Preface

The Workshop in Computational Mathematics is organized by the Laboratory for Computational Mathematics (LCM) of the Centre for Mathematics of the University of Coimbra (CMUC) that promotes research in computational mathematics and scientific computing.

Computational mathematics and scientific computing are growing and fast changing areas whose applications to various branches of science, engineering, medicine, economics and others are increasing in number and relevance every day. On account of that, the activity of LCM includes interdisciplinary research, high performance computing and development of numerical software and collaboration with the industry.

This meeting is the second meeting of a series that we expect will be held every year, to provide a forum for discussion on recent aspects of numerical mathematics promoted by the LCM and worldwide. They seek to convene leading experts with special emphasis on contributions from Portugal. All speakers were invited and this small text collects the abstracts of those speakers.

José Augusto Ferreira
Sílvia Barbeiro
Ercília Sousa

Location

Department of Mathematics, room 2.4, Largo D. Dinis, Coimbra

Organizers

José Augusto Ferreira, Sílvia Barbeiro, Ercília Sousa

Support

Centre for Mathematics of University of Coimbra Department of Mathematics, Faculty of Sciences and Technology of University of Coimbra

Scientific programme

	THURSDAY, FEBRUARY 1	FRIDAY, FEBRUARY 2
9.00- 9.30	*Reception*	
9.30-10.30	Linda Green	Robert Mattheij
10.30-11.00	Adérito Araújo	João Luís Soares
11.00-11.30	*Coffee Break*	*Coffee Break*
11.30-12.00	Isabel Narra Figueiredo	Luís Nunes Vicente
12.00-12.30	Georg Stadler	Ana Luísa Custódio
12.30-13.00	Paula de Oliveira	Ismael Vaz
13.00-14.30	*Lunch*	*Lunch*
14.30-15.10	Luís Gouveia	Luís Trabucho de Campos
15.10-15.50	Luís Filipe Menezes	José Francisco Rodrigues
15.50-16.20	*Cofffee Break*	*Coffee Break*
16.20-17.00	Filomena D'Almeida	António Mendes Ferreira
17.00-17.40	Paulo Oliveira	Adélia Sequeira
20.00	*Workshop Dinner*	

Abstracts

Segmenting medical images using level sets

Adérito Araújo⋆*, D. M. G. Comissiong, G. Stadler*

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Image segmentation is the process by which objects are separated from background information. Structural segmentation from 2D and 3D images is an important first step in the analysis of medical data. In this talk we will present some results obtained by a level set algorithm on the segmentation of two and three-dimensional images. Besides synthetic data, we also use magnetic resonance images of the human brain provided by the Institute of Biomedical Research in Light and Images of the University of Coimbra (IBILI).

Improving Efficiency in Direct Search Methods

Ana Luísa Custódio⋆*, L. N. Vicente*

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Direct search methods are widely used in practice but have the major drawback of sometimes being very slow. In this talk we will introduce a number of ways of making directional direct search (pattern search in particular) more efficient by reusing previous evaluations of the objective function,based on the computation of simplex derivatives (e.g., simplex gradients). At each iteration, one can attempt to compute an accurate simplex gradient by identifying a sampling set of previous evaluated points with good geometrical properties. The simplex gradient can then be used to reorder the evaluations of the objective function associated with the directions used in the poll step or to update the mesh size parameter according to a sufficient decrease criterion, neither of which requires new function evaluations. We will present mathematical support for these procedures and describe them in detail. Numerical results will be reported for a set of problems which includes problems from the CUTEr collection and one application problem (related to the simulation of a mechanical system). Numerical experience shows that these procedures can enhance significantly the practical performance of directional direct search methods.

Local Approximate Inverse and Spectral Computations for an Integral Operator

Filomena Dias d' Almeida [⋆], *P. Vasconcelos, M. Ahues, A. Largillier*

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Let us consider an integral formulation of the transfer problem that represents the restriction of a strongly coupled system of nonlinear equations dealing with radiative transfer in stellar atmospheres. This restriction comes from considering that the temperature and the pressure are given. The original form of this model was proposed by Groupe de Transfert de l'Observatoire de Lyon to the Équipe d'Analyse Numérique of the Université de Saint Etienne and to us. The interest of the underlying integral operator is not restricted to the solution of the corresponding Fredholm integral equations of the second kind it is also useful to compute its spectral elements. They will be computed by a projection method on a subspace of small dimension followed by iterative refinement methods based on defect correction. This technique needs the construction of an appropriate local approximate inverse, and in order to do that, in this case, we have to use a definition of this that generalizes the notion of defect correction introduced by Stetter. Numerical results with the radiative transfer operator are presented.

Radial basis functions for the analysis of laminated structures

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Radial basis are a very precise meshfree method for interpolation of data and PDEs. The method we use is based on a collocation technique for both boundary and domain nodes. The method was originally applied to PDEs by Edward Kansa in early 1990's, with great accuracy. In the early 2000's our group produced a number of results for the analysis of laminated beams, plates and shells by using various forms of RBfs and some coupling with pseudospectrals. The quality of the method in its global form is highly dependent on a shape parameter. This parameter was recently optimized by Ferreira and Fasshauer producing highly accurate results for static deformations and free vibrations of beams and plates. More recently (unpublished) work is being performed on adaptive methods for the analysis of beams and plates using radial basis functions, by a residual subsampling technique. The lecture will briefly address all mentioned aspects.

Analysis and design of smart structures and piezoelectric devices

Isabel Narra Figueiredo⋆*, Team of the Project POCI/MAT/59502/2004 (FCT-Portugal Research Project)*

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Smart structures are advanced structures that consist generally of a host structure (for instance a plate, a beam or a shell) with integrated surface-bonded or embedded devices of active or smart materials. These devices have the capability to change the structure's behavior acting as sensors and actuators, with the purpose of obtaining a self-controlled and self-adaptive structure able to react and adapt to the environment. The sensors give information about the state of the structure, while the actuators can generate modifications in its mechanical behavior. The most used smart materials are piezoelectric materials, which have the property to convert mechanical energy into electric energy and vice-versa. Therefore piezoelectric devices are both actuators and sensors. This makes them useful in a wide range of practical applications (as for instance in aerospace, aeronautic, automotive, industrial, biomedical, underwater communications, medical imaging, therapy and control applications). In a large number of applications, its geometries are those of thin plates or thin rods (i.e. for a plate, the thickness is very small when compared to the area of the middle plane of the plate, and, for a rod, the area of the cross section is very small with respect to the axis's length). In this talk new asymptotic models for static nonhomogeneous anisotropic piezoelectric thin plates, rods or smart structures (the latter made of elastic plates with integrated piezoelectric patches) are described and mathematically justified. In addition, we report on our numerical tests to study the actuator and sensor effect for thin piezoelectric plates. By "asymptotic model" we mean a reduced (i.e. lower-dimensional) electro-mechanical equilibrium model. It corresponds to the limit model which is derived, when in the three-dimensional system of equations, the thickness or the area of the cross section tends to zero. We emphasize that these asymptotic models are reliable. In fact their justification relies on rigorous mathematical proofs demonstrating the weak and strong convergence of the solutions of the three-dimensional models when the asymptotic parameter, either the thickness or the area of the cross section, tends to zero. Besides the simple structure of asymptotic models, they can be numerically solved fast compared to the original threedimensional models. For plates, it has been found that the two unknowns of the asymptotic models are the Kirchhoff-Love mechanical displacement and the electric potential. While in the three dimensional partial differential formulation of these models these two variables are coupled, in the asymptotic plate models the electric potential can be derived as an explicit function of the mechanical displacement. Regarding the numerical tests, two different optimization approaches are used to study the actuator effect of the asymptotic plate model. The first one is a non-differentiable multi-objective optimization problem while in the second approach, an optimal control formulation is used. Our tests are performed using a finite element code, which has been developed to solve the asymptotic plate model for the case of a laminated plate made of different piezoelectric materials.

On reformulations by discretization

Luís Gouveia

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MIP packages depend strongly on the MIP formulation given to be solved. We describe and survey a reformulation technique (the so-called reformulation by discretization) for solving several classes of MIP problems. In general terms, "Discretization"is a reformulation technique that is used to transform a discrete optimization model with at least two sets of variables associated to objects of the problem (one set of binary variables indicates whether each object is in the solution and the other set, of integer variables, indicates an amount associated to each object) into another with at least one set multiple-indexed binary variables where the information associated to the extra index corresponds to the values of the integer variables of the original model. Although this technique has an obvious disadvantage, namely the creation of many discretized binary variables, the discretized variables permit us to i) model variations of the problem with more general cost functions and ii) generate new sets of strong valid inequalities which lead to models with a much stronger linear programming relaxation. Our talk and main results, are focused on Capacitated Concentrator Location problem with modular costs where we will show the two advantages mentioned before. At the end, other problems where this technique has been used with success will be briefly surveyed: variable sized bin packing problem, lot sizong, degree constraint spanning tree with node dependent costs and (time dependent) travelling salesman problem.

Using stationary queueing models to set staffing levels in non-stationary service systems

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A common feature of many service systems is that demand for service often varies greatly by time of day. In many cases, including telephone call centers, police patrol, and hospital emergency rooms, staffing levels are adjusted in an attempt to provide a uniform level of service at all times. Analyzing these systems is not straightforward because standard queueing theory focuses on the long-run steady-state behavior of stationary models. In this talk, I'll discuss how stationary queueing models can be adapted for use in non-stationary environments so that time-dependent performance is captured and staffing requirements can be identified. Specific applications to telephone call centers and hospital emergency rooms will be described.

Some industrial problems from Eindhoven

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We will discuss a number of problems that have come to us from industrial companies. Rather than concentrating on a single theme, we will show a variety of problems, like cooling machinery for the 75 K region, drilling of holes in alloys by lasers or electrochemistry, pressing and/or blowing of viscous material, oscillating flames and tracer transport. All these problems are related to larger projects carried out at TU/e for and with industry. If time permits we will also discuss the use of local defect correction used in some of these problems to deal with largely varying numerical grids needed to solve such problems accurately.

Trimming and splitting of 3D solid hexahedral finite element meshes

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Deep drawing is a forming process controlled by a large number of parameters. The numerical simulation of this technological process is not simple and involve, besides the complex task of simulate the deformation process, other algorithms that allow to execute all the production stages, from the initial blank sheet to the final part ready to assembly. One example of this is the algorithms to trimming and/or splitting finite element meshes that are frequently necessary to fully simulate multi-step stamping processes. During the presentation it will be described some strategies to perform trimming and/or splitting operations on 3D solid hexahedral finite element meshes. The remapping of finite element meshes, necessary after the geometrical adjustments during the trimming operation, will be described, presenting a method called Incremental Volumetric Remapping (IVR). The IVR method is based in a volumetric approach where the calculus of the remapped state variables is obtained by means of a weighted average of the intersection volume between the meshes. An example of application of the trimming algorithm will be presented. This example consists in a method to determine the optimal initial blank shape for a rectangular box using finite element simulations and NURBS surfaces. The optimisation procedure involves an initial blank shape which is iteratively trimmed according to the deep drawing simulations results to achieve the final optimal blank shape. Parametric NURBS surfaces are used to optimise the initial blank shape based on the deformation behaviour predicted by numerical simulation.

A phenomenological model for desorption in polymers

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In desorption phenomena in polymers an overall outward flux triggers a change from a rubbery state to a glassy state that are separated by a moving front. Experimental results exhibit features that can not be completely explained by Fick's Law. To overcome this difficulty several authors have proposed these last years mathematical models with a viscoelastic stress term in the flux. These models exhibit a global non Fickian character. Nevertheless, the numerical simulations obtained using this modified flux exhibit sharp fronts which in some cases do not agree with experimental data

The idea underlying the model presented in this talk lies on the observation of experimentalists that the non Fickian character is local: if one considers a system where a front separates two different states the only obvious violation of Fick's law takes place only at the moving front. As a consequence, if a particular kinetics is taken into account by imposing an upper limit on the flux or on the speed of the front, there may be no need to invoke a global violation of Fick's law. The new model uses Fick's law in the rubbery and glassy regions and a parameter rate controlled motion of the moving front .

The model is studied from a theoretical point of view. The well-posedeness of the model is established. Analytical expressions for the glassy and rubbery concentrations are computed using an integral method developped by Boyle for standard diffusion problems. The qualitative behaviour of these concentrations are studied for short and long times. Particular attention is devoted to the dependence of the speed and the flux on the parameter. Numerical simulations illustrating the behavior of the model are included showing agreement with experimental data.

Approximating from sparse discrete observations

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It happens quite often that we are faced with a sparse number of observations over a finite number of cells and we are interested in the estimation of the cell probabilities. The simple histogram produces approximations with the zero value for too many cells. Some polynomial smoothers have been proposed to circumvent this problem which show good properties in the analysis of such sparse situations but have the drawback of producing negative values. We propose a penalized polynomial smoothing for this problem. The estimators that are proposed are always positive and a simulation study show a very good behaviour with respect to natural error criteria.

If the distribution is bidimensional, we may further have the knowledge of one of the marginal distributions. Even with nonsparse observations it is useful to construct approximations that use the partial information. The techniques developed provide an answer to this problem. The proposed estimators perform well for sparse and nonsparse observations, in this bidimensional framework.

Systems of unilateral problems and applications

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Dual estimates for T-monotone operators are important to characterize properties of solutions to abstract unilateral problems leading to existence and regularity results. For second order elliptic or parabolic differential operators, those estimates are also called Lewy-Stampacchia inequalities and imply well-known regularity results for the solution to obstacle type problems. Developing these ideas we have obtained recently new results in two directions. In the N-membranes problem for quasi-linear degenerate systems, the dual estimates have a simple iterated expression in terms of the data and considering this problem as a system coupled through the characteristic functions of the sets where at least two membranes are in contact, it is possible to characterize the stability of the coincidence sets. For other unilateral problems, that include convex sets of the type of Gibbs simplex, the combined Lewy-Stampacchia inequalities imply that the regularity of the solution to multi-phase constrained diffusion systems is the same as the one corresponding to linear parabolic systems of second order. This has interesting consequences in phase field models with constraints for ternary mixtures, for a system of two grains and for a diffuse interface model for simultaneous order-disorder and phase separation that have been used in the material science literature.

Blood rheology: mathematical models and numerical simulations

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Cardiovascular diseases are among the major causes of death in developed countries, having a great social and economic impact. The simulation of the cardiovascular system is hence of utmost importance, helping to understand blood circulation and medical prediction of vascular diseases, without using invasive techniques. The complexity of the problems at hand, which can involve the coupling of different mathematical models to capture phenomena that occur at multiple scales in time and space, are very challenging and often stimulates the use of innovative mathematical and computational techniques.

Blood is a multi-component mixture with complex rheological characteristics. It consists of multiple particles, red blood cells (erythrocytes) white blood cells (leukocytes) and platelets (thrombocytes), suspended in an aqueous polymer solution, the plasma (Newtonian fluid). The arterial wall is a complex multi-layer structure that deforms under blood pressure. In the large vessels where shear rates are high enough, it is reasonable to assume that blood has a constant viscosity and a Newtonian behaviour. However in smaller vessels and capillaries or in some diseased conditions, the presence of the cells induces low shear rate and blood exhibits remarkable non-Newtonian properties, like shear-thinning viscosity, thixotropy and viscoelasticity. We refer to [1,2] as recent review papers on mathematical models of blood rheology.

In this talk we present a short overview of some constitutive models that can mathematically characterize the rheology of blood and some numerical simulations to illustrate its phenomenological behaviour. Using a mesoscopic lattice Boltzmann flow solver for non- Newtonian shear thinning fluids, we present a three-dimensional numerical study of the dynamics of leukocytes rolling and recruitment by the endothelial wall, based on in vivo experimental measurements in Wistar rats venules [3]. Preliminary numerical results obtained for a comprehensive model of blood coagulation and clot formation, that integrates physiologic, rheologic and biochemical factors will also be presented [4]. The corresponding threedimensional simulations were obtained for a shear-thinning blood model using a finite volume semi-discretization in space and a three-stage Runge-Kutta time integration method.

References:

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[2] A. M. Robertson, A. Sequeira and M. Kameneva, Hemorheology. In: Hemodynamical Flows: Modelling, Analysis and Simulation, G. P. Galdi, R. Rannacher, A. Robertson and S. Turek (eds.), Birkhauser, 2007, to appear.

[3] A.M. Artoli, A. Sequeira, A.S. Silva and C. Saldanha, Leukocyte rolling and recruitment by endothelial cells: hemorheological experiments and numerical simulations, Journal of Biomechanics, 2007, submitted.

[4] T. Bodnár and A. Sequeira, Shear-thinning effects of blood flow past a formed clot, WSEAS Transactions on Fluid Mechanics, Issue 3, Vol. 1, pp. 207-214, 2006.

Call Center Staffing: a practical application

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Capacity management in call centers is critical and the staffing of human resources is the most pro-eminent problem. Gans et al (2003) report that capacity costs in general, and human resource costs in particular, account for 60-70% of the operating expenses in a call center.

However, many small and mid-sized call centers make staffing decisions with minimum scientific support. Workforce scheduling software tools that address these staffing issues are extremely expensive. Moreover, the investment is risky because the effectiveness of these tools is difficult to validate, due to the unpredictable nature of the arrival stream, service duration and other process complexities.

In this talk, we will report on a recent, and ongoing, project with a Portuguese call center where no such workforce scheduling software tool is in place. We are helping them setting staffing levels and finding adequate staffing schedules based on our previous research experience on nonstationary queueing models for staffing.

Gans, N., G. Koole, A. Mandelbaum. 2003. Telephone Call Centers: Tutorial, Review, and Research Prospects. Manufacturing & Service Oper. Management 5 79-141.

Examples and numerical solution for large-scale inverse problems

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Modelling of physical systems allows us to draw conclustions of the following type: Given a complete discription of the system, we predict the outcome of measurements. This is usually referred to as *simulation* or *foreward problem* or, more casually, just as *solving the equation*. On the contrary, *inverse problems* consist of using the actual results of some measurement to infer the values of the parameters that characterize the system. These problems occur in many practical applications, in which one cannot measure the relevant parameters directly. Inverse problems are illposed and thus appropriate regularization techniques are required. In this talk, I will present two inverse problems with systems governed by partial differential equations. After discretization by finite elements, they lead to large-scale (i.e., several 100.000s unknowns) systems.

The first problem is an image registration problem: Given a so-called reference image and a so-called template image, we intend to find a reasonable transformation that makes the transformed template image as similar as possible to the reference image. The problem of finding such a transformation is an inverse problem, where the template image is the "measured data" and the deformation has to be inverted for. Among others, there are applications in brain mapping and in surgery planning.

The second example deals with inverse seismic wave propagation. Here, reflections of waves inside the earth that are measured on the earth's surface are used to study the rock (and eventually fluid) formations inside the earth. Even for only one space dimension, for realistic data this time-dependent problem leads to large systems.

To tackle these large nonlinear systems numerically, we use Newton-like schemes and iterative solvers for the linear systems. Moreover, a multilevel approach is used to speed up the iteration and to avoid local solutions. For both the registration and the seismic wave inversion problem numerical results are shown. The results for the inverse seismic wave propagation problem are kindly provided by my collegue Carsten Burstedde.

On the curvature and torsion effects in one and two dimensional waveguides

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When considering Schrödinger's equation, with an infinite potential at the boundary, for a curved tube or for a thin shell, the wave function turns out to be a solution of an eigenvalue problem for Laplace's operator, whose eigenvalues are associted with different energy levels. In this work, we study the limit problem as the diameter of the tube's cross section or the thickness of the shell goes to zero and show the effect of the curvature and of the torsion functions on the energy levels (eigenvalues) and on the wave functions (eigenvectors).

Application of direct search methods to parameter estimation in astrophysics

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The purpose of this talk is twofold. First, we present a new algorithm for the global minimization of a function subject to simple bounds, without the use of its derivatives. The underlying algorithm is a pattern search method, more specifically a coordinate search method, which guarantees convergence to stationary points from arbitrary starting points. In the optional search phase of pattern search the algorithm incorporates a particle swarm scheme to globally explore the possible nonconvexity of the objective function. Our extensive numerical experiments showed that the resulting algorithm is highly competitive with other global optimization methods also based on function values. In the second part of the talk we discuss the application of optimization methods, and in particular of the abovementioned method, to identify optimal parameters in astrophysics models. The main goal is to estimate stellar masses and ages, as well as other parameters such as initial individual abundance of helium and hydrogen, from the observed stellar surface temperatures and total luminosities. The estimation problems consist of the minimization a least-squares type residual function subject to boundson the variables and to linear constraints. Due to the simulation process involved, derivatives of the objective function are unavailable.

Large-scale nonlinear programming using interior-point and filter methods

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This talk describes the development of an optimization solver (ipfilter) for large scale nonlinear programming problems. The underlying algorithm is based on the primal-dual interior-point filter framework developed in the paper by M. Ulbrich, S. Ulbrich, and L. N. Vicente, A globally convergent primal-dual interior-point filter method for nonlinear programming, Mathematical Programming, 100 (2004) 379-410. This method is based on the application of the filter technique to the globalization of the primal-dual interior-point algorithm, avoiding the use of merit functions and the updating of penalty parameters. The algorithm decomposes the primal-dual step obtained from the perturbed first-order necessary conditions into a normal and a tangential step. Each entry in the filter is a pair of coordinates: one resulting from feasibility and centrality, and associated with the normal step; the other resulting from optimality (complementarity and duality), and related with the tangential step. The method possesses global convergence to first-order critical points. We will describe some of the features of ipfilter, its current capabilities and limitations. We will present numerical results for large-scale problems and if time permits discuss extensions of the original algorithm and of its convergence theory.

List of participants

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Adérito Araújo, University of Coimbra
Alzira Mota, Instituto Superior de Engenharia do Porto
Ana Luísa Custódio, New University of Lisbon
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