Energy & Environment

Bentonite Buffer in Nuclear Waste Management

Executive summary

Helsinki University of Technology[1], University of Jyväskylä and Numerola Oy have co-operated in a research project which investigates the numerical modelling of bentonite buffer in nuclear waste management.

Challenge overview

Professor Rolf Stenberg from Helsinki University of Technology suggested Numerola Oy to take part in the Finnish research programme on nuclear waste management to develop the numerical modelling of bentonite buffer. Motivation for the initiative was to improve the software development in the project, especially to make it more continuous and consistent. During the past ten years, Numerola has developed its own software platform called Numerrin for numerical modelling and optimization. This was seen as a suitable tool to continue the development of numerical models and methods to study the behaviour of bentonite buffer.

Implementation of the initiative

The project was initiated by preparing a research plan for a funding application to the national research programme. The Department of Physics at the University of Jyväskylä participated in the application as a third partner. Their role was to coordinate experimental studies and to develop physical modelling of the bentonite buffer. The group at the Helsinki University of Technology concentrated on the development of numerical methods while Numerola was responsible for the software development.

The problem

Previous research work had already resulted in a thermo-hydro-mechanical multiphase model, which gave a starting point for this project. However, more efficient and robust methods and implementations were needed for the numerical solution of the equations. Also the models needed to be improved and extended to more complicated situations. Currently chemical reactions are being coupled to the physical equations.

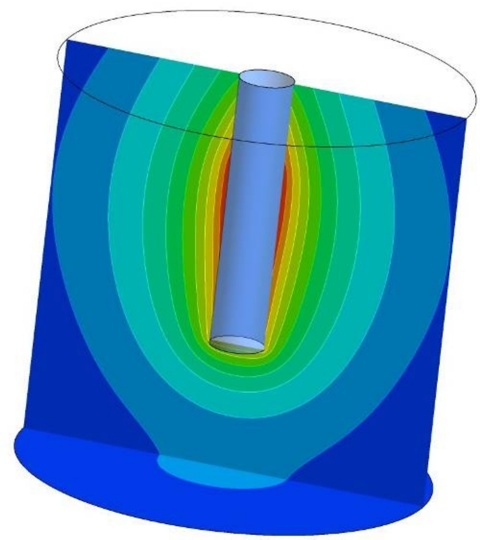
[1] Starting from 2010 Helsinki University of Technology is a part of the new Aalto University.

Results and achievements

The project has proceeded as expected in the research plan, and is still active. Both the mathematical models and numerical methods have been improved as a result of the co-operation. Recently the Technical Research Centre and Geological Survey of Finland have joined the project as two new partners.

Lessons learned and replicability

The co-operation has been fruitful and it has provided a concrete sample problem to test and develop the capabilities of the Numerrin platform. It has turned out to be a flexible and efficient tool for various modelling purposes and it is currently used in many research projects around Finland as a computational tool. It thereby supports both academic work and practical utilisation of the research results.



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Intelligent Video Understanding Applied to Plasma Facing Component Monitoring

Executive summary

Infrared thermography has become a routine diagnostic in many magnetic fusion devices to monitor the heat loads on plasma facing components (PFCs) for both physics studies and machine protection. In ITER[2] perspective, the development of a versatile, reliable and fully automatic system for the real-time monitoring of PFCs becomes essential.

Challenge overview

The understanding of the observed phenomena is not a trivial task and requires a high degree of expertise in both image/video processing and plasma physics. This research project aims at applying the scene understanding framework developed at INRIA for activity recognition to PFC monitoring during plasma operation.

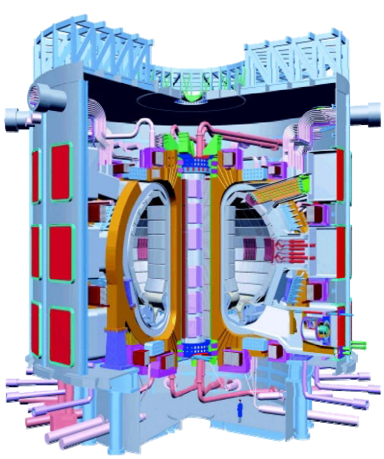

Figure 1. ITER

Implementation of the initiative

The cooperation between INRIA and CEA was born in September 2005 from the common goal to put together efforts for the success of ITER. In 2008, a research collaboration project named *moniTORE*[3] between INRIA project team PULSAR and the PFC group of CEA/IRFM at Cadarache and financially supported by INRIA was permitted to recruit a post-doctoral researcher and several master trainees. This project is now supported at the national level by the French Federation for Magnetic Fusion Research and at European level by EFDA (European Fusion Development Agreement) through a research fellowship.

The problem

Many operational tasks such as machine protection functions can be assured on the basis of qualitative imaging. The main problem is thus to be able to automatically perform a semantic interpretation of a dynamic scene from multi-sensor numerical data. From a mathematical point of view, semantics can be extracted using statistical models or fuzzy logic. The second problem relies on real-time constraints imposed by the control system during plasma operation. Vision algorithms must then be designed with the help of high computational performance hardware such as FPGAs to perform in real-time.

Results and achievements

A major achievement resulting from this partnership is the implementation at Tore Supra (a French Tokamak producing long plasma discharges) of a unique prototype of infrared imaging diagnostic relying on intelligent reasoning for real-time detection and recognition of abnormal thermal events during plasma operation. This constitutes a good starting point toward a real-time automatic feedback control system based on intelligent signal and image processing. We hope that this control system will be part of the foreseen infrared viewing system of ITER, which aims to protect its PFC components.

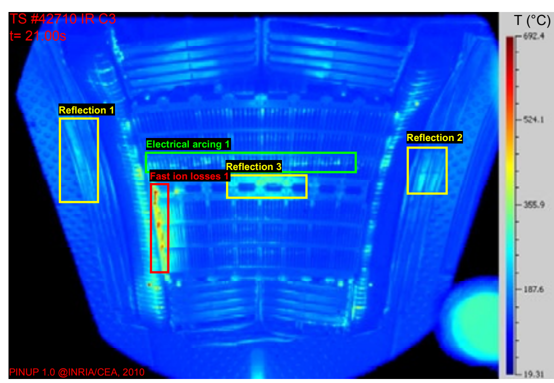

Figure 2. Automatic thermal event recognition from infrared images of Tore Supra PFCs during plasma operation

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[2] International Thermonuclear Experimental Reactor
[3] real-time *moni*toring of imaging diagnostic applied to *TORE* plasma operation

Modelling Coal Combustion

Executive summary

Mathematical models and numerical methods for the simulation of pulverised coal furnaces of power plants were developed under contract for the company ENDESA.

Challenge overview

The contact with ENDESA started in 1989 through Prof. Juan Casares, who was the director of the Department of Analysis of Results in the Power Plant of As Pontes (Spain). This plant had numerous problems with slagging, fouling and pollutant emissions (due to a more restrictive normative). The non-existence of well established commercial packages for numerical simulation of coal combustion prevented a good understanding of the phenomena taking place in the interior of a pulverised coal furnace. This lack of knowledge in turn prevented the company from adopting strategies to improve the installation through a modification in the operating conditions. The group then tried to establish and numerically solve a 3D mathematical model for the behaviour of a pulverised coal furnace. The results provided by the program were used by the engineers to improve the efficiency of the generation groups of the As Pontes power plant, as well as to state guidelines for their adaptation to the combustion of coal blends (lignite of the local mine and imported sub-bituminous coals).

Implementation of the initiative

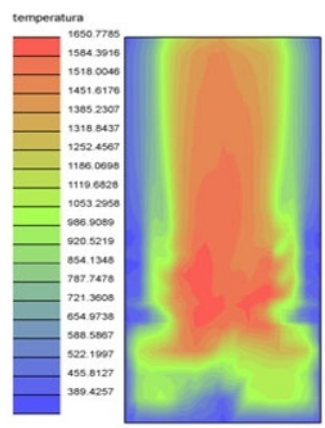
Using funds of the PIE program, an investigation project was agreed for a period of three years (1991-93) with an equivalent budget of Euro 127,000 between ENDESA and the Department of Applied Mathematics of the USC. This project gave rise to the group in mathematical modelling of combustion, directed by Prof Alfredo Bermúdez, and complemented with two pre-doctoral students. The international expert Prof. Amable Liñán provided an introduction into the theory of combustion. The project was subsequently extended for a period of one year and a budget of Euro 87,500, with the objective of including a graphical user interface and the corresponding user guides in the computer code, as well as a training program for the technicians of the company in the As Pontes power plant.

The problem

The mathematical model must contain the fluid dynamics equations for a turbulent, multiphase and reactive flow, where energy transport by radiation is important. The dispersed character of the coal particles led to an Eulerian description for the gas phase and a Lagrangian description for the solid phase being considered. The main outcome was the development of a completely new model for the combustion of coal particles by using the high activation energy asymptotics methodology. With respect to numerical solution, we developed high-order semi-Lagrangian finite element methods for the discretisation of the partial differential equations of the gas phase model. This choice was encouraged from the experience of the group in the analysis of this kind of methods. Finally, in order to determine and adjust the boundary conditions and some of the parameters involved in the models, the staff of the Plant carried out different measurement campaigns.

Results and achievements

From the obtained results, some of the problems observed in furnaces were justified and thereby some modifications in operating conditions or in the geometrical design could be proposed in order to improve the efficiency. New projects have since been agreed between ENDESA and the research group for simulating new installations and operating conditions.



Lessons learned and replicability

This initiative has been the seed of the research group in combustion which is now composed of 3 permanent positions and 3 doctoral students. Other students subsequently secured positions in private companies. The computational tool SC3D, which can be seen as a precursor of the present combustion commercial packages, is now being updated to include new models and improved numerical methods.

endesa generación

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Optimal Flames

Executive summary

Temperature distribution in industrial furnaces strongly affects the quality of ceramic products: optimal control techniques may help to improve the production.

Challenge overview

Edilcuoghi, a leading Italian producer of ceramic tiles, estimated that 12% of the production did not satisfy the high standards of the company. This was mainly due to excessive temperature oscillations inside the furnaces in which the tiles were processed. Moreover, it was observed that by changing the furnace burners, flames with different shapes are obtained, causing very different temperature distributions. Hence, the R&D department came up with the idea of finding an "optimal flame shape" that makes the temperature of processed tiles as close as possible to a desired value. Indeed, based on this information, the corresponding optimal nozzles can be designed. However, the available commercial softwares were inadequate for such analysis. *Edilcuoghi* contacted the Modelling and Scientific Computing Laboratory (MOX, Politecnico di Milano) to develop in-house optimisation algorithms and softwares that could serve their purposes.

Implementation

A two-year research contract was signed between MOX and *Edilcuoghi*. The research was initially set up based on internal resources, including a Master degree student, and later by hiring an engineer working on the established guidelines. First, a mathematical model of heat exchange was developed. Radiative heat transfer was taken into account by representing flames as radiating surfaces at high temperatures, and by non-local boundary conditions for the heat equation inside the furnace walls. Then, Optimal Control techniques were used to derive the equations expressing the sensitivity of the temperature with respect to surface variations. The numerical approximation of the model was performed by the Boundary Element Method. A Constrained Gradient Method was developed for the minimisation of a "cost functional" measuring the deviation of the temperature from the target profile. Different optimisation algorithms (genetic algorithms) and more complex heat transfer modes (convection) were considered as well.

Results and achievements

The critical dependence of the temperature profile on the radiative shapes was confirmed by computer simulations. Moreover, the optimal shapes were found to be non-symmetric, with a reduced width and an increased height. The quantitative results on the optimal shapes and on the temperature profiles were useful for *Edilcuoghi* to design specific nozzles for their furnaces.

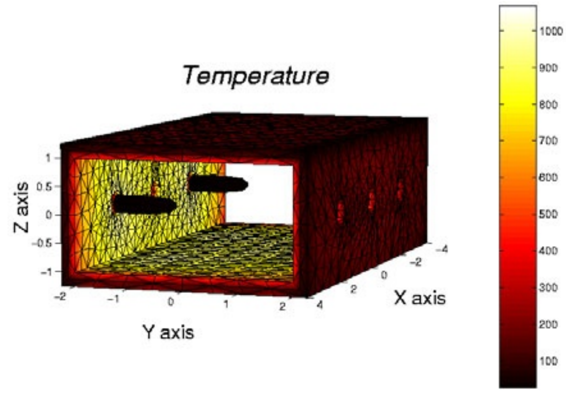

Figure 1. Temperature (Kelvin) inside a section of the furnace. The internal, lower horizontal surface is where tiles are processed and temperature is controlled.

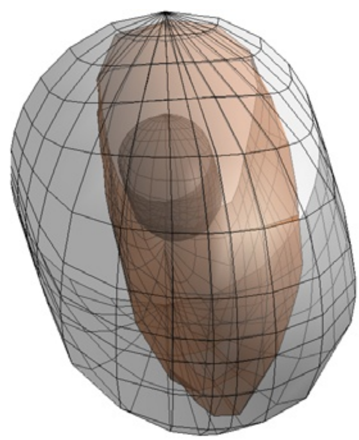

Figure 2. Optimal radiative shape (enclosed between the maximal and minimal admissible shapes).

Replicability

The scientific consultancy conducted for *Edilcuoghi* proved that optimal control techniques and shape optimisation can be effective tools to improve industrial production involving thermal processes, also when complex radiative heat exchange conditions have to be accounted for. The developed software can be used or expanded to treat similar problems, supporting the engineers in designing radiative surfaces and heat exchangers.

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Optimising a Complex Hydroelectric Cascade in an Electricity Market

Executive summary

In hydroelectric power stations it is possible to manage the storage of water in reservoirs and to release water downstream, thus producing energy. The profit resulting from this process depends on the price of energy at times of energy consumption and energy production. Having the possibility of pumping water upstream at times when the energy price is low, the energy stored may then be made available at a later time when prices are higher. This study considered a branched model for a hydroelectric power station interacting in a cascade arrangement, in order to provide guidance in decision-making aimed at maximising the profit.

Challenge overview

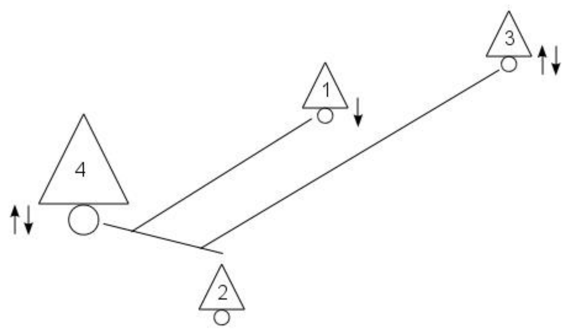
The problem involving a specific hydroelectric cascade power station was posed as a case study by the Portuguese electricity and gas transmission supply operator, "Redes Energéticas Nacionais, S.A." (REN), to the 69th European Study Group (ESGI69) which took place at the University of Coimbra in 2009. Some turbines in that power station are able to pump water up from a downstream reservoir to an upstream one. Pumping water upstream can be advantageous, for instance if done at times of low demand for electricity, to build up reserves in order to be able to produce energy during peak hours, thus balancing the load. The problem proposed was focused on profit maximisation when operating such a system, and on how to decide which upstream reservoir to pump to, when there is a choice.

Implementation of the initiative

A team of mathematicians from European universities participating in the ESGI69 gathered for one week to learn about and discuss the problem and to mathematically model it. A representation of the hydroelectric cascade as an optimal control set of equations was formulated and some conclusions were drawn for particular cases and simplified versions of the whole model. Finally a non-linear optimisation program resulting from the discretisation of a one day period into one hour time steps was developed. After the meeting was over the team associated with this problem presented a report of the study.

The problem

In the case of reversible hydroelectric power stations it is possible to bring water from a downstream reservoir to an upstream one. This is usually desirable at times of low demand, in order to be able to produce energy during peak hours. While this might not be worthwhile from an energy point of view, the fact that the price of electricity varies along the day makes it possible to use cheaper energy to produce energy at future times when it will be more expensive. While in the case of one single power station the solution of the problem is more or less straightforward, it becomes more complex in the case of a system of power stations in a cascade configuration with the possibility of pumping water from one reservoir to two reservoirs. Moreover, the different characteristics (dimension and location) of reservoirs give rise to different consumptions and productions of energy. This type of problems can be treated by various fields of mathematics, from optimal control to network flow optimisation, among others. In practice major model simplifications often lead to inaccurate solutions, which can have a high impact on companies' revenues.



Results and achievements

The report produced presents the models and the conclusions drawn during and after the ESGI69, as well as recommendations to REN. It includes also a detailed analysis of a simple reservoir configuration, some simple relationships between price and timing of decisions, and a numerical algorithm based on the non-linear program. A paper based on this final report has been submitted for publication in a scientific journal.

Lessons learned and replicability

The complexity of the hydroelectric power station and the multiple variables involved made it difficult to come up with an accurate system's representation in terms of the problem formulation, capable of answering the issues raised by REN. Nevertheless the process benefited from an intensive contact with the industry representative, and in the end it was possible to point out models and ways to find an (eventually approximate) optimal solution.

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Mathematical Problems in Oil Pipelines

Executive summary

We have developed some mathematical models for wax precipitation in waxy crude oils (oils with high content of heavy hydrocarbons), studying the dynamics of wax deposition in pipelines crossing cold regions (subsea pipelines).

Challenge overview

The research is the result of a contract with Eni (Milan). The main objective was modelling the mechanism of the segregation of wax, of its migration induced by temperature gradients, and its deposition on the pipeline walls. This was the first research contract of the company with mathematicians. We were asked to develop mathematical models and numerical codes apt to predict the possibility of occurrence of precipitation and deposition of wax on the walls of pipelines, depending on the temperature of the environment.

Figure 1. Section of a pipeline with deposited wax

Implementation of the initiative

The research was carried in continuous contact with the company. Every step was checked by means of experiments carried out by the company itself or by other departments of our university. Confidentiality issues just caused delays in the publication of the results.

The problem

We have modelled various aspects of wax precipitation and deposition, both in the cases when thermodynamical equilibrium (between solid and liquid phases) can be assumed and when kinetics of precipitation has to be taken into account. We have considered static and dynamical situations in laboratory devices (cold finger, loop) and in real field pipelines. We have developed models for predicting wax precipitation, wax deposition and wax gelification.

We adopted a multi-scale approach, taking into account microscopic phenomena (such as crystal nucleation and growth) and studying the time scale at which different phenomena occur. A main difficulty encountered in the research consisted in the lack of the experimental data which are useful for the development and validation of the model. In recent years this problem has been overcome thanks to the collaboration with the Department of Chemistry of the University of Florence where some experiments were performed and the input data for the model were found.

Results and achievements

The models we have proposed are capable to predict the amount of precipitated wax in specific thermal conditions. Moreover they can predict the amount of deposited wax (by molecular diffusion) on the pipeline walls.

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Eni

STUDIORUM UNIVERSITAS FLORENTINA

Let the Oil Flow!

Executive summary

Bringing together the IFP and the Laboratoire Jacques-Louis Lions, a technological research team was set up to develop new computing methods to improve the simulation of multiphase flows in pipelines.

Challenge overview

A mixture of hydrocarbons flowing in a pipeline usually gives rise to very complex phenomena because liquid and gas coexist over very long range and under highly varying temperature and pressure conditions. The challenging case of the « severe slugging » is the paramount of a violent chaotic problem. Oil companies request numerical simulations that are robust, accurate and fast in order to pilot the installations. Stemming from a long-term collaboration between the two institutions, through thesis and internships, the idea of tackling this difficult problem originated during Cemracs 2003 with a project involving Quang-Huy Tran (IFP), Frédéric Coquel (LJLL) and Marie Postel (LJLL).

Implementation of the initiative

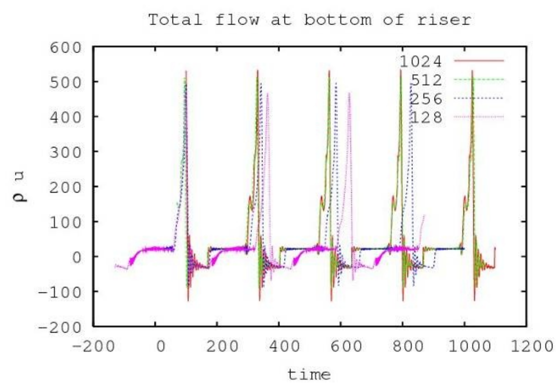
An “internal technological research team” was formed and financed by both the IFP and the French Ministry of Research. Experts in complex fluids and in adaptive methods for hyperbolic systems were already in the LJLL, and just had to be motivated on this specific problem. IFP was willing to involve one permanent researcher and to welcome temporary staff. It turned out that for almost four years a base kernel of two academics and one industrial researcher met weekly at the LJLL. They carried out in their stream two master internships, one post-doc (N. Andrianov) and one PhD thesis (Q.-L. Nguyen) and occasional collaborations. Most of the numerical algorithms were designed during the weekly sessions at the LJLL, and then checked, implemented and tested by both partners. A C++ program was developed jointly at IFP and at LJLL with a huge effort made on collaborative development. Four papers and numerous proceedings were published to formalise and illustrate the results.

The problem

The transport of hydrocarbons from the well site to the separation facility can be modelled by a system of hyperbolic PDEs whose unknowns are the density, speed of the different components of the fluid mixture, as a function of time and position in the pipeline. The main difficulties encountered in the design of numerical schemes to solve these equations are three-fold: physical laws linking the gas and liquid phases of the mixture are highly non-linear and very costly to evaluate. In operating mode, the transport is monitored at both ends of the pipeline by pumps, which amount to very stiff time-varying boundary conditions. Last but not least, the changes in the pipeline geometry induce source terms and non-conservative terms in the PDEs. We have attacked these challenging issues from two fronts, both ensuring the robustness of the resulting schemes: large time-steps relaxation methods to handle the non-linearities and multiresolution analysis to monitor a space- and time-varying grid.

Results and achievements

The difficult part for the academics was to confront our algorithms and programs to realistic test cases. If no real comparison with experimental results was possible at this stage, at least a good knowledge of the expected qualitative behaviour of the solution was available. The software developed during the project was able to reproduce difficult test cases already handled by the company home software TACITE. The adaptivity in time and space allowed drastic computing time reductions.



Lessons learned and replicability

This type of collaboration has proved itself fruitful for both parties. At the end of the four-year contract a new technological research team has been set up on another challenging problem, namely, in oil reservoir modelling.

Partners in the project

http://www.ann.jussieu/ERTint

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Ministère de l’enseignement supérieur et de la recherche

Near Real-Time FCC Riser Simulation and Visualisation

Executive summary

A lightweight physical model and a fast numerical solver have been designed for the near real-time rendering of fluid catalytic cracking (FCC) in the riser cylinder reactor part. For real-time requirements, a trade-off between the model fidelity and the numerical complexity was needed. The choice of the physical model and numerical schemes are here completely driven by the requirement of real-time rendering virtual reality on a standard (powerful) PC. It has been possible to design a real-time numerical rendering model able to show the three-phase flow dynamics depending on design parameters (number of oil injection inlets, injection angles, flow rates, temperature of catalyst powder). Open source technologies were used for the software design: gcc, python, SWIG C++ Python wrapper, wxPython, pyVTK.

Challenge overview

The problem was expressed by the French Petroleum TOTAL company, Head of Scientific Division. The challenge was to produce a software able to “render” in quasi real-time on a standard PC a three-phase three-dimensional flow into a Fluid Catalytic Cracking riser reactor with runtime visualisation and human interaction capability. The model is expected to return most of the expected flow feature like gas expansion near liquid oil inlets, turbulent fluidised bed, emergence of privileged gas paths, recirculation patterns, etc. The goal was also to be able to directly act on some design parameters like the number of oil inlets, the inlet attack angles, the oil flow rates, the temperature of regenerated catalyst powder. The industrial interest for such a tool is the use of a lightweight simulator for training and understanding of the process but also for numerical engineering design. Because of internal review deadlines, it was asked to produce such a tool in record deadline: 3 months!

Implementation of the initiative

So the duration of the contract was three months. A multidisciplinary academic team of 5 people was set up: three specialists of fluid mechanics and particle methods, a software engineer and an expert of scientific visualisation and VTK toolkit. A transversal manager was also chosen for project coherence: interfaces between the model components, interface between the models and the visualisation component, interface between the models and the interactive graphic user interface. During the first month, weekly meetings between academics and the company were necessary for a precise definition of the requirements. Then every 15 days, a project review in the company was scheduled to check the agreement between the industrial expectations and the work in progress. The software was delivered on a laptop PC with dedicated integrated development environments and high-performance graphic hardware accelerator.

The problem

From the mathematical and computational point of view, multiphase flows are known to be very difficult to model and simulate. A model designed for a full system of volume-averaged multiphase flow equations would require several weeks of CPU time for only a few seconds of physical time! Therefore a strong effort of model reduction was necessary in this work. Moreover, very fast solvers were designed in order to reduce the CPU time of about one or two orders of magnitude. It appeared that a coupled system of Lagrange particle solvers for both liquid and solid phase and an Eulerian finite volume solver for the gas were good candidates to get a good trade-off between performance and accuracy of the whole numerical model.

Results and achievements

The work and the resulting software were much appreciated by the company. Almost real-time was reached on the PC laptop with the expected flow description. The software was built using pure open source tools under GPL-like public licences. A company’s internal project review highly rated the project. Now the labs involved in this success story are still working with TOTAL on related projects. We thank Bruno Frogé for his advices concerning VTK.

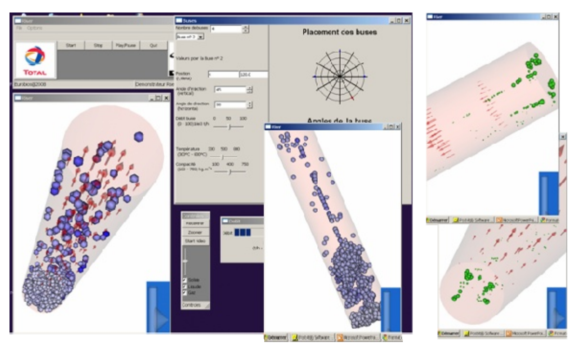

Figure 1. FCC riser software: near real-time simulation with interactive graphic user interface and three-dimensional three-phase visualisation during runtime.

TOTAL

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SmartGrid.gc: Intelligent Agent Based Modelling and Simulation of Electrical Grids

Executive summary

This project deals with the development of a framework that allows simulation of island power systems at market and operational levels. Complex situations that occur in the management of electricity networks are modelled based on the interaction of multiple decision making units, with bounded rationality and self-interest. For system behaviour studies the paradigm of Agent Based Modelling and Simulation (ABMS) is used. It is conceived as a tool for modelling and simulating scenarios, that is configurations and situations in electrical grids. Special emphasis is focused on the study and simulation of the effects of technological trends regarding generation, storage and processing in order to evolve towards future smart grids. This project has received financial support from by the Canary Islands Agency for Research, Innovation and Information Society (ACIISI) of the Canary Islands Government and with the participation of the important utilities sector, UNELCO-ENDESA (Canary Islands electrical generation company) and *Red Eléctrica de España* (Spanish electrical transportation company).

The results of this project are:

- The study of solutions to future scenarios for restructuring and management of island power systems (like Gran Canaria island electrical grid) can simulate situations in order to maximise renewable energy sources (RES) integration into the grid, ensuring the service quality and reducing dependence on fossil fuels and environmental contamination.
- Studies towards the definition of smart power grid management solutions, like the ones related to the maximisation, the RES integration and use of electrified vehicle fleet as storage element.

Implementation of the initiative

The initiative has been developed by the Artificial Intelligence and System Division with Prof. Mario Hernández (fhernandez@siani.es) as scientific director. The research group is composed by a multi-disciplinary team of engineers, computer science graduates and scientists working together in research and innovation for industry and government departments.

The problem

Electrical systems are facing major challenges due to:

- The new environmental needs related to climate change control.
- The introduction of market structure at different levels of electrical business.
- The economic and geostrategic problems related to the electrical energy production from fossil fuels.
- The massive introduction of unmanaged RES in the electrical grid.
- The revolutionary changes that are occurring in the automotive industry due to the planned production of plug in electrical vehicles (PHEV).
- The technological changes that are necessary for grid management with the introduction of the Smart Grid concept.

Lessons learned and replicability

Over 97% of domestic energy demand of Gran Canaria is covered with refined oil (more than 10 million barrels per year), with an annual consumption of oil of 1.4 million Tm of which 0.8 million Tm are dedicated to produce electricity and 0.6 million Tm to transport and others. This situation occurs in the island of Gran Canaria with the best wind resources in Europe. The integration of a substantial amount of RES in an isolated electrical system of medium size like the island of Gran Canaria grid (3800 GWh of annual production), demands intelligent management systems to guarantee their effectiveness and stability. Both of them can be increased if it is done with storage systems, acting in a buffering mode, as PHEV can be. The case of Gran Canaria's electrical grid is similar to many other medium size grids around the world and is a good laboratory exemplar to evaluate different technological approaches and market solutions for future grid studies.

Contact

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A Kinetic Model of Blast Furnace Automation

Executive summary

Blast furnaces have been used for iron production for centuries. In today's competitive engineering markets, math-based furnace simulation can cover operating conditions which are not accessible by experiment.

Challenge overview

Siemens VAI is one of the world´s leading engineering and plant-building companies for the iron & steel industries, based in Linz, Austria, which has been cooperating with mathematical research institutions since the 1980s. They became a partner in the Industrial Mathematics Competence Center (IMCC), which was established in 2002 and is co-financed between industry and the public sector. The support of the Austrian Ministry for Economy and Labour and the Upper Austrian Government is gratefully acknowledged.

The modernisation of steel mills around the world requires a thorough understanding of the processes going on in a blast furnace and quantitative simulation tools for analysing the influence of different raw materials and of different operating conditions.

Implementation of the initiative

The joint research team consisted of experts in metallurgical and chemical engineering, in numerical mathematics and in computer science. Regular meetings between the team members, especially in the modelling stage, were essential for success.

The problem

The mathematical model of a blast furnace should cover at least: (a) the transient movement of layers of coke and of iron ore and the shrinking of the coke layers, (b) the movement of gas through the furnace, (c) the chemical reactions taking place (up to 50 of them taken into account), and (d) balances of energy. This leads to a system of (around 50) highly nonlinear partial differential equations with the unknowns depending on position and time. Assuming a rotational symmetry seems reasonable, leading to a (2D + time) problem. The discretised version (finite elements combined with method of lines for some reactions) led to systems with up to 800,000 unknowns.

Results and achievements

The simulation tool which was developed is able to simulate e.g. various mixings of raw materials. The computation of one real-world blast furnace day takes typically 3 hours on a standard PC and therefore allows the user to simulate different operating conditions and thus to optimise, e.g., energy consumption. The kinetic blast furnace model is part of Siemens VAI's automation offerings. From the academic point of view, such cooperations allow for industry-driven PhD theses, as the complexity of the coupling between the differential equations is extremely high, and this prepares young scientist for industrial problem solving. Other projects for the iron and steel industry carried out at math institutions in Linz were in the fields of sintering, continuous casting of steel or hot rolling.

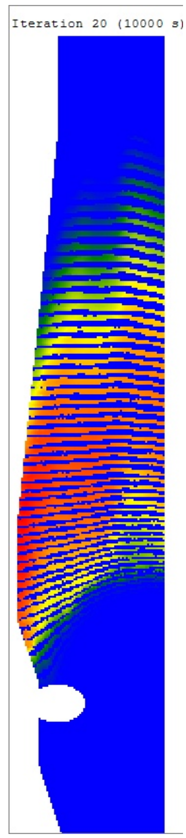

Figure 1. Concentration of FeO (red = high) in the layers of a blast furnace. Note that there is no FeO in the (blue) coke layers.

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IMCC

Numerical Modelling of Heterogeous Porous Media

Executive summary

This project is concerned with the numerical modelling of the flow and transport of radionuclides in heterogeneous porous media.

Challenge overview

The responsible officer of the division modelling and scientific computing division at IRSN/Radioactive Waste Safety Department contacted the Universite de Pau et des Pays de l'Adour for a collaboration in the upgrade of the 3D MELODIE code. This code performs radionuclide transport calculations within the field of technical expertise of the French radioactive waste underground repository project.

Implementation of the initiative

The collaboration began in 2000; it has mobilised research engineers from IRSN, Professors from the University and Master, PhD and Post-doctoral students.

The problem

The problem is to perform efficient and robust numerical methods for the numerical simulation of coupled systems arising in multiphase flow in porous media. For this we utilised finite volume methods & upscaling.

Results and achievements

During this collaboration, several codes have been performed, a PhD thesis, several publications and reports have been produced. The contract is ongoing until at least 2012.

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IRSN
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DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

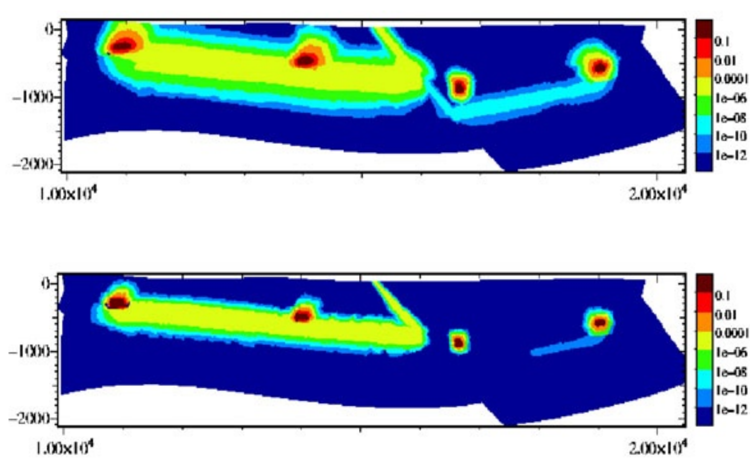

Figure 1. Radionuclide transport calculations by finite volume method for a scenario of radioactive waste underground repository.

Aero-Acoustic Virtual Design of Exhaust Systems

Executive summary

Swenox is a leading manufacturer of exhaust systems for the European car industry, with an established cooperation with the Marcus Wallenberg Laboratory for Sound and Vibration Research (MWL) at the Royal Institute of Technology (KTH) in Stockholm. Applied mathematicians of the Computational Technology Laboratory (CTL) at KTH now participate in a project together with Swenox and MWL to develop new tools for modelling and simulation of turbulent flow fluid-structure-acoustic interaction in exhaust systems.

Challenge overview

After a discussion at a chance meeting in 2007, the project was initiated when it was realized that the work at CTL on simulation of blood flow in flexible arteries relied on similar mathematical technology as would be needed to address the outstanding problem of simulating aero-acoustics of the flow of air in exhaust systems. The use of existing simulation tools for such problems is limited since the problem is too challenging to address without extensive simplifications, so that many aspects of key importance for design are not part of the model.

Implementation of the initiative

The collaboration was in 2007 funded by Swenox and the Swedish Governmental Agency for Innovation Systems (Vinnova), and was later continued in 2009 as a new 3-year project funded by Swenox and the Swedish Energy Agency. Swenox acted as project coordinator through regular meetings and workshops with a core group of 3 senior researchers and 3 PhD students, of which one of the students was recruited specifically for this project. The meetings were the key to find a common language between the engineers, experimentalists and mathematicians involved, and to indentify suitable project goals to both break new ground in mathematics research and to advance the frontier of aero-acoustics simulation in industry.

The problem

An exhaust system consists of flexible parts interacting with the airflow from the engine, and the problem is to predict aero-acoustic properties of such a system. The basic model is the Navier-Stokes equations describing velocity, pressure and density of the exhaust air, together with corresponding equations for the solid structures of the system. The main challenges are: (i) to model turbulent fluid flow, with several open problems with respect to the mathematics of the model and the computational cost of resolving the turbulent scales, (ii) coupling of the fluid and the structure models, which is typically very unstable, and (iii) extracting acoustic information from the model, in the form of very small pressure fluctuations.

Results and achievements

The mathematical technology used in the project to simulate both the turbulent airflow and the solid structure is adaptive finite element methods. The algorithms are implemented in the open source software project fenics.org, in the form of the simulation software Unicorn, developed by CTL. To address the industrial problem of complex geometry and realistic physics, the computer code had to be redesiged to run efficiently on the most advanced supercomputers available in Sweden. The coupling of the fluid and the structure was handled by a monolithic approach where the fluid and solid were formulated as one unified continuum, to achieve robustness. The project is still running, and today fluid-structure interaction simulations are routinely carried out at CTL, which are validated against experimental tests at Swenox and MWL. The aero-acoustic sources can now be extracted from the simulations, and the next step of the project is to allow for a fully coupled fluid-structure-acoustic coupling of the problem. Dissemination of the new technology developed at CTL is also in process, in the form of software tools adapted to the needs of Swenox.

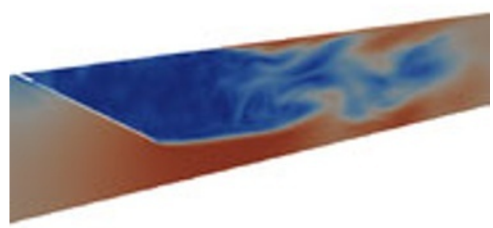

Figure 1. Simulation of the turbulent flow of air past a mixer plate in an exhaust system (simulations by Rodrigo Vilela De Abreu and Johan Jansson at CTL).

Contacts

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Numerical Simulation for Environmental Prediction

Executive summary

This project deals with the numerical simulation of four important environmental problems: the realistic prediction of wind fields, solar radiation, air pollution and forest fires.

Challenge overview

Three groups (Laboratori de Càlcul Numèric, LaCàN, from Universitat Politècnica de Catalunya, Instituto de Física Fundamental y Matemáticas from Universidad de Salamanca and Instituto Universitario de Sistemas Inteligentes y Aplicaciones Numéricas en Ingeniería, SIANI, from Universidad de Las Palmas de Gran Canaria) have been working since ten years ago on these environmental problems and together they have finished three previous coordinated projects sponsored by Spanish Goverment and FEDER. At present (2009-2011) these groups are developing the project entitled Predictive Numerical Models for Environmental Management where the Agencia Estatal de Meteorología (AEMET), Desarrollos Eólicos, S.A. (DESA) and Instituto Tecnológico de Canarias, S.A. (ITC) are the three main companies involved.

Implementation of the initiative

The present environmental problems (wind fields, air pollution, fire propagation and solar radiation) have a great social, economic and scientific impact. Nowadays, climate change is being considered as one of the most important problems of our planet. Because of that efficient use of renewable energies (such as wind and solar) is increasing exponentially. Moreover, decreasing of air pollution and forest fires is needed for maintaining the quality of ecosystems and human environment. Many companies and institutions are interested on the results of this project.

The problem

The main objective of the project is the combination of our local approaches with predictive mesoscale models such as MM5, WRF, HIRLAM or HARMONIE for weather, and CMAQ or MOCAGE for air quality. These models usually solve the problems by using finite difference methods on a structured grid (defined on several nested domains) and can predict atmospheric magnitudes with a maximum resolution of about 1km. The combination of these predictive models with our adaptive finite element models (see figure), which work with triangular or tetrahedral unstructured meshes, allows us to carry out predictive simulations in a local scale accurately (about a few metres). In this way, the terrain characteristics and solution will be efficiently approximated according to a desired precision.

Results and achievements

The scientific aims proposed in this project are clear, reachable and suitable. We do not try to reproduce tools that already exist. We try to solve problems that cannot be solved by known standard codes. Our wind model will be able to construct a wind field starting from few experimental measures. This is important for the diagnosis or evaluation of the wind power in a zone. However, companies are also interested on the prediction of such power. For this purpose, our adaptive local models (with a resolution of a few metres) must be connected with predictive mesoscale models (with a resolution of kilometres). We have initially focused in the MM5 and WRF codes since they are widely used by the community of meteorological phenomena prediction, although other predictive mesoscale models are also considered. In the framework of air pollution, the aims are similar. The adaptive local code that we are developing will extract the meteorological and air quality information from the MM5-CMAQ codes. The forest fire model will also be connected with MM5. The solar radiation model will be designed for both diagnosis and prediction. The integration of GIS tools will provide all these codes with the necessary information for carrying out realistic simulations.

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Predicting Climate Change

Executive summary

Increasing global temperatures, rising sea levels and the disruption of fragile ecosystems: climate change is one of the greatest challenges humanity has ever faced, and could potentially affect billions of lives in the coming century. Scientists around the world are working to tackle the problem with detailed models of our changing climate, and mathematicians are at the heart of these models, solving the difficult equations that no one else can. Researchers in meteorology, physics, geography and a host of other fields all contribute their expertise, but mathematics is the unifying language that enables this diverse group of people to implement their ideas in climate models.

Challenge overview

At the centre of all climate models are the Navier-Stokes equations, which describe the movement of liquids and gases such as the atmosphere and ocean. Translating the Navier-Stokes equations into computational code is undertaken by Paul Williams, a Royal Society Research Fellow at the University of Reading, who aims to improve the time-stepping calculation, making it more accurate without losing computational efficiency.

The problem

As a linked set of four nonlinear partial differential equations the Navier-Stokes equations are impossible to solve analytically in all but a few trivial cases, hence the need for numerical approximation methods. These methods allow us to apply the Navier-Stokes equations to a range of practical situations.

There are a variety of time-stepping methods, each with their own strengths and weaknesses, but because climate modelling is so complex, the different methods don't always produce results that agree. Determining which method to use can be beneficial as it allows climate scientists to investigate uncertainties.

Other aspects of the climate aren't captured by the Navier-Stokes equations, and some atmospheric phenomena lack fundamental mathematical theory behind them. Clouds are the leading source of uncertainty in climate modelling because they occupy a scale much smaller than the 100 km grids currently in use in climate models, so the full details of their behaviour are lost.

These unanswered questions show that while current climate models have served us well, demonstrating that increased carbon dioxide levels lead to a rise in temperature, we must still gain a deeper understanding of all the mechanisms within our atmosphere and ocean if we are to effectively fight global warming.

Climate scientists use many different varieties of time-stepping methods to power their models, and the choice of method can influence the resulting predictions. The most widely used is the “leapfrog” method, so-called because the function and its derivative get from the previous time to the future time by “leaping” over the current time.

Results and achievements

The method's success is due to its ease of use and low computational complexity, but its jumping nature can lead to discrepancies between even and odd steps. This can be solved by using the Robert-Asselin filter to smooth the discontinuities, but at the cost of a loss in accuracy. Williams' research modifies the filter in a way that counteracts this loss, producing better models with no noticeable reduction in calculation speed.

University of Reading

THE ROYAL SOCIETY

Institute of mathematics & its applications

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Stepping in Sherlock Holmes's Shoes: Where is the Underground Water? Is it Still Drinkable?

Executive summary

This document describes the multidisciplinary collaboration between four universities, two in Europe (Oviedo and Bordeaux1 Universities) and two in Morocco (D'ElJadida and Meknès Universities). By putting together their knowledge in applied mathematics and optimisation, geology, applied geophysics and geostatistics, a common language was created and we were able to solve important environmental problems using hydrogeophysical methods. These methodologies were then used to solve underground water problems in the Sahel des Doukkala and Saïss basins of Morocco. In particular, the contamination of underground water by salt water intrusion is a problem that interests most of the industries and local administrations in countries belonging to the Mediterranean basin. These methods are versatile and low cost in their implementation and can be easily applied to underground water exploration in countries where other geophysical methods cannot be used due to technological and economic constraints.

Challenge overview

First contact was made at the XI International Congress of Mathematical Geology held in Liege, Belgium in 2006. The Spanish and French teams quickly discovered our commonalities and that we had much to gain by sharing knowledge, experiences, software and data. An Atlantic Spanish-French team was immediately formed and was soon joined by our Moroccan colleagues who brought a wide variety of interesting environmental problems and a large volume of field data. Thus, our scientific and human collaboration was built across continents and now is based on strong cultural respect and friendship.

Implementation of the initiative

The first steps of our collaboration were facilitated by the exchange of professors and researchers of the different universities, first in France (Bordeaux) and later in Spain (Oviedo). Agreements were signed to share the available data and the mathematical models. Support was given by interchange programs: one Franco-Spanish (Hubert Curien PICASSO) and the other Franco-Moroccan (Hubert Curien VOLUBILIS).

The problem

Hydrogeophysics is made of a set of geophysical techniques that serve to study underground aquifers, and eventually all the problems (such as contamination) related to their exploitation and management. Currently it is a very active subject of research due to the increasing impact that drinkable water has in any country's economy. Some methods are more sophisticated, while others such as the Vertical Electrical Soundings or the Spontaneous Potential are more low-cost. Implicit to these methods are their respective inverse problems which are crucial for retrieving information from the underlying earth structure (including the aquifers). The low number of parameters facilitates the use of global methodologies to perform risk analyses on the final decisions that often have a very important environmental character.

Results and achievements

We were able to create simple methodologies to help assessment and risk analysis in applied hydrogeology. These methodologies have recently become very important for local industries and administrations that are highly dependent on the amount and quality of the underground water resources.

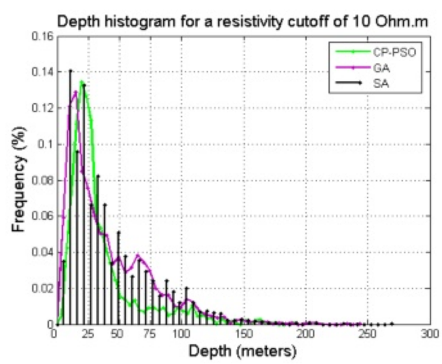

Figure 1. Depth of a salt water intrusion on a coastal aquifer in southern Spain.

Lessons learned

One of the most important lessons learned from this experience is that in science, problems have an international character and we should cooperate across borders in their solution. Usually teams compete to arrive first to the target, but when a common language is created that respects the uniqueness of cultures, the success is the normal outcome of these initiatives. These developments can have a great impact when knowledge is transferred to developing communities. Mathematics and science can be used to improve people's life.

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Modelling and Simulation of Environmental Problems

Executive summary

Mathematical models and numerical methods for simulation of free surface flows including the treatment of the geometry, the turbulence, and the transport or dispersion of pollutants have been developed and applied to some aquatic environmental problems.

Challenge overview

The contact with the COTOP ("Consellería de Ordenación do Territorío e Obras Públicas") of the Government of Galicia started in 1986. They were interested in the construction and the location of submarine outfalls in the Galician coast. From the mathematical point of view, in order to solve the problem, it is necessary first to obtain the velocity fields and the water surface elevation in the coastal region, second to apply a mathematical model giving the evolution of the Dissolved Oxygen (DO) and the Biochemical Oxygen Demand (DBO) and third to formulate and solve some constrained optimal control problems. The non-existence of well-established commercial packages for this topic in 1986 was the motivation to develop our own codes. We considered two numerical strategies, finite elements and finite volumes methods in order to discretise the partial differential equations involved in the mathematical models. Non-standard finite elements were used for the shallow water equations. Concerning the finite volume approach, a new numerical treatment of the geometry terms (source terms) was proposed and analysed.

Implementation of the initiative

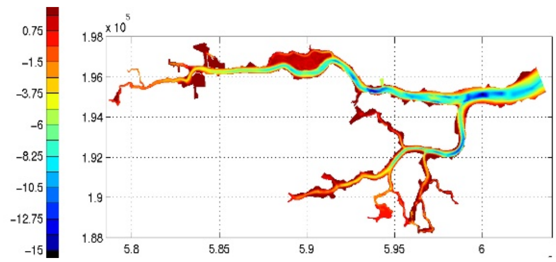
Using funds of the COTOP, three research contracts were agreed from 1986 to 1990 between this institution and the Department of Applied Mathematics of the USC. These contracts gave rise to a group in mathematical modelling directed by Prof Alfredo Bermúdez and complemented with four pre-doctoral students. For the finite volume topic, Profs Alain Dervieux and Antoine Desideri, from the well-known French Institute, INRIA, were contacted due to a previous collaboration in the HERMES European project. At the end of this project the group developed a FORTRAN code to solve the problem and wrote a report with the proposed location for the submarine outfalls in the "rias" of Pontevedra and Vigo.

The problem

The mathematical model of the shallow water equations is a system of hyperbolic conservation laws with source term, the latter arising from the bottom geometry. The main outcome in the context of the finite volume methods was the development of a completely new methodology to upwind these source terms.

Results and achievements

This contract was the initial motivation of a now consolidated research line. Since the preliminary application to the Galician rias, other geographical areas have been considered. Moreover, many theoretical and numerical contributions have been published by the group.



From an academic point of view, the research led to four PhD theses.

Lessons learned and replicability

This initiative was the origin of the research group in hydrodynamics modelling which is now composed of 5 permanent positions and 2 doctoral students. The methodology developed, from this contract in finite volumes, was tested experimentally in the context of the CADAM (Concerted Action on Dam-Break modelling) project (1998-2000). The developed computational tools are now implemented in two codes: SOS with the finite element method, which also include optimisation of systems of treatment plants, and TURBILLON with the finite volume method. The latter was registered in 2005 by the Universities of A Coruña and Santiago de Compostela and used to model shallow water flows in many coastal areas and rivers around the world: Arosa and Barqueiro rias in Galicia, Strait of Gibraltar, Ebro river in Spain, BioBio river in Chile, and the Crouch in estuary in the UK.

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New Storm Surge Forecasting Model in the Netherlands

Executive summary

The bottom topography of the North Sea used in a numerical tidal model was reconstructed more accurately by using a new parameter estimation method.

Challenge overview

Operational storm surge forecasting is very important for the Netherlands. The forecasts are computed by using a detailed numerical tidal model of the North Sea and adjacent areas developed by the research institute Deltares. A weak point in the model is that the bottom topography is not known very accurately.

At Delft Institute of Applied Mathematics (DIAM) of the Delft University of Technology, research has been carried out on efficient methods for parameter estimation in large scale numerical models. Deltares and DIAM have cooperated already for many years with each other on different research topics, so it was quite natural to formulate a joint project where the new parameter estimation algorithm would be applied to reconstruct the bottom topography of the storm surge forecasting model.

Implementation of the initiative

The initiative was carried out in the framework of a PhD project, partly financed by Deltares. Here first the general methodology was developed and tested for relatively simple problems. In the last year of the project the methodology was applied to the new tidal model of Deltares.

The problem

The so called adjoint method has often been used for the calibration of large scale numerical flow models. Here a number of unknown parameters are introduced into the numerical model. Using the given data these parameters are identified by minimising a cost function that measures the difference between model results and data (observations). The drawback of the adjoint method is the programming effort required for the implementation of the adjoint model code. In this research, a method of parameter estimation has been developed based on model reduction using Proper Orthogonal Decomposition (POD) for a large-scale shallow sea model of the entire European continental shelf. The POD based method shifts the minimisation problem into lower dimensional space and avoids the implementation of the adjoint of the tangent linear approximation of the original nonlinear model.

Results and achievements

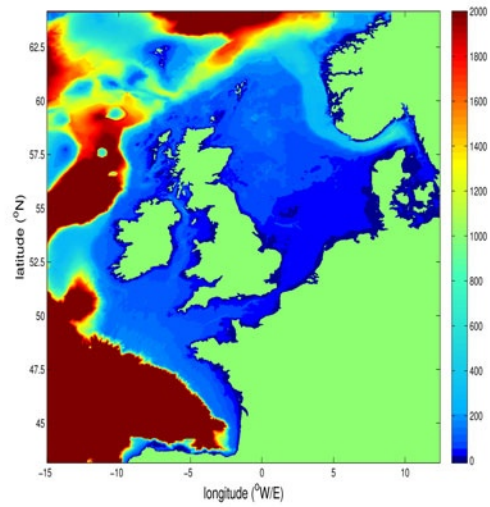

Figure 1. The bathymetry in meters. Bathymetry greater than 2000 m is shown as 2000 m. The North Sea is much shallower, with maximum depth around 200 m.

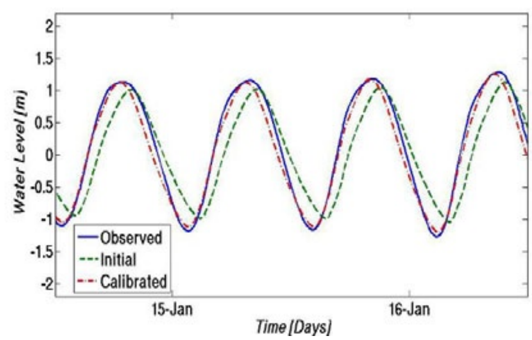

Figure 2. Water level time series at tide gauge station Delfzijl for a two days period from observations and the numerical model before and after calibration.

Validating the new model using long series of data showed that the Root Mean Square error reduced from approximately 20 cm to 10 cm.

TU Delft

GOFIM – Simulation and Optimisation of Waste Water Filtration

Executive summary

Mathematical models have been the basis for a new management protocol to improve the filtration process for drinking water treatment.

Challenge overview

The initiative started by the collaboration between the Mathematics Department and the Environmental Engineering Department of Firenze University. The latter has many collaborative projects with *Publiacqua*, the company in charge for the management of municipal waters in Firenze (Italy) and a wide region around the city. The continuous discussions taking place within this network led to the idea of applying mathematical models in order to improve the efficiency of the filtration plants, focusing on water treatment based on membrane filters.

Implementation of the initiative

The start of this collaboration was the contribution made by the Fondazione per la Ricerca e l'Innovazione – Firenze. Publiacqua decided to join the project GOFIM, coordinated by our Department, in which the company contributed by making available one of the filtration plants managed by the company. Such a plant was the reference point for the initiative, which started in January 2009 for the duration of one year.

The problem

We studied the filtration process based on hollow-fibres made of polymeric membranes. These fibres are arranged in cassettes like the one shown in the figure. The problem consists of describing the evolution of the transmembrane pressure, which is the quantity driving the filtration. To address this problem, a set of ODEs was defined and the system was solved numerically. The major challenge of the research was the experimental determination of parameters involved in the model, since it is difficult to link the qualitative description of the process taking place at the membranes with the experimental results referring to the global plant.

Results and achievements

The numerical code was implemented in the language Python, developing also a prototype for a graphical user interface to simulate the filtration process, and so a useful tool for managing the plant has been obtained. The methods experienced in this initiative were used by our Department to participate in a larger project on a similar subject. The project (named PURIFAST) has been funded by the European Community, within the programme LIFE+.

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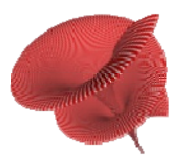


Solar Reflector Design

Executive summary

Methods were investigated to optimise the collection of solar energy on a roof.

Challenge overview

Erin Energy initiated contact with MACSI and sought help to optimise the design and cost of solar reflectors.

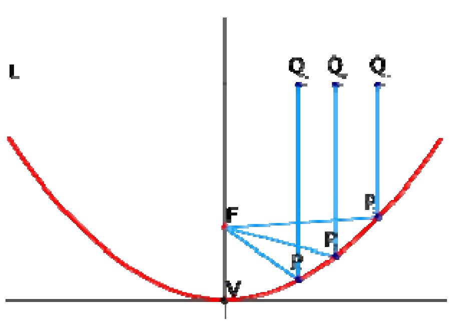
The company were aware that their panels were too thick. They needed guidance on how to approach this problem and required theoretical knowledge on how to solve it. The depth of the panels was also problematic for the construction industry. The company needed to find an economical way of reducing the depth of panels without compromising energy efficiency.

Implementation of the initiative

After initial analysis of the problem MACSI decided that the problem would benefit from an intensive brainstorming session involving experts from a wide range of mathematical disciplines. Therefore the problem was included in the 70th European Study Group with Industry: the second industrial study group held in Ireland, organised by MACSI at the University of Limerick. The study group format also simplified the consideration of intellectual property and confidentiality issues since results obtained by study groups are released into the public domain.

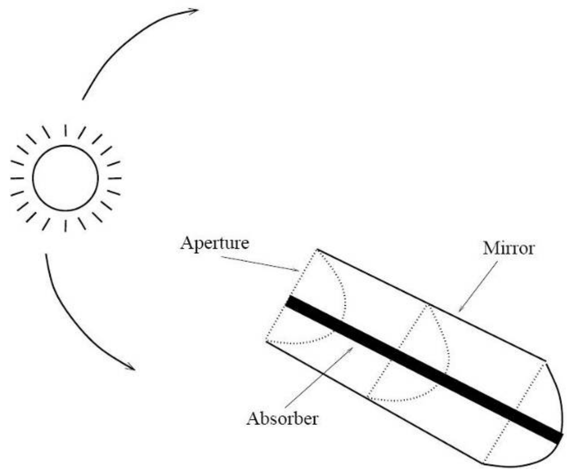
The problem

The device considered in this study collects solar energy on the roof of a house using an energy absorber. The solar energy is first collected, then transported and stored in a chemically based energy tank. Ideally, the roof should be completely covered with energy collectors but they are quite expensive. To reduce the amount of collectors necessary, the roof is covered with mirrors. The challenge was to optimise their shape in order to maximise the solar energy collected and minimise the costs.



Results and achievements

The solar radiation was studied and a ray tracing algorithm was developed by the academics involved. These models were used in simulations during which several techniques were considered to calculate the shape of the mirrors. The optimisation process shows that wide mirrors are not as energy efficient as smaller ones when the depth of the mirror is forced to remain shallow as is preferred in the construction industry. This simple rule is now used in the design of the solar reflector.



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MACSI
Mathematics Applications Consortium for Science & Industry

sfi Science Foundation Ireland

The Birth of CELMEC

Executive summary

The international meetings on Celestial Mechanics CELMEC, now worldwide recognised as focal points of the community, are born by a strong collaboration between the University of Roma Tor Vergata and Telespazio SpA, Roma.

Challenge overview

Modern Celestial Mechanics deals with the study of the motion of celestial bodies, natural or man-made. It can be approached from different points of view: a purely theoretical analysis of the models which may lead to results which are or little relevance for applications or a numerical investigation aimed to assess mission strategies but often without a solid theoretical foundation. We needed a bridge which would allow the merging of the mathematical analysis and the numerical experiments and the mission developments. A group of mathematicians together with some researchers working at Telespazio, Roma (Italy) decided in 1993 to try to find common ground through the organisation of a meeting encompassing both theory and applications.

Implementation of the initiative

The first meeting was organised on a national basis in 1993 at the University of L'Aquila in collaboration with Telespazio, Roma; it was followed in 1997 by a national second meeting. Due to the interest shown by the overseas community, the meeting was upgraded to an international congress in 2001. Since then, it is organised every 4 years by the Dept. of Mathematics, University of Roma Tor Vergata and Telespazio, Roma, which act as main sponsors of the meeting.

The problem

Modern Celestial Mechanics has a basic interdisciplinary nature. Its methods and applications are developed by mathematicians, physicists and engineers working in widely different contexts: universities, research institutions, astronomical observatories, space agencies and the aerospace industry. Within this framework the CELMEC meetings aim to establish a common ground among people working in this field, to provide a reference event open to discussions and collaborations, and to maintain a knowledge network at an international level.

Results and achievements

CELMEC is now recognised worldwide as the meeting point of the three "souls" of modern celestial mechanics: *Perturbation Theories* (stability and evolution of dynamical systems), *Solar System and Stellar Systems* (dynamics of solar system bodies) and *Spaceflight Dynamics* (near-Earth spacecraft orbits and interplanetary missions). The success obtained by the CELMEC meetings has brought to a steady increase in the number of participants, from 30 people in 1993 to 153 in 2009. The last meeting was attended by researchers coming from 25 countries. CELMEC contributed also to increase the development of common projects between mathematicians and space industries. The strong link between Universities and Telespazio established thanks to CELMEC have proven essential for building up the winning teams of contracts within the framework of the ESA NEO Space Mission Initiative, the ASI Vision for Moon Exploration and the ESA Space Situational Awareness Program. Moreover, CELMEC gave birth to the "Italian Society of Celestial Mechanics and Astrodynamics", which was founded in 2001 and it is presently composed by 130 members (http://www.mat.uniroma2.it/simca/). The association is very active in promoting collaborations between universities and industries.

Lessons learned and replicability

In the ever-increasing differentiation of the scientific disciplines CELMEC has demonstrated that there is a great demand for interaction among different topics, from purely mathematical subjects to space applications. CELMEC greatly contributed to the activities of the Space Academy Foundation, whose founder members are Telespazio, Thales-Alenia Space and the University of L'Aquila, and whose activities are devoted to high-level learning and training on space science. Science, technology and the socio-cultural aspects of merging together people working in different topics and institutions, all contributed to this end.

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Simulation of a Moving Bed Reactor Used in the Pulp and Paper Industry

Executive summary

This project gathered a group of experts in mathematics and chemical engineering to model and simulate numerically the dynamical behaviour of a moving bed reactor, the so-called digester, used in the pulp and paper industry. The main goal was to develop a software package, based on innovative numerical methods, to simulate experiments that could be expensive or risky in an industrial context.

Challenge overview

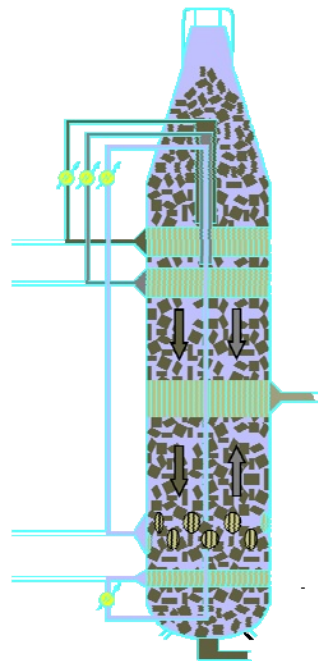
The pulp and paper business is one of Portugal's most important industries. Near Coimbra is located an important mill of the major Portuguese firm Portucel, which is one of the world's biggest producers of bleached eucalyptus Kraft pulp for the packaging industry and one of Europe's top five producers of uncoated wood-free paper. The most critical piece of equipment in a Kraft pulp and paper plant is the digester, known as the heart of the mill. It is a very special and complex heterogeneous reactor where a moving bed of wood chips contacts and reacts with sodium hydroxide and sodium sulphide in a liquid phase (Kraft process), in order to dissolve lignin and therefore to release the fibres of cellulose. In order to optimise the quality of the pulp, this industry has a real need for tools that enable the simulation of experiments that cannot be afforded or that might be risky in a real industrial context.

Implementation of the initiative

The problem was tackled under the scope of a research project financed by the Portuguese Science Foundation. The project involved two chemical engineers, five mathematicians and three graduate students, and it was accomplished in three years. The incidence of the work was twofold: from an engineering point of view, the description of the transient behaviour of the digester which allows the prediction of the quality of the pulp when some changes in the wood properties occur; from a mathematical point of view, the project gave the possibility to study new numerical methods, specially tailored to the phenomena that take place in each part of the digester.

The problem

The dynamical behaviour of the reactor can be represented by a system of hyperbolic nonlinear partial differential equations. Among the equations of the system, we can identify three main types: the equations that describe the temperature and the concentration of the solid, the entrapped liquid, and the free liquid phase. Each one of these types of equations presents a certain complexity, making its numerical simulation a hard task. Several factors contribute to the complexity in the numerical simulation: (i) the high non-linearity of the functions that represent the chemical reactions; (ii) the discontinuities induced by the extraction, enrichment and heat of the free liquor; (iii) the discontinuities in the convection velocity of the free liquor - positive where the liquid flows downwards and negative where the free liquid flows upwards.



Results and achievements

An open-source software package to simulate the dynamic behaviour of the digester was developed and is available by request. This package was tested by the company to simulate the steady-state case with very promising results. The scientific activity is reflected in five papers in international journals and one PhD thesis.

Lessons learned and replicability

The translation of the mathematical technology into practical terms and its efficient implementation in applicable paradigm is not straightforward. To enhance the process of communication between academia and industry there is a need for academic careers in industrial mathematics to demonstrate the complexity and value of application-driven research.

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Dynamic Image Based Lighting for Highly Realistic Lighting in Building Design

Executive summary

Arup hosted an Industrial Mathematics Intern from the University of Warwick to assist in the production of algorithms for re-lighting virtual objects using videos.

Challenge overview

The natural world presents our visual system with an ever changing and wide range of light, colours and intensities. The difference in average luminance level between a starlit night and daylight scene spans eight orders of magnitude. A human eye can see detail in regions that vary by 1 in 10,000 at any given eye adaptation level.

Existing video cameras are only capable of capturing a limited part of this wide range of light, colour and detail with sufficient resolution. High Dynamic Range (HDR) imagery can represent most real world luminances, but until now the capture of HDR images with a linear response function has been limited to static scenes rather than 'moving images'. In July 2009, the University of Warwick took delivery of the world's first true HDR video system.

Image Based Lighting (IBL) is a technique for artificially re-lighting real world or synthetic objects. The project sought to develop a new mathematical approach to IBL to cope with the dynamic nature of the lighting captured by the HDR video camera.

Additionally, the project sought to integrate accurate dynamic real world lighting captured from this HDR video system into Arup's existing visualisation system in order to significantly improve the fidelity of images used for building design.

Implementation of the initiative

Arup and Warwick University successfully applied to the Industrial Mathematics Knowledge Transfer Network for an Industrial Mathematics Internship, a mechanism which is co-funded from the UK's Engineering and Physical Sciences Research Council and is designed to expose current PhD students to real industrial problems in a business environment for 3-6 months to stimulate new relationships between industry and academia.

The problem

Dynamic IBL will play a key role in improving the visual fidelity of computer generated imagery for building design. High-fidelity rendering techniques, such as image based lighting are physically based and thus require a robust mathematical foundation in order to deliver the desired perceptual equivalence between the real scene and its virtual counterpart. A novel mathematical method for dynamic image based lighting is required to cope with the nature of the video streams now possible with the HDR video camera.

The new mathematical method can then be used to define algorithms for IBL using images or videos. Of particular interest are temporal IBL algorithms applicable to the newly acquired HDR video.

Results and achievements

An important achievement of the project was the production of a series of algorithms for re-lighting virtual objects using videos. Of particular interest was the re-lighting of high contrast videos, i.e. videos with a high dynamic range.

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Optimisation of Electricity Production

Executive summary

Every day, EDF (French Electricity Board) has to compute production schedules of its power plants for the next day. This is a difficult, large-scale, heterogeneous optimisation problem.

Challenge overview

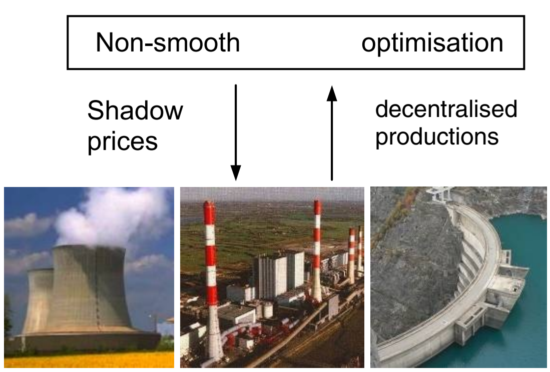
In the mid eighties, a meeting was organised between INRIA and EDF R&D. The idea was to let EDF present some of their applications, to explore possible collaborations. Indeed, EDF has a long tradition of scientific work, in particular with academics. Their production optimisation problem was presented among others. Its mathematical model was clearly established; even the relevant software existed, but the solution approach needed improvement. The mathematics required turned out to perfectly fit with INRIA competences.

Implementation of the initiative

Collaborative work therefore started immediately. No difficulty appeared with administrative issues such as intellectual property or industrial confidentiality. It was a long-term research project, so deadlines posed no problem either.

The problem

The solution approach is by decomposition: each power plant (EDF software) optimises its own production on the basis of “shadow prices” remunerating it; these prices are iteratively updated (INRIA software) so as to satisfy the balance equation. The engine to compute the prices is a non-smooth optimisation algorithm.



The difficulty was to join the EDF and INRIA-software. This turned out to be harder than expected. The model appeared as not mature enough and significant bugs were revealed. The project was basically abandoned and it is only in the mid nineties that intensive collaboration resumed on a renewed model.

Results and achievements

This time, the collaboration was successful and the new software became operational a few years later. This relatively long delay was due to necessary industrial requirements (mainly aimed at achieving reasonable reliability). Substantial improvements in cost and robustness were achieved. EDF is highly satisfied with this collaboration, which continues and will probably continue for many years.

Current research focuses on developing more accurate models of the power plants, entailing more delicate price optimisation.

Several academic outcomes resulted from this operation:

- To understand better and to improve highly sophisticated optimisation methods;
- To assess these methods in the “real world”, thereby introducing them for new applications;
- To exhibit the practical merits of a mathematical theory (convex analysis, duality), generally considered so far as highly abstract (and taught as such in the university curriculum).

Lessons learned

Beyond science and techniques, a lesson of this success story is that any academic-industrial collaboration should be undertaken with strong mutual esteem and confidence.

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