detection stage, the fuzzy distance between the vectors of the color image $x_i$ and $x_j$ was used, which is given by the following function:
where \((x_i (1), x_i (2), x_i (3))\) is the color vector for the pixel \(x_i\) in space color RGB. In [6], \(k = 1024\) was shown to be an appropriate setting, and this was therefore the value that was used in the present study. Fuzzy distance measure is employed in peer group \(P(x_i, d)\), giving the central pixel \(x_i\) in a window \(W\) with size \(n \times n\) and \(d \in [0,1]\); \(P(x_i, d)\) represents the set:

\[
\{x_j \in W : M(x_i, x_j) \geq d\}.
\]

The peer group associated with the central pixel of \(W\) is a set consisting of the central pixel \(x_i\) and its neighbors belonging to \(W\), whose distance from \(x_i\) exceeds \(d\). After several tests, \(d = 0.95\) proved to be a good value for \(d\).

Detection was also divided into two phases, with two kernels for execution. In the first step (described in algorithm 1), the image was divided into \((N_1 \times N_2)/n\) windows \(W\) disjointed with dimension \(n \times n\), where \(n \in \{3,5,7, \ldots\}\); in the present case, \(n = 3\) was considered and the kernel was configured to set \((N_1 \times N_2)/n\) threads. Each thread analyzes their \(n \times n\) pixels of \(W\), \(x_i\) as the central pixel in \(W\), and \((f, c)\) for the thread. Given the parameter \(d\), each thread calculates its peer group.

**Require:** \(m, d\), image noise

1: Each thread defines the row and column corresponding to the central pixel \(x_i\) of the windows \(W\) disjoint.
2: Each thread builds its Windows \(W\) of pixels.
3: Calculate \(P(x_i, d)\) in \(W\).
4: **If** \((\#P(x_i, d) \geq m + 1)\)**
   5: thread mark:
   6: \(\forall x_j \in P(x_i, d), x_j\) as uncorrupted.
   7: \(\forall x_k \in W, x_k \notin P(x_i, d), x_k\) as undiagnosed.
5: **else**
   9: thread mark:
10: pixel \(x_i\) as provisionally corrupted.
11: \(\forall x_j \in W, j \neq i, x_j\) as undiagnosed.
12: **end if**

Algorithm 1: S1P1 - Step 1 Phase 1 Detection of erroneous pixels.

Once the value of \(m\) has been established (the optimal value according to [6], if the window is \(n \times n\), is \(m = n - 1\); in our case \(n = 3\) and \(m = 2\), if the peer group contains...
at least $m+1$ elements, then the thread labels the central pixel $x_i$ as uncorrupted and peer group members as uncorrupted. On the other hand, if the central pixel is declared as corrupted, members of the peer group are left as undiagnosed, and also as members of the window outside the peer group.

In the second step (described in algorithm 2), the kernel was reconfigured to set more threads in each block and many threads were set so that each thread processed one item of pixel data. The thread corresponding to the pixel $x_i$ (central pixel of a $n \times n$ window) labeled as undiagnosed calculates the peer group and if this satisfies the cardinality $m+1$, the central pixel is diagnosed as uncorrupted; if not, it is diagnosed as corrupted.

**Require:** m,d, threads corresponding to the pixels labeled as not diagnosed

Each thread defines the row and column corresponding to the central pixel $x_i$.

Each thread builds its Windows $W$ of pixels.

1: Calculate $\mathcal{F}(x_i, d)$ in $W$.
2: If ($\#\mathcal{F}(x_i, d) \geq m + 1$)
3: thread mark:
4: pixel $x_i$ as uncorrupted.
5: else
6: thread mark:
7: pixel $x_i$ as corrupted.
10: end if

Algorithm 2: S1P2 - Step 1 Phase 2 Detection of erroneous pixels.

In the correction step (described in algorithm 3), we used an equal number of threads for kernel 2. The threads corresponding to pixel $x_i$ apply filtering by substitution where this has been labeled as corrupted in step 1. The replacement value is determined by creating a window $W$ for the pixel $x_i$ and calculating the AMF (Arithmetic Mean Filter) on corrupted pixels $W$. Threads with uncorrupted pixel values continue as before.

**Require:** n, threads corresponding to the pixels labeled as corrupted

Each thread defines the row and column corresponding to the central pixel $x_i$.

Each thread builds its Windows $W$ of pixels.

1: Calculate the AMF of uncorrupted pixels $W$.
2: Thread corresponding to the pixel $x_i$ replaces value obtained by the AMF.

Algorithm 3: S2 - Step 2 Elimination of erroneous pixels.

To determine the number of threads per block that best fits the application, a heuristic study concluded that $64 \times 64$ threads per block gave lowest computational costs. The function `cudaMallocPitch` was used to ensure optimal global memory alignment of the pixels through textures.
As can be observed in section 2, a series of choices must be considered in order to implement an algorithm on CUDA. In the present case, two strategies were employed:

- Storing the image with 3 channels per pixel or 4 channels per pixel.
- Accessing data through the texture memory or not

Deciding whether to store the image in RGB (three channels) or RGBA (3 channels + padding) is necessary since the RGB format uses 3 bytes and thus does not achieve access coalescence. However, if a padding byte is added, even using a time for it, the accesses will fit in blocks of 4 bytes and performance may improve. Furthermore, the addition of a fourth byte can be used to indicate pixel status: corrupted, uncorrupted or undiagnosed.

In addition, we evaluated the improvements deriving from the use or not of texture memory. For this research, two textures were used: one in the first phase of detection, another in phase 2 and in the elimination phase. In all cases, these were used with the purpose of reading \(x_i\) neighboring pixels in the fuzzy and peer group calculations. In the detection phase, and once the pixels are in the device memory, each block thread reads its corresponding pixel for analysis, together with its neighbors, through two texture. At the end of this stage, the RGB fill channel contains the state of the pixel: corrupted, uncorrupted or undiagnosed.

In the elimination phase, each thread reads its corresponding pixel, together with its neighbors, through the two texture. Once this is completed, the new values are written onto the pixel which has been analyzed.

4. Experimental results

This section presents the results obtained for the implementations discussed in section 3. The CPU used was a Mac OS X Intel Xeon Quad-Core processor at 2 x 2.26 GHz with 8GB memory. The GPU was an NVIDIA GeForce GT 120 with 512MB of memory. Our implementation used C language. Many images are used in the area of image processing; for the present research, the lenna image [6] was employed, with RGB format square dimensions 256, 512, 1024 and 2048 pixels and 5 and 10% noise impulse.

For each algorithm, we designed both the CPU serial code and the GPU parallel code and then compared execution time. When calculating execution time, data transfer time from host memory to device memory was not considered.

The first experiment on GPU was to run the three algorithms for correction of erroneous pixels in RGB and RGBA format (strategy a Section 3), whilst the second experiment used textures (strategy b of section 3). Table 1 and Figure 1 show a comparison of computational costs obtained by the process described.
IMPLEMENTING A GPU FUZZY

Table 1. Processing time (msec) for the CPU and GPU-based implementations.

<table>
<thead>
<tr>
<th>Size</th>
<th>5% noise</th>
<th>10% noise</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RGB</td>
<td>RGBA</td>
</tr>
<tr>
<td>246</td>
<td>4.25</td>
<td>3.09</td>
</tr>
<tr>
<td>512</td>
<td>20.56</td>
<td>12.59</td>
</tr>
<tr>
<td>1024</td>
<td>87.14</td>
<td>51.01</td>
</tr>
<tr>
<td>2048</td>
<td>408.67</td>
<td>250.96</td>
</tr>
</tbody>
</table>

Figure 1. Comparison GPU for RGB, RGBA and Texture. 5% impulse noise.

It can be seen that in the case of using the RGBA format on GPU with 5% noise, the improvement is at worst 27% for the 256 image size and at best, 41% for the 1024 image size, compared to RGB implementation. On the other hand, with 10% noise, the performance is at worst 27% for the 256 image size and at best, 44% for 2048 image size. The best performance was obtained when using GPU with texture, since the improvement is approximately 45% with 5% noise and 43% to 49% with 10% noise compared to RGBA (without texture) implementation. The results regarding relative GPU time spent by each kernel are shown in Table 2.

As can be seen, the computational cost of S1P1 is less than that for S1P2 in all cases. For RGB strategy S2, computational cost is less than that for S1P2 with image sizes 2048.
IMPLEMENTING A GPU FUZZY

<table>
<thead>
<tr>
<th>Strategy</th>
<th>Kernel</th>
<th>Step 1 Phase 1</th>
<th>Step 1 Phase 2</th>
<th>Step 2</th>
</tr>
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<tr>
<td></td>
<td></td>
<td>(S1P1)</td>
<td>(S1P2)</td>
<td>(S2)</td>
</tr>
<tr>
<td>GPU time</td>
<td>RGB</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>256</td>
<td>0.59</td>
<td>1.77</td>
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<td>512</td>
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<td>1024</td>
<td>17.41</td>
<td>34.61</td>
<td>35.12</td>
<td></td>
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<tr>
<td>2048</td>
<td>77.56</td>
<td>175.03</td>
<td>156.08</td>
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<tr>
<td>GPU time</td>
<td>RGBA</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>256</td>
<td>0.44</td>
<td>1.29</td>
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</tr>
<tr>
<td>512</td>
<td>2.33</td>
<td>4.61</td>
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<td></td>
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<tr>
<td>1024</td>
<td>11.03</td>
<td>17.40</td>
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<td>GPU time</td>
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<tr>
<td>256</td>
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<td>0.63</td>
<td>0.73</td>
<td></td>
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<tr>
<td>512</td>
<td>1.69</td>
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<td>2.88</td>
<td></td>
</tr>
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<td>7.34</td>
<td>10.22</td>
<td>11.76</td>
<td></td>
</tr>
<tr>
<td>2048</td>
<td>40.36</td>
<td>44.05</td>
<td>52.51</td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Computational times for kernels.

To conclude the comparison, CPU times are compared with GPU times (image with textures) in Table 3 and Figure 2.

<table>
<thead>
<tr>
<th>Size</th>
<th>Textures GPU</th>
<th>CPU</th>
<th>Speedup</th>
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<tr>
<td>246</td>
<td>1.79</td>
<td>111.88</td>
<td>62.30</td>
</tr>
<tr>
<td>512</td>
<td>7.11</td>
<td>467.63</td>
<td>65.69</td>
</tr>
<tr>
<td>1024</td>
<td>29.33</td>
<td>1932.72</td>
<td>65.89</td>
</tr>
<tr>
<td>2048</td>
<td>136.92</td>
<td>7907.12</td>
<td>57.75</td>
</tr>
</tbody>
</table>

Table 3. Speedup for different image sizes.

Figure 2. Comparison GPU (texture strategy) and CPU.
As can be seen, excellent results were obtained by using optimization with textures on GPU compared with CPU for this application. Figure 3 shows the speedup (speed performance of one implementation with respect to another) when comparing the sequential version running on CPU and the parallel version on GPU using textures. As can be seen, even the worst result for the GPU version is 57 times faster than sequential, which is an excellent outcome.

![Graph showing speedup for different image sizes](image)

Figure 3. GPU vs CPU speed-up for different image sizes.

Finally, although not the objective of this research, we would highlight the quality obtained for impulse noise correction using the method described in Section 3, of 5 and 10% in different image sizes compared with the result in [6]. Table 4 shows the results using the measures PSNR (Peak Signal-to-Noise Ratio) [12], MAE (Mean Absolute Error) and NCD (Normalized Color Difference).

<table>
<thead>
<tr>
<th>Filter</th>
<th>5%</th>
<th>10%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MAE</td>
<td>PSNR (10^-2)</td>
</tr>
<tr>
<td>VMF</td>
<td>2.775</td>
<td>32.051</td>
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<tr>
<td>DDF</td>
<td>2.764</td>
<td>31.808</td>
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<tr>
<td>BVDF</td>
<td>2.985</td>
<td>31.382</td>
</tr>
<tr>
<td>FIVF</td>
<td>0.414</td>
<td>35.685</td>
</tr>
<tr>
<td>PGF m=2</td>
<td>0.404</td>
<td>37.996</td>
</tr>
<tr>
<td>FMPGF m=2</td>
<td>0.521</td>
<td>36.196</td>
</tr>
<tr>
<td>GPU FMPGF m=2</td>
<td>0.500</td>
<td>36.220</td>
</tr>
</tbody>
</table>

Table 4. Quality Comparison.

As can be seen, the quality achieved by implementing this algorithm in parallel is competitive.
5. Conclusions

In this paper we have described a study conducted in order to determine the best method for implementing image correction processing in RGB format with impulsive noise on a GPU using a CUDA platform. This processing was divided into two steps: noise detection and noise elimination. For detection, the fuzzy measure and the concept of peer group were used, obtaining a set with pixels similar to a given and then deciding, according to the cardinality of the set, whether the pixel was noisy or not. In the correction stage, corrupted pixel values were replaced by calculating the mean of those neighbors not labeled as corrupted in the first stage.

The experimental results show that if the accesses are coalescing, the results improve significantly. This is demonstrated by the versions in which we added one padding byte to the three-byte RGB format dedicated to each pixel. Additionally, this byte is useful for storing the assessment of whether the associated pixel is corrupted or not, making it unnecessary to access another area of global memory for this purpose. Furthermore, we have also shown that the use of textures for accessing data in global memory is less complex compared, for example, with versions used in multiprocessor caches to avoid accesses to the global memory (since this would have to include codes performing the copy.) Likewise, through the use of textures we have obtained outstanding results in speed, compared to sequential versions of the implementation, in the order of approximately 65%.

Based on the results of this study, we would suggest two future lines of research. Firstly, optimal utilization of CUDA on GPUs would be interesting in order to obtain implementations for large images, spread the processing load between multiple GPUs available in the system and evaluate performance. The second line of research would be GPU implementation of the improvements in computational times and quality achieved using the implementation developed in this work.

6. Acknowledgements

This work was funded by the Spanish Ministry of Science and Innovation (Project TIN2008-06570-C04-04) and Ma. Gpe. would also like to acknowledge DGEST-ITCG for the scholarship awarded through the PROMEP program (Mexico).

References

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Gas Transport in the Near-Surface Porous Layers of Cosmic Bodies

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Abstract

The gas transport through non-volatile random porous media is investigated numerically. We extend our previous research of the transport of molecules inside the uppermost layers of space bodies, assess the validity of the simplified capillary model and its assumptions to simulate the gas flux through the porous non-volatile layer as it has been applied in planetary physics. A microphysical computational model for molecular transport in random porous media formed by packed spheres is presented. The main transport characteristics such as the mean free path distribution and the permeability are calculated for a wide range of model parameters and compared with those obtained by more idealized models. Finally a practical way is suggested to adjust the algebraic Clausing formula taking into consideration the nonlinear dependence of permeability on layer porosity. The retrieved dependence allows us to accurately calculate the permeability of layers whose thickness and porosity vary in the range of values expected for the near-surface regions of a cometary nucleus.

Key words: gas, porous media, planetary physics

As the physical models of the surface layer structure become more sophisticated and possibly more realistic (e.g. material may be porous, its composition may include a variety of volatile and non-volatile additives, etc.) determination of the
GAS TRANSPORT IN THE SURFACE LAYER

effective gas production is becoming a more and more complicated problem. Various aspects of this fundamental problem of planetary physics were considered by us in numerous articles published over the past few years (e.g., [1], [2]). Here we focus on the release of gas through a porous non-volatile surface layer of a cosmic body.

1. Capillary models of gas transfer through a porous dust layer

The vast majority of publications containing theoretical modeling of gas transfer in the uppermost porous layers of a space body uses one and the same basic algebraic formula to calculate effective gas activity - namely, the formula of Knudsen, that describes the mass flow rate per unit capillary area

$$\Psi_K = \left( \frac{32m}{9\pi k} \right)^{1/2} \frac{r}{L} \left( \frac{P_t(T_t)}{\sqrt{T_t}} - \frac{P_b(T_b)}{\sqrt{T_b}} \right)$$

where $r$ is the channel radius, $L$ is the length, $(P_b, T_b)$ and $(P_t, T_t)$ are pressures and temperatures at the bottom and top of the channel, respectively. This formula is very popular in planetary physics and has been used without change for almost thirty years [3]. The Knudsen formula refers to a very simple model of the porous medium as a bundle of disjoint, straight cylindrical capillary channels of radius $r$, and length $L$ with diffusively scattering walls. The gas in the channel is in the free-molecular regime, i.e. the intermolecular collisions are negligible, whereas scattering by the walls plays a major role. A simple generalization of the Knudsen approach exists which allows us to calculate the rarefied gas flow in a Knudsen regime through a cylindrical tube of arbitrary length with diffusion scattering walls with high accuracy. This is the Clausing formula which apparently was for the first time considered in cometary physics by Steiner [4]:

$$\Psi_C = \left( \frac{m}{2\pi k} \right)^{1/2} \frac{20 + 8(L/r)}{20 + 19(L/r) + 3(L/r)^2} \left( \frac{P_t}{\sqrt{T_t}} - \frac{P_b}{\sqrt{T_b}} \right)$$

He also performed a quantitative comparison of the Knudsen and the Clausing formulas and showed that even for a sufficiently long channel in which the ratio of length to radius equals 10, the gas flow calculated using the former formula is overestimated by 50%, while for short tubes ($L \approx r$) the relative error is about eight times higher. Later Skorov et al. [1] applied this approach for modeling a gas flow through a cylindrical tube with icy walls of varying temperature.

Both formulae considered above were obtained for the molecular gas flow in a tube, while our ultimate goal is the calculation of gas flow in natural stochastic porous media, where statistically the length of a void is the same in any arbitrary
direction. The transition from the model of a single pipe to the model of porous medium can not be realized in a simple way when the capillary approach is used. The other serious obstacle for use of the capillary models in planetary physics applications is the anisotropic character of the model generated medium. In order to compensate for this problem an additional model parameter the above-mentioned tortuosity, $\tau$, is usually added. The formal purpose is to replace a straight cylindrical channel by a broken one of greater length and thereby to make the model environment more isotropic. Unfortunately the tortuosity can be introduced in a non-unique way into the simplest capillary model. For a natural porous media the tortuosity is an empirical quantity, that should be determined from the experiments. Note that, in contrast to porosity, tortuosity can not be easily measured directly. Often it is derived from independent measurements of the Knudsen diffusion coefficient and porosity.

2. Models of granular packed bed

There is an alternative way to describe the Knudsen diffusion in a porous medium - a way where the molecular gas flow is regarded to be external to the nonvolatile matrix: “flow around obstacles”. The matrix itself is constructed (composed) of elementary scattering or absorbing objects, for example, spheres. Interaction of gas molecules with the surfaces of matrix elements is similar to interaction with the walls of a capillary in the models of the first type. Thus, the weakening of gas flow and reduction of effective diffusion rate can be well modeled as before.

We generate porous media consisting of mono-disperse spheres using two different methods: ballistic deposition (RBD) and random sequential packing (RSP). For RBD spheres are dropped one by one vertically into a control volume where they touch either the bottom or another sphere. The porosity of media generated by RBD is about 0.85, with a more compact base and a fluffier top. For RSP spheres are placed one by one at random locations within a control volume. Locations that would result in overlapping spheres are rejected. This results in a homogeneous, isotropic medium with a porosity that can be determined by specifying the total number of spheres used. We generated media with porosities of 0.65, 0.70, 0.75, 0.80 and 0.85.

In order to estimate the transport properties of the model media we apply the random walk algorithm used extensively in studies of disordered granular media. The major characteristics of a porous layer that are important for planetary applications are the permeability and the resulting return flux. These characteristics are examined by tracing the geometric paths of a large number of test particles through the medium using the Monte Carlo method. We use 100,000 test particles for each simulation. Since the outflow is assumed to be rarefied, intermolecular collisions and particle velocities are not considered. Therefore, the geometric paths of test particles only are a result of their starting direction and
subsequent interactions with the spheres that represent the nonvolatile matrix. These interactions are modeled as either specular reflections or diffuse scattering.

3. **Results and conclusions**

The present work aims at three primary goals:

- Revise or adjust the capillary models used in planetary physics to describe the transport of sublimation products through porous nonvolatile layer accurately.
- Present alternative description of porous media based on ballistic deposition and random sequential packing methods. Use direct statistical simulation to retrieve major geometrical and transport properties of model media as a function of porosity and layer thickness.
- Suggest a way to adjust the Clausing formula taking into consideration the nonlinear dependence of permeability on layer porosity.

In view of these goals we summarize below the main results:

Knudsen’s formula is not applicable for modeling the gas transport through short channels. Satisfactory agreement with experimental data is achieved only when the channel radius is much smaller than its length. As an alternative, Clausing’s formula can be used. This formula gives an exact agreement with the experimental data for straight cylindrical channels with an arbitrary ratio of radius to length. However, the spatial anisotropy of the capillary model leads to the fact that its transfer characteristics are highly different for different directions. The transition from the permeability of one channel to the permeability of the medium can not be accurately and correctly generalized. Adding an additional linear factor - tortuosity to the formula does not solve the problem, but on the contrary, only confuses the situation.

To avoid these inconsistencies accurate statistical calculations are performed for media formed either by ballistic deposition (RDB) of test particles or by random filling of a control volume (RSP). Two types of interaction of molecules with scattering spheres are tested: diffuse and specular scattering. It turns out that for the random model of the porous medium the permeability is virtually independent of the type of interaction. We show that a relatively small variation of porosity (not more than 30%) leads to a strong change of permeability. The permeability depends on the medium porosity in a nonlinear way.

In order to overcome the resource consuming calculations for direct use of the statistical models, we present a practical way to calculate the effective permeability. We preserve the overall structure of Clausing’s formula, accurately describing the kinetics of transport through a single cylindrical capillary. To take into consideration the porosity of the medium in an appropriate manner we
assume that the effective radius of the capillary is an unknown function of porosity. The explicit form of this functional dependence is derived from a nonlinear approximation based on statistical modeling results. Thus, the effective permeability, as before, depends on the thickness of the layer and its effective pore size, which in turn is a function of porosity. The retrieved algebraic expression allows us to accurately calculate the permeability of layers whose thickness and porosity vary in the range of values expected for the near-surface regions of a cometary nucleus. The simplicity of this approach makes it practical to include the computational block that accurately describes the transport of gas in the overall thermal model of a cometary nucleus.

This work was supported by the German Research Foundation (DFG grant BI 298/9-1).

4. References

Fuzzy Model for Improving Accuracy in Real-Time Location Systems

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Abstract

Wireless Sensor Networks (WSN) have become much more relevant in recent years, mainly because they can be used in a wide diversity of applications. Real-Time Location Systems (RTLS) are one of these applications and represent a currently growing market. However, accuracy in RTLS is still a problem requiring novel solutions. This paper presents an innovative mathematical fuzzy model for improving the accuracy of RTLS. The proposed approach and the preliminary results obtained are presented in this paper.

Key words: Wireless Sensor Networks, Real-Time Location Systems, Location Algorithms, Fuzzy Logic, Artificial Neural Networks.

1. Introduction

Wireless Sensor Networks allow us to obtain information about the environment and act on this, expanding users’ capabilities and automating daily actions. One of the most interesting applications for WSN is the Real Time Localization System (RTLS). Although outdoor localization is covered to a large degree by systems such as GPS, indoor localization is still an area in need of development, especially with respect to locating people or objects within an enclosure [13] [14].
Mathematical model for a temporal-bounded classifier in security environments
Therefore, it is in indoor spaces that localization presents the most difficulty. For this, it has become necessary to develop systems that allow the performance of efficient localization in terms of precision and optimization of resources (for example, sensor infrastructure and calculation capacity). The process necessary for carrying out localization must take into account the type of sensors used and the algorithm applied for the calculation of the final position based on the information recovered by these sensors.

Amongst the technologies that are currently used most in the development of RTLS are, RFID (Radio Frequency IDentification), Wi-Fi y ZigBee [3] [4] [5]. However, in addition to the technology used, it is necessary to establish mathematic models that allow us to determine the position from the signals recovered. For this, various algorithms exist, such as Triangulation, Fingerprinting and Multilateration [10]. However, these models present important disadvantages when developing a precise localization system, especially indoors. Therefore, it is necessary to define new models that allow the improvement of precision in this type of system.

In this article, a new model based on fuzzy logic is presented in order to improve the precision of localization systems based on wireless sensor networks, in real time. The basic functioning of these systems is as follows: Firstly, it is necessary to place a fixed node network within the space where localization will be carried out. In turn, a series of mobile nodes exist, generally called "tags", which periodically transmit a signal that contains their identifier in the network. That signal is detected by the fixed nodes within their coverage area, containing power measurements (RSSI: Received Signal Strength Indication) and quality (LQI: Link Quality Indicator) of the signal received. A central node compiles all the reference measurements from all of the fixed nodes in the network and sends them to a computer to be processed. The model proposed in this article takes RSSI as inputs and based on this executes an estimation of the position of each of the mobile nodes in the system. In a first stage, the model establishes the most probable position of each mobile node based on the RSSI levels. In the second stage, the data generated is used by the diffused model to train an MLP neuronal network [2] which will be what finally estimates the positions when the system has already been trained.

The paper is structured as follows: Section 2 presents different localization techniques. Section 3 describes the planning model. Section 4 describes a set of tests evaluating our proposal.

2. Localization Systems

Localization Systems allow the identification and localization of different elements in an environment. Localization Systems are composed of two elements: sensors and tags. The tags are placed on the elements while the sensors are normally placed in fixed points, that way generating a sensor network which allows us to locate different devices.
Mathematical model for a temporal-bounded classifier in security environments

Currently, different systems of localization exist based on the technology used, and the different alternatives are:

- **GPS:** The operation of a real time localization system based on GPS (Global Positioning System) basically consists of a set of satellites (fixed transmitters) that constantly send information, which is collected by mobile devices (receivers). The receivers calculate their position based on the coordinates of the satellites, so the more satellite references had, the better the precision. It is necessary to have at least 3 satellite references in order to be able to calculate the position.

- **GSM/GPRS:** Mobile phone operators also offer localization services. Their operation is based on using the same network of antennas that the telephone service provides. In this case, localization can be carried out as much by the mobile device as by the service provider, due to the fact that antennas and devices both act as transmitters and receivers. To calculate localization, they use parameters such as the time of arrival of the signal, incidence angles, triangulation of signals or belonging cells.

- **RFID:** Radio Frequency IDentification (RFID) [3] is another of the alternatives used for the development of real time localization systems. Its operation is based on a network of RFID readers and tags. The readers transmit a constant RF signal, which is collected by the tags, which in turn respond to the readers by sending a number of identification. In this type of localization, each reader covers a determined zone through its RF signal (reading field) When a tag passes through the reading field of the reader, it is said that the tag is in that zone. An RFID system is mainly composed of four elements: 1) Tags, 2) Readers, 3) Antennas and Radios and 4) Processing Hardware [4] [5]. RFID tags or chips can be passive (without batteries), in which case they are called transponders [3]. Transponders are much cheaper and smaller than active chips (with batteries), but have much less of a reach range. The main RFID technology applications have taken place in industrial, transport environments, etc., but their application in other sectors, including medicine, is increasingly important [3][4] [5].

- **Wi-Fi:** Localization systems based on WiFi [6] employ wireless network devices to calculation position. A mesh of nodes is employed (fixed transmitters and receivers) which function as a reference for mobile nodes. The system calculates the position of the mobile nodes starting from the signals received by the fixed nodes. A large amount of techniques exist for processing these signals and determining their position, including symbolic or signpost localization, triangulation, trilateration, etc. Localization based on Wi-Fi has three main components: 1) An RFID tag that transmits and receives signals under the regulation 802.11 [7], 2) a WLAN infrastructure, formed by access and controller points, and 3) a localization engine, consisting of software capable of interpreting
Mathematical model for a temporal-bounded classifier in security environments

information provided by the Wi-Fi infrastructure and tags to provide data
relating to the location of users [6].

- The ZigBee standard allows operation in the ISM (Industrial, Scientific
  and Medical) band, which includes 2.4GHz almost all over the world. The
underlying IEEE 802.15.4 standard is designed to work with low-power
nodes with limited resources. ZigBee adds network and application layers
over IEEE 802.15.4 and allows more than 65,000 nodes to be connected in
a mesh topology WSN. Another standard for deploying WSNs is
Bluetooth. This standard also operates in the 2.4GHz band and allows
the creation of star topology WSNs of up to 8 devices, one acting as master
and the rest as slaves, but it is possible to create larger WSNs through
devices that belong simultaneously to several WSNs. However, it is not
easy to integrate devices from different technologies into a single WSN
[1]. The lack of a common architecture may lead to additional costs due to
the necessity of deploying interconnection elements amongst different
WSNs.

The most adequate technology for indoor localization is that based on ZigBee
since others such as GPS can only be used outdoors as it is necessary to receive
satellite signal. Other networks like GSM allow the implementation of
localization but the margin of error is too high so it is not considered to be
adequate for use as is the case with WI-FI.

3. Localization Algorithms

There are three main algorithms employed by real time localization systems for
determining the position of mobile nodes (tags): Triangulation, Fingerprinting and
Multilateration [10]. Triangulation allows us to obtain localization coordinates
through the calculation of longitude of the sides of a triangle from the input angles
of the received signal in each antenna, for which it is necessary to provide at least
3 reference points [10]. Fingerprinting, also known as signpost or symbolic
localization, is based on the study of the characteristics of each area of
localization, carrying out measurements of radio frequency characteristics and
estimating in which area of influence each tag is found [1][11]. Finally,
Multilateration is based on the estimation of distances from the readers to the tags
by measuring parameters such as RSSI (Received Signal Strength Indication) or
TDOA (Time Difference of Arrival) [12], so that intersecting the estimated
differences from each tag to three or more fixed nodes can determine the points
where these tags are found. Multilateration allows us to obtain better results
outdoors than with triangulation, but its performance lowers notably indoors. This
is because indoor RSSI levels will vary in function of the presence of elements
(people, objects or animals) and are also based on the calculation of distances, so
that it is necessary to carry out a prior estimation of these distances starting from
RSSI values which change constantly.
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For this, we propose a new model which makes use of fuzzy logic and neural networks to improve the calculation of the position of mobile nodes. This model is described below.

3.1. New Fuzzy Model

The model proposed in this article is based on the level of the RSSI signal (Received Signal Strength Indication) detected by the nodes (sensors). The absolute value of RSSI is exponentially related to the distance that is found. Therefore, initially it seeks to convert these values in such a way that the connection is more linear although it is not necessary to carry out a precise conversion. In figure 1, there is an example of the operation of a sensor network and a tag. The sensors have been represented in red and the tag in the centre of the image is represented in blue. For each of the sensors, some circles have been represented related to a logarithm of the absolute value of the RSSI detected. The colour of the circles is related to the radio coverage. Thus, it can be seen that the circles intersecting different regions so that the darkest region is the one found closest to the point.

![Figure 1. Graphic representation of localization based on RSSI levels.](image)

From the information shown in the previous figure, we can proceed to making an estimation as to the most likely regions in which there is a tag. For this, for each one of the cells a relevance index is calculated based on the circles that are drawn...
Mathematical model for a temporal-bounded classifier in security environments over it, finally having something similar to that shown in Figure 2. The darker the colour of the cell, the greater the possibility of finding a tag in this cell.

![Graphic representation of the possibility of localization in each of the cells. The darker the cell is, the higher the probability.](image)

**Figure 2.** Graphic representation of the possibility of localization in each of the cells. The darker the cell is, the higher the probability.

Finally, once the region with the most possibility is determined, the midpoint, which will represent the estimated location of the node, is calculated. Due to the fact that the RSSI level does not remain constant and that it will vary according to rebounds from appropriate waves emitted by the sensors, it is necessary to stabilize the positions through the use previously estimated values. For this, the relevance index for each cell is calculated depending on what has previously been observed. Thus, the calculation process of levels follows the algorithm below. In equation (1) the calculation of each relevance index of the tags to each cell is shown.

\[
w_{ij}(t+1) = \frac{w_{ij}(t) + f_r(\vec{r}(t)) \cdot k}{k+1}
\]

(1)

where t represents the sequence, \(w_{ij}\) the index of pertinence of the tag to the cell \(ij\), \(k\) the rate of update and \(f_r\) the function of calculation of the new index based on the vector \(r\) of sensitivities. \(f_r\) is defined in function of the equation (2).

\[
f_r(\vec{r}(t)) = \sum_{k=1}^{n} \frac{1}{|r_k(t)|}
\]

(2)
Mathematical model for a temporal-bounded classifier in security environments \( \tilde{r}(t) \) is the vector of signal intensities corresponding to the sensors that have detected the tag. In this vector, only the sensor readings for the distances between them are included and the cell is less than the range of the sensor for the sensitivity detected. Namely, the vector only stores the sensor component if the cell that is found within the circle corresponds to the sensor as in Figure 1. Formally \( \tilde{r}(t) \) is described in the following manner:

\[
\tilde{r}(t) = \{ \log(|RSSI_j| \* p_j(RSSI) / d(c, s_j)) < \log(|RSSI_j|) \} 
\]

(3)

where \( j \) represents each one of the sensors that detect the tag \( y \) \( d(c, s_j) \) the Euclidian distance between the cell \( c \) and the sensor \( j \). \( p_j \) represents a weighting based on the levels of RSSI detected. The weighting is used due to the fact that not all the RSSI levels are equally reliable due to interference. Thus the values obtained between -51 and -80 are less reliable than those obtained from 80 and much less than values near 1 so that a weighting is defined based on these values. The weighting chosen follows the equation below (4).

\[
p_j(RSSI) = \begin{cases} 
  k_1 & -1 < RSSI < l_1 \\
  \vdots \\
  k_r & l_{r-1} < RSSI < l_r \\
  \vdots \\
  k_n & RSSI > l_{n-1} 
\end{cases} 
\]

(4)

The final position of the sensor is estimated according to the middle position of the cells with a greater probability rate of belonging to equation (5).

\[
l = \frac{\sum_{i=1}^{n} p_j}{n} 
\]

(5)

### 3.2. Operation Stage

As the fuzzy model is capturing data, from the signals and estimating positions, it stores these in a memory to subsequently use to carry out the training of an MLP. The neural network allows us to make the fastest estimations and is more responsive to variations resulting from the reflections of the waves emitted. Input data from the neural network corresponds with the intensity values detected by a pre-fixed number of sensors. Output has two coordinates, one for the space coordinate. The number of neurons in the hidden layer is \( 2n+1 \), where \( n \) is the number of neurons in the input layer. Finally, there is one neuron in the output layer. The activation function selected for the different layers has been the
Mathematical model for a temporal-bounded classifier in security environments sigmoid. Taking into account the activation function $f_j$, the calculation of output values is given by the following expression

$$y_j^p = f_j\left(\sum_{i=1}^{N} w_{ji}(t) x_i^p(t) + \theta_j\right)$$

(6)

The neurons exiting from the hidden layer of the neural network contain sigmoidal neurons. Network training is carried out through the error Backpropagation Algorithm [2].

4. Results and Conclusions

To analyze the system we proceeded to install a network of ZigBee devices in a laboratory. The sensor network was formed by 15 fixed devices distributed in 3 rooms, following the distribution shown in figure 3. The dimensions in meters are 19x19m.

![Figure 3. Distribution of the network of ZigBee devices in the laboratory](image)

To analyze the results, an estimation of error was carried out in 19 measurements and the error during the training and estimation phases was calculated. Figure 4 shows the sensors, the real location of the tags and the estimated locations using the multilateration and fuzzy methods.

![Figure 4. Location of tags using Multilateration and Fuzzy](image)
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Figure 5 shows the estimated errors obtained using the fuzzy, Multilateration and the localization models described in section 3. The X axis represents the different measurements and the Y axis, the Euclidian distance in meters from the estimated position to the real position of the tag.

![Figure 5. Prediction Errors in meters](image)

The proposed model is capable of carrying out localization of the tags in a more precise way. Furthermore, it allows us to carry out an estimation which subsequently makes the estimation of positions though the use of a neural network possible. The neural network improves the operation of the fuzzy model since it has a greater capacity for adaptation than fuzzy models. Thus, measuring errors due to noise have less effect.

Acknowledgements

This work has been supported by the MICINN TIN 2009-13839-C03-03 project and the Professional Excellence Program 2006-2010 IFARHU-SENACYT-Panama.

References

Mathematical model for a temporal-bounded classifier in security environments
Solving Multi Objective Stochastic Programming Problems using Differential Evolution

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Abstract

Stochastic (or probabilistic) programming is an optimization technique in which the constraints and/or the objective function of an optimization problem contains random variables. The mathematical models of these problems may follow any particular probability distribution for model coefficients. The objective here is to determine the proper values for model parameters influenced by random events. In this study, DE and its two recent variants LDE1 and LDE2 are presented for solving multi objective linear stochastic programming (MOSLP) problems, having several conflicting objectives. The numerical results obtained by DE and its variants are compared with the available results from where it is observed that the DE and its variants significantly improve the quality of solution of the given considered problem in comparison with the quoted results in the literature.

Key words: Differential Evolution, stochastic programming, multiobjective optimization.

1 Introduction

Stochastic programming (SP) is a mathematical programming where stochastic element is present in the data. In contrast to deterministic mathematical
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programming where the data (coefficients) are known numbers in stochastic programming these numbers follow a probability distribution. Thus we can say that SP is a framework for modeling optimization problems that involve uncertainty. The goal here is to find some policy that is feasible for all (or almost all) the possible data instances and maximizes the expectation of some function of the decisions and the random variables. More generally, such models are formulated, solved analytically or numerically, and analyzed in order to provide useful information to a decision-maker.

In the recent past, SP has been applied to the problems having multiple, conflicting and non-commensurable objectives where generally there does not exist a single solution which can optimize all the objectives. Several methods for solving Multi-Objective Stochastic Linear Programming (MOSLP) problems and their applications to various fields are available in literature [1] – [7]. Most of the probabilistic models assume normal distribution for model coefficients. Sahoo and Biswal [8] presented some deterministic equivalents for the probabilistic problem involving normal and log-normal random variables for joint constraints. Charles et al. [9] addressed different forms of distributions like Power Function distribution, Pareto distribution, Beta distribution of first kind, Weibull distribution and Burr type XII distribution. In the present study we have followed the models proposed by Charles et al [9] and have solved them using Differential Evolution (DE).

The rest of the paper is organized as follows: Section 2 briefly describes the classical DE, LDE1 and LDE2 algorithms. The problem definition is given in section 3. In section 4; the experimental settings and numerical results are discussed. Finally the paper concludes with section 5.

2 Differential Evolution Algorithms

2.1 Classical Differential Evolution (DE)

Differential Evolution (DE) [10] is a population based metaheuristics that has been consistently ranked as one of the best search algorithm for solving benchmark as well as real life problems in several case studies. The algorithm mainly has three advantages; finding the true global minimum regardless of the initial parameter values, fast convergence, and uses a few control parameters [11]. DE has been successfully applied to solve a wide range of real life application problems such as clustering [12], unsupervised image classification [13], digital filter design [14], optimization of non-linear functions [15], global optimization of non-linear chemical engineering processes [16] and multi-objective optimization [17] etc. Also it has reportedly outperformed other optimization techniques [18] – [20].
A general DE variant may be denoted as $DE/X/Y/Z$, where $X$ denotes the vector to be mutated, $Y$ specifies the number of difference vectors used and $Z$ specifies the crossover scheme which may be binomial (bin) or exponential (exp). Throughout the study we shall consider the mutation strategy $DE/rand/1/bin$ [10] which is perhaps the most frequently used version of DE.

For a D-dimensional search space, each target vector $x_{i,g}$, a mutant vector is generated by

$$v_{i,g+1} = x_{r_1,g} + F \times (x_{r_2,g} - x_{r_3,g})$$

(1)

where $r_1, r_2, r_3 \in \{1, 2, \ldots, NP\}$ are randomly chosen integers, must be different from each other and also different from the running index $i$. $F (> 0)$ is a scaling factor which controls the amplification of the differential evolution $(x_{r_2,g} - x_{r_3,g})$. In order to increase the diversity of the perturbed parameter vectors, crossover is introduced. The parent vector is mixed with the mutated vector to produce a trial vector $u_{j,i,g+1}$,

$$u_{j,i,g+1} = \begin{cases} v_{j,i,g+1} & \text{if } \text{rand } j \leq CR \lor j = k \\ x_{j,i,g+1} & \text{otherwise} \end{cases}$$

(2)

where $j = 1, 2, \ldots, D$; rand $j \in [0, 1]$; CR is the crossover constant takes values in the range $[0, 1]$ and $j_{\text{rand}} \in \{1, 2, \ldots, D\}$ is the randomly chosen index.

The final phase of DE algorithm is selection. Here the population for the next generation is selected from the individual in current population and its corresponding trial vector according to the following rule:

$$x_{i,G+1} = \begin{cases} u_{i,G+1} & \text{if } f(u_{i,G+1}) \leq f(x_{i,G}) \\ x_{i,G} & \text{otherwise} \end{cases}$$

(3)

Thus, each individual of the advance (trial) population is compared with its counterpart in the current population. The one with the lower objective function value will survive from the tournament selection to the population of the next generation. As a result, all the individuals of the next generation are as good as or better than their counterparts in the current generation.

### 2.2 Laplace Differential Evolution (LDE)

The LDE algorithms are proposed by Thangaraj et al. [21]. These algorithms differ from the classical DE in the mutation phase in a twofold manner. These schemes make use the absolute weighted difference between the two vector points in place of the usual vector difference as in classical DE and secondly, in LDE schemes amplification factor, $F$ (of the usual DE), is replaced by $L$, a random variable following Laplace distribution.

The mutation schemes of LDE1 and LDE2 algorithms are defined as follows:
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2.2.1 LDE1 Scheme

\[ v_{i,g+1} = x_{\text{best},g} + L \cdot |x_{h_,g} - x_{r_2,g}| \]  

(4)

In LDE1 scheme, the base vector is the one having the best fitness function value; whereas the other two individuals are randomly selected.

2.2.2 LDE2 scheme

\begin{align*}
& \text{If } U(0,1) < 0.5 \text{ then} \\
& v_{i,g+1} = x_{\text{best},g} + L \cdot |x_{h_,g} - x_{r_2,g}| \\
& \text{Else} \\
& v_{i,g+1} = x_{r_1,g} + F \cdot (x_{r_2,g} - x_{r_3,g})
\end{align*}

In LDE2 scheme, mutant vector using equation (4) and the basic mutant vector equation are applied probabilistically using a predefined value. A random variable following normal distribution \( U(0,1) \) is generated. If it is less than 0.5 then LDE1 scheme is applied otherwise Eqn. (1) is applied. Both the modified versions, LDE1 and LDE2 have reportedly given good performances for solving benchmark as well as real life problems [21].

3 Problem Definition

Mathematical model of a constrained MOLSP may be given as [9]:

Maximize \[ z_k = \sum_{j=1}^{n} c_j^k x_j, \quad k = 1,2,\ldots,K \]

Subject to \[ P \left( \sum_{j=1}^{n} a_{1j} x_j \leq b_1, \sum_{j=1}^{n} a_{2j} x_j \leq b_2, \ldots, \sum_{j=1}^{n} a_{mj} x_j \leq b_m \right) \geq p \]

\[ x_j \geq 0, \quad j = 1,2,\ldots,n \]

Where \( 0 < p < 1 \) is usually close to 1. It has been assumed that the parameters \( a_{ij} \) and \( c_j \) are deterministic constants and \( b_i \) are random variables. For more details the interested reader may please refer to [9]. In the present study, we have considered the two test problems which are used in [9]. These problems are multi-objective stochastic linear programming problems (MOSLP) involving random variables following different distributions.

Test problem 1: MOSLP1:

Maximize \[ z_1 = 5x_1 + 6x_2 + 3x_3 \]
Maximize \[ z_2 = 6x_1 + 3x_2 + 5x_3 \]
Maximize \[ z_3 = 2x_1 + 5x_2 + 8x_3 \]

Subject to \[ P(3x_1 + 2x_2 + 2x_3 \leq b_4) \geq 0.90 \]
Here, $b_1$ follow Power Function distribution, $b_2$ follow Pareto distribution, $b_3$ follow Beta distribution, $b_4$ follow Weibull distribution; $b_5$ follow Burr type XII distribution. The problem is converted to deterministic model as follows:

**Maximize** $z = \lambda_1(5x_1 + 6x_2 + 3x_3) + \lambda_2(6x_1 + 3x_2 + 5x_3) + \lambda_3(2x_1 + 5x_2 + 8x_3)$

Subject to

\begin{align*}
3x_1 + 2x_2 + 2x_3 &\leq 6.3096, \quad 2x_1 + 8x_2 + 5x_3 \leq 8.0812 \\
5x_1 + 3x_2 + 2x_3 &\leq 4.7115, \quad 0.5x_1 + 0.5x_2 + 0.25x_3 \leq 0.9379 \\
8x_1 + 3x_2 + 4x_3 &\leq 10.0321, \quad \lambda_1 + \lambda_2 + \lambda_3 = 1 \\
x_1, x_2, x_3, \lambda_1, \lambda_2, \lambda_3 &\geq 0
\end{align*}

**Test problem 2: MOSLP2:**

*Maximize* $z_1 = 3x_1 + 8x_2 + 5x_3$

*Maximize* $z_2 = 7x_1 + 4x_2 + 3x_3$

*Maximize* $z_3 = 6x_1 + 7x_2 + 10.5x_3$

Subject to

\begin{align*}
P(5x_1 + 4x_2 + 2x_3 \leq b_1) &\geq 0.95 \\
P(7x_1 + 3x_2 + x_3 \leq b_2) &\geq 0.95 \\
P(2x_1 + 7x_2 + 3x_3 \leq b_3) &\geq 0.95 \\
P(0.5x_1 + 0.5x_2 + 0.25x_3 \leq b_4) &\geq 0.95 \\
P(5x_1 + 2x_2 + 1.5x_3 \leq b_5) &\geq 0.95 \\
x_1, x_2, x_3 &\geq 0
\end{align*}

Here $b_1$ follow Power Function distribution; $b_2$ follow Pareto distribution; $b_3$ follow Beta distribution of first kind; $b_4$ follow Weibull distribution and $b_5$ follow Burr type XII distribution. The deterministic model of the problem is given as:

**Maximize** $z = \lambda_1(3x_1 + 8x_2 + 5x_3) + \lambda_2(7x_1 + 4x_2 + 3x_3) + \lambda_3(6x_1 + 7x_2 + 10.5x_3)$
Subject to

\[
\begin{bmatrix}
\frac{y_1^2}{9} - 100 \\
y_2^2 - 100 \\
y_3^2 - 5 \\
\frac{e^{2y_4} - 1}{e^{2y_4}} \\
\frac{3y_5^2}{1 + 3y_5^2}
\end{bmatrix} \geq 0.95
\]

\[5x_1 + 4x_2 + 2x_3 = y_1, \quad 7x_1 + 3x_3 + x_3 = y_2\]
\[2x_1 + 7x_2 + 3x_3 = y_3, \quad 2x_1 + 3x_2 + 2.5x_3 = y_4\]
\[5x_1 + 2x_2 + 1.5x_3 = y_5, \quad \lambda_1 + \lambda_2 + \lambda_3 = 1\]
\[x_1, x_2, x_3, y_1, y_2, y_3, y_4, y_5, \lambda_1, \lambda_2, \lambda_3 \geq 0\]

4 Experimental Settings and Numerical Results

4.1 Parameter Settings

DE has three main control parameters; population size, crossover rate Cr and Scaling factor F which are fixed as 50, 0.5 and 0.5 respectively. For LDE schemes the scaling factor is a random variable, L, following Laplace distribution. For each algorithm, the stopping criterion is to terminate the search process when the maximum number of generations is reached (assumed 1000 generations). Constraints are handled according to the approach based on repair methods suggested in [22]. A total of 50 runs for each experimental setting were conducted and the best solution throughout the run was recorded as global optimum. Results obtained by basic DE and LDE versions are also compared with previously quoted results [9].

4.2 Numerical Results

We have considered four test cases in each of the test problems. Since, \(\lambda_1 + \lambda_2 + \lambda_3 = 1\), one of \(\lambda_i\), \(i = 1, 2, 3\) could be eliminated to reduce the number of dependent variables from the expression of objective function. So, we assigned equal weights to two terms at a time in the objective expression. The resultant test cases are as follows:

(i) \(\lambda_i = W, \lambda_j = \lambda_k = \frac{1-W}{2}\), \(0 \leq W \leq 1\)

(ii) \(\lambda_2 = W, \lambda_1 = \lambda_3 = \frac{1-W}{2}\), \(0 \leq W \leq 1\)

(iii) \(\lambda_3 = W, \lambda_1 = \lambda_2 = \frac{1-W}{2}\), \(0 \leq W \leq 1\)

(iv) \(\lambda_1, \lambda_2, \text{ and } \lambda_3\) are dependent variables.

The numerical results of the given two test problems MOSLP1 and MOSLP2 are recorded in Tables 1 and 2 respectively. The best solution obtained by DE and
LDE algorithms for MOSLP1 in terms of optimal decision variable values and objective function value are given in Table 1. For the test case (i), the performance of LDE1 is better than all the other algorithms. For the remaining 3 test cases, LDE2 performs better than other compared algorithms. If we compare the LDE algorithms with classical DE algorithm then from the numerical results we can see that LDE algorithms are superior with classical DE algorithm. There is an improvement of 52% in objective function value when the problem is solved by LDE2 in comparison with the quoted result [9], where the problem is solved by Genetic Algorithm. The results of test problem MOSLP2 are given in Table 2. From this table also we can see that LDE2 algorithm is superior with others in all the test cases. The improvement of LDE2 algorithm in comparison with the results in the literature is 141%. Figure 1 shows the performance of DE and LDE algorithms in terms of objective function value.

<table>
<thead>
<tr>
<th>Table 1 Results of MOSLP1</th>
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<tr>
<td></td>
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<tr>
<td>Z</td>
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<tr>
<td>x1</td>
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<td>x2</td>
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<td>x3</td>
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<td>Z</td>
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<tr>
<td>x1</td>
</tr>
<tr>
<td>x2</td>
</tr>
<tr>
<td>x3</td>
</tr>
</tbody>
</table>

Problem described as in [9]

| Z                        | 9.48978  | 11.3988  | 12.9299  | 8.5089   |
| x1                       | 0.352147 | 0.334378 | 0        | 0.3727   |
| x2                       | 2.12479e-007 | 0.00514505 | 0        | 0.2319   |
| x3                       | 1.47538  | 1.47426  | 1.61624  | 1.0761   |
Table 2 Results of MOSLP2

<table>
<thead>
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<th></th>
<th>DE</th>
<th>LDE1</th>
<th>LDE2</th>
<th>GA [9]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_1 = W, \lambda_2 = (1-W)/2, 0 \leq W \leq 1$</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$z$</td>
<td>5.5452</td>
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<td>6.86328</td>
<td></td>
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Figure 1 Performance of DE and LDE algorithms in terms of objective function value

5 Conclusion

The Stochastic Programming is an optimization technique in which the constraints and/or the objective function of an optimization problem contains certain random variables following different probability distributions. In the present study DE and two of its recent variants LDE1 and LDE2 are used to solve two constrained multiobjective stochastic linear programming problems. Four test cases were considered with respect to the weighing factors and the results were produced in terms of objective function value and decision variable values. From the experimental results it was observed that the DE algorithm and its variants significantly improve the quality of solution of the considered problems in comparison with the quoted results in the literature. As expected the modified versions LDE1 and LDE2 performed better than the basic version of DE because of the presence of the Laplace mutation operator. In conclusion we can say that DE’s present an attractive option for solving stochastic programming problems.

Acknowledgement

This work was carried out during the tenure of an ERCIM “Alain Bensoussan” Fellowship Programme.
6 References


Short Abstracts

New Approaches to Characterizing the Information Theory of MIMO Wireless Channel

Yang Chen\(^1\) and Matthew McKay\(^2\)
\(^1\)Department of Mathematics, Imperial College London, UK
\(^2\)Electronic and Computer Engineering Department Hong Kong University of Science and Technology Clear Water Bay, Hong Kong

Abstract

In this talk we compute the Shannon capacity of multi-antenna Gaussian channel through its moment generating function. It transpires that such a quantity can be described as a particular Hankel determinant of a \((n \times n)\) moment matrix generated by a perturbed Laguerre weight, with a parameter \(t\). We show that the logarithmic derivative of the Hankel determinant with respect to \(t\), satisfies the Jimbo-Miwa-Okamoto sigma form of a Painlevé V.

We show how to reconcile the Coulomb Fluid approach (valid for large \(n\)) with the moment generating function with this PV and obtain \(1/n\) and higher order corrections.

On a degenerative version of the Favard’s theorem

R.S. Costas-Santos and J.F. Sánchez-Lara

Abstract

We state a degenerate version of Favard’s theorem that allow us to extend the orthogonality properties valid up to some integer degree \(N\) to Sobolev type orthogonality properties. We also present the process to obtain the factorization and the non-standard Sobolev-type orthogonality property for those families of classical orthogonal polynomials which satisfy a finite orthogonality property, i.e. it consists in sum of finite number of masspoints.
Public-Key Cryptography based on Modular Lattices

Marcus Greferath and Jens Zumbrägel (University College Dublin)

Abstract

This contribution seeks to generalize pairing-based public-key cryptography to more general algebraic structures. It focuses on modular lattices, presents a pairing on such lattices, and studies a projective-geometry based cryptosystem.

A class of asymptotic preserving schemes for kinetic equations and related problems with stiff sources

Shi Jin

University of Wisconsin-Madison, USA

Abstract

We propose a general time discrete framework to design asymptotic preserving schemes for initial value problem of the Boltzmann kinetic and related equations. Numerically solving these equations are challenging due to the nonlinear stiff collision (source) terms induced by small mean free or relaxation time. We propose to penalize the nonlinear collision term by a BGK-type relaxation term, which can be solved explicitly even if discretized implicitly in time. Moreover, the BGK-type relaxation operator helps to drive the density distribution toward the local Maxwellian, thus naturally imposes an asymptotic-preserving scheme in the Euler limit. The scheme so designed does not need any nonlinear iterative solver or the use of Wild Sum. It is uniformly stable in terms of the (possibly small) Knudsen number, and can capture the macroscopic fluid dynamic (Euler) limit even if the small scale determined by the Knudsen number is not numerically resolved. It is also consistent to the compressible Navier-Stokes equations if the viscosity and heat conductivity are numerically resolved. The method is applicable to many other related problems, such as hyperbolic systems with stiff relaxation, and high order parabolic equations.
New results on Laguerre-type orthogonal polynomials

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¹Departamento de Matemáticas, Escuela Politécnica Superior, Universidad Carlos III, Leganés-Madrid, Spain.
²Departamento de Matemáticas, Universidad Nacional de Colombia, Ciudad Universitaria, Bogotá, Colombia.

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Abstract

This contribution is devoted to the study of the Laguerre-type monic orthogonal polynomial sequences (MOPS, in short) defined by an Uvarov’s canonical spectral transformation of the Laguerre weight supported on the positive semi-axis of the real line. In such a way, we state a comparative analysis with the behavior of the standard Laguerre-type polynomials, taking into account that, in our case, we are dealing with a mass point located outside the support of the measure. The outline of the talk is the following. In the first part we introduce the representation of the perturbed MOPS in terms of the classical ones, we deduce the three term recurrence relation that they satisfy, as well as the behavior of their coefficients. Next, we obtain the lowering and raising operators associated with these polynomials, and thus the corresponding holonomic equation follows in a natural way. The second part of the talk is devoted to the study of the behavior of the zeros of these polynomials in terms of the mass $M$. We also provide an electrostatic interpretation of them. Finally, we analyze the outer relative asymptotics as well as the Mehler-Heine formula for these polynomials.

Key words: Orthogonal polynomials, Zeros of polynomials, Christoffel transforms, Uvarov transforms, Connection Formula, Structure relation.

MSC 2000: 33C47.

References


The Seysen reduction algorithm and its application to MIMO systems

Gerard Maze

Mathematical Institute, University of Zurich, Switzerland email: gmaze@math.uzh.ch

Abstract

Given a lattice $L$, a basis $B$ of $L$ together with its dual $B^*$, the orthogonality measure $S(B) = \sum_i ||b_i||^2 ||b_i^*||^2$ of $B$ was introduced by M. Seysen [5] in 1993. This measure is at the heart of the Seysen lattice reduction algorithm and is linked with different geometrical properties of the lattice [2, 3, 6, 7]. In this talk, we will derive different expressions for this measure as well as new inequalities related to the Frobenius norm and the condition number of a matrix. This approach allows us to improve known upper bounds for the Seysen measure and the orthogonality defect.

We will then review the Seysen reduction algorithm [5, 1] and describe its application to the field of MIMO systems [4]. We will concentrate on the conceptual differences between the LLL algorithm and the Seysen reduction algorithm. The LLL algorithm focuses on local optimization (i.e., on 2 dimensional sublattices) but Seysen’s algorithm performs global angle optimization to produce a reduced lattice. As a consequence, Seysen’s scheme can achieve a better BER performance. We will also present the work of [4] showing that it requires less computational time than the LLL algorithm in the linear detection case.

References


On numerical integration of perturbed rigid body problems

A. Pascual and J. M. Ferrándiz

University of Alicante, Department of Applied Mathematics, Spain

Abstract

The accurate numerical integration of rigid and non-rigid solid bodies is an important issue in Space Geodesy. Its main difficulty is that a very high level of accuracy is required in many cases, as well as long-term validity of the solution. For instance, in the case of the Earth rotation the accuracy must be better than 0.15 milli arcseconds during time periods spanning several decades. Besides, the problem includes dissipations which prevents the use of the of symplectic or other geometric integrators and the variables that have been successful when deriving asymptotic analytical solutions give rise to virtual singularities. This presentation reports on the last progress we have made in the derivation of systems of variables and of equations of motion convenient for the numerical integration of such problems. An application to a simplified Earth rotation problem is included.
Building Public Key Crypto-Systems

Joachim Rosenthal

University of Zürich, Mathematics Institute, Switzerland

Abstract

Cryptography has a long history and its main objective is the transmission of data between two parties in a way which guarantees the privacy of the information. There are other interesting applications such as digital signatures, the problem of authentication and the concept of digital cash to name a few. The proliferation of computer networks resulted in a large demand for cryptography from the private sector.

A basic building block in public key cryptography are the one-way trapdoor functions. These are one-one functions which can be efficiently computed. The inverse function can however only be computed if some additional trapdoor is known. The best known one-way trapdoor function is the RSA function whose difficulty of inverting is related to the difficulty of factoring. Other one-way trapdoor functions use the arithmetic of elliptic curves and more general abelian varieties.

In this talk we will first provide a survey for the non-specialists. We then explain some new ideas on how to build one-way trapdoor functions from actions of finite simple semi-rings on finite semi-modules. The presented results constitute joint work with Elisa Gorla, Gerard Maze and Chris Monico and Jens Zumbrägel.

Multiphysics Simulation

Pablo Vallejos

Applications Department, COMSOL Multiphysics Sweden

Abstract

Simulation is a necessary task for every researcher and design engineer. Multiphysics simulation takes this task to the next level by introducing everything required to build precise comprehensive models. That is why multiphysics simulation is one of the fastest growing research fields in industrial engineering and academic research. In this presentation, you will be introduced to COMSOL Multiphysics. It is a simulation environment that facilitates all steps in the modeling process - defining your geometry, meshing, specifying your physics, solving, and then visualizing your results.

We will present the mechanics of the new (COMSOL Multiphysics 4.0) model-builder-based user interface which not only is much more efficient and quick to use, but also provides new functionality to the user to modify and quickly adapt models. We will work through a 3-physics coupled example to demonstrate the speed and efficiency of the new work flow. This will be of interest to both new and existing users of COMSOL Multiphysics.
Coupled Heat Transfer in Simulations

Pablo Vallejos
Applications Department, COMSOL Multiphysics Sweden

Abstract
In almost every manufacturing or product design process one must consider the effects of thermal fluctuations. A combination of capabilities to model heat transfer via conduction, convection, and radiation, as well as the ability to couple these to other physics is presented. In addition a case story of Ugitech S.A., a manufacturer of stainless steel in France is presented. It runs its continuing casting machines as fast as possible while maintaining quality. Yet, if it cuts off individual pieces from the square bloom coming out of the casts prematurely, the inside of the steel section will not completely solidify, and a molten metal well with as much as 1.5 tons of liquid steel can empty into the bottom sections of the vertical concast machine, causing major damage. Through modeling, Ugitech has optimized the proper temperatures and process speeds for each of the 150 different steel grades the company produces.

Randomization Techniques on Lattice Reduction Algorithms

U. Wagner

Abstract
Lattice reduction algorithms are of crucial importance in many cryptographic protocols. The goal of reduction algorithms is hereby to output lattice bases that consist of short and nearly orthogonal vectors. The notion of reducedness is not uniquely defined and several measurements of reducedness like the Seysen measure [1,6] and the Gram-Schmidt log [2] exist. Often the output of the shortest vector in a lattice is desired. However it is hard in general to find short vectors in lattices in higher dimensions and known reduction algorithms such as LLL can tackle the problem of finding the shortest vector in a lattice only to a certain (low) dimension [3,4]. Our work builds on the fact that most algorithms are not deterministic for the given lattice,
i.e. the basis to apply the reduction algorithm on influences the performance of the algorithm. Hence randomization of the lattice basis randomizes the whole algorithm. Our interest lies in randomization techniques in order to find suitable bases, on which the reduction algorithms perform better than on the average basis. In order to recognize a considerable improvement the average behaviour of the reduction algorithms have to be known. Fortunately results in this direction exist ([2] and [5]), where extensive tests on the behaviour of LLL and BKZ have been done. In special the Hermite factor of the reduced bases is computed, which gives information on the quality of the shortest vector found by the reduction algorithm. Hence our goal is to have a comparison of the different randomization techniques by means of the Hermite factor.

References


