Scientific Computing
Calcul scientifique
(Org: **Christine Bernardi** (CNRS-Paris VI), **Anne Bourlioux** (Montréal) and/et **Brian Wetton** (UBC))

MOHAMMED AMARA, IPRA–LMA UMR5142, Université de Pau, 64013 Pau Cedex, France
Mixed finite element approximation of a coupled reservoir-wellbore model with heat transfer

In order to interpret recorded temperatures in wellbores as well as a flowrate history at the surface and thus to better characterize reservoirs, we are interested in the thermomechanical coupling of a petroleum reservoir with a vertical wellbore, both written in 2D axisymmetric form.

The reservoir model, assumed to be a monophasic multi-layered porous medium, is described by a Darcy–Forchheimer equation together with a non-standard energy balance. The wellbore model is based on the compressible Navier–Stokes equations and an energy equation. The coupling between these two models is achieved by adequate transmission conditions at the perforations.

We obtain, at each time step, a mixed formulation and the uniqueness of the solution is established by means of a generalization of the Babuska–Brezzi theorem.

Concerning the spatial discretization, we approximate the heat and mass fluxes by the lowest-order Raviart–Thomas mixed elements, the pressure and the temperature by piecewise constant elements, the fluid's velocity by Q_1 continuous elements while the Lagrange multipliers on the interface are taken piecewise constant. The density is updated by means of a thermodynamic module and the convective terms are treated by appropriated upwind schemes. A technical analysis of the discrete mixed formulation is carried on and the well-posedness of the problem is proved.

Numerical tests including real cases will be presented.

FAKER BEN BELGACEM, Université de Technologie de Compiègne, Centre de Recherches de Royallieu, BP 20529, 60205 Compiègne Cedex, France
On the Lavrentiev Regularization of the Ill-posed Data Completion Problem

The Lavrentiev regularization method is naturally fitted to the data completion problem, put under the variational form proposed in Ben Belgacem and El Fekih (Inverse Problems, 2005). We address the important issue of selecting the regularizing parameter. We study an a priori choice and the a posteriori choice by means of the discrepancy principle written on the Kohn–Vogelius function. In both cases, we prove that the Lavrentiev method, though its simplicity, is *super-convergent* as we state estimates similar to those expected for Tikhonov's method.

ZAKARIA BELHACHMI, Université Paul Verlaine–Metz
Computing Neumann–Laplacian eigenvalues in nonsmooth domains and applications

The study of shape optimization problems involving the eigenvalues of an elliptic operator (the Laplacian-Δ for instance) has strong relations with several applications (stability of vibrating bodies, ...). When Dirichlet boundary conditions are imposed on the free boundary $\partial\Omega$, there are several situations where solving the optimization problem is made easier, in both theoretical and computational aspects, by the existence of a relaxation process. The same problems for the Laplace operator with Neumann conditions on the free boundary is a difficult subject where up to now very few results are available. In fact, proving existence of solutions in this case is related to the (deep) understanding of the behavior of the Neumann spectrum on non-smooth domains (highly oscillating boundaries, cracks, etc). This is a challenging question and it is largely open.

In this talk, we consider the Neumann–Laplacian eigenvalue problem in domains with multiple cracks. We derive a mixed variational formulation which holds on the whole geometric domain (including the cracks) and implement efficient finite element discretizations for the computation of eigenvalues. Optimal error estimates are given and several numerical examples are presented, confirming the efficiency of the method. As applications, we numerically investigate the behavior of the low eigenvalues of the Neumann–Laplacian in domains with a high number of cracks. For particular cases of highly oscillating boundaries, these computations allows us to identify formally the problems with the limit spectra.

ADEL BLOUZA, Université de Rouen

Finite element approximations of Naghdi's shell model in cartesian coordinates

We present a mixed formulation of Naghdi's model for linearly elastic shells with little regularity, and a conforming finite element approximation thereof. The a posteriori analysis of the discrete problem leads to the construction of error indicators which satisfy optimal estimates. We then describe a mesh adaptativity strategy based on these indicators. We also use them to optimize the choice of the penalty parameter of our discretization. Numerical tests are given that validate and illustrate our approach.

ANDRÉ FORTIN, Université Laval

An adaptive remeshing method for free surface viscoelastic fluid flow problems

In this work, we describe an adaptive remeshing method which can be applied to the computation of viscoelastic fluid flow problems involving free surfaces. We first introduce a log-conformation formulation of the constitutive equation and a level set method for the computation of free surfaces.

The methodology is then applied to the deformation of droplets in shear flow and to put in evidence the importance of secondary flows in coextrusion problems.

FRÉDÉRIC HECHT, UPMC Univ. Paris 06, UMR 7598, Laboratoire Jacques-Louis Lions, F-75005, Paris, France

Some mesh adaptation schemes for solving PDE with high order finite element method

Aujourd'hui il existe des générateurs de maillage triangulaire ($d = 2$) ou tétraédrique ($d = 3$) qui utilisent des métriques pour prescrire les tailles de maille. Ces métriques $\mathcal{M}$ sont données comme des champs de matrice symétrique définie positive en tout point de l'espace. Ces champs dans le cas d'une interpolation élément fini P_1 Lagrange, ces métriques dérivent directement du Hessien de la solution à approcher.

L'idée pour généraliser cette construction est de définir une représentation infinitésimale de l'erreur d'une fonction u donnée. Pour une approximation d'ordre $k+1$ (polynôme de dégre k), nous utiliserons simplement le reste de la formule de Taylor à l'ordre $k+1$, c'est à dire la dérivée $D^{k+1}u$ (une forme $k+1$ linéaire) à l'ordre $k+1$ en négligant les termes d'ordre supérieur.

Alors nous construirons une métrique telle que:

$$\frac{1}{(k+1)!}|D^{k+1}u(\xi,\ldots,\xi)| \leq (\xi,\mathcal{M}\xi), \qquad \forall \xi \in \mathbb{R}^d, \|\xi\| = 1.$$

Nous proposerons des schémas numériques pour construire des métriques respectant cette inégalité. Puis nous expliquerons comment construire des champs de métrique quasi-optimaux asymptotiquement, pour construire un maillage

- avec un nombre de maille minimal pour une erreur donnée,
- avec un nombre de maille donné qui minimise l'erreur;

où l'erreur est l'erreur d'interpolation en norme L^p ou $W^{1,p}$.

Pour finir, nous présenterons le logiciel FreeFem++ pour illustrer ces propos.

NICHOLAS KEVLAHAN, McMaster University, Hamilton, ON L8S 4K1
Stochastic Coherent Adaptive Large Eddy Simulation

Stochastic Coherent Adaptive Large Eddy Simulation (SCALES) is an extension of Large Eddy Simulation that uses a wavelet-based dynamic grid adaptation strategy to solve for the most energetic coherent structures in a turbulent flow field, while modelling the effect of the less energetic ones. A localized dynamic subgrid scale model is needed to fully exploit the ability of the method to track coherent structures. In this paper, new local Lagrangian models based on a modified Germano dynamic procedure, redefined in terms of wavelet thresholding filters, are proposed. These models extend the original path-line formulation of Meneveau *et al.* (J. Fluid Mech. **319**, 1996) in two ways: as Lagrangian path-line diffusive and Lagrangian path-tube averaging procedures. The proposed models are tested for freely decaying homogeneous turbulence with initial $Re_\lambda = 72$. It is shown that the SCALES results, obtained with fewer than 0.4% of the total non-adaptive nodes required for a DNS with the same wavelet solver, closely match reference DNS data. In contrast to classical LES, this agreement holds not only for large scale global statistical quantities, but also for energy and, more importantly, enstrophy spectra up to the dissipative wavenumber range.

BOUALEM KHOUIDER, University of Victoria
Convectively coupled waves in a simple multicloud model

Organized convection in the tropics involves a hierarchy of spacial and temporal scales ranging from the individual clouds of a few kilometres and a few hours to the mesoscale cloud clusters and superclusters and their intraseasonal/planetary scale wave envelopes, known as the Madden–Julian oscillation (Nakazawa, 1988). Interactions between large scale dynamics (and thermodynamics) and small scale convective processes are believed to play a crucial role in the generation and maintenance of these organized features. The analysis of Wheeler and Kiladis (1999) and Heartel and Kiladis (2004) showed that the dynamical fields and the power spectral peaks of the synoptic scale superclusters—identified as the convectively coupled waves, are closely related to the first few equatorially-trapped linear waves of Matsuno (1966), but with a significantly reduced equivalent depth (*i.e.*, phase speed). Despite recent research efforts and significant progress in computing power, current general circulation models (GCM), used for long-term weather and climate predictions, often simulate poorly the dynamics and structure of convectively coupled waves, and particularly the MJO, due to an inadequate treatment of organized convection by the convective parametrizations currently used by the GCMs (Moncrieff, 2004). To study these interesting waves, from both a practical and a theoretical perspective, we designed and used an idealized multicloud model that captures many of the physical and dynamical features attributed to the large scale organized convective systems.

Joint work with Andrew J. Majda.

EMMANUEL LORIN, University of Ontario I.T.
Numerical Modeling of Intense and High Frequency Laser-Gas Interactions

In this communication we are interested in mathematical, numerical and modeling tools for ultrashort, high intensity and high frequency laser-matter interactions in dense gaseous media. These last 15 years, in this extreme regime, several new phenomena have been experimentally discovered (High Harmonic Generation, Filamentation, ATI), and will likely be very useful for practical applications in laser technology (virtual antennas, atmospheric applications, communications, dynamic imaging, etc). We have recently presented one of the first multiscale models and a corresponding numerical 3-D scheme for laser-gas interaction in this regime. The model involves the coupling of macroscopic non-homogeneous Maxwell's equations with Time-Dependent Schroedinger Equations (TDSE's). Indeed, in order to consider high order nonlinearities, the polarization, response of the gas to the electromagnetic field, is computed using quantum-level laser-molecule TDSE's; in contrast, perturbative nonlinear expansions are used in classical nonlinear Schroedinger models that do not model precisely important small scale phenomena and ionization. The complexity of the model requires the accurate computation in parallel of Maxwell's equations and thousands of 3D TDSE's.

In this contribution after a discussion on the mathematical modeling, we will present some recent numerical and mathematical results that involve in particular artificial boundary conditions for laser-molecule TDSE's and domain decomposition techniques for these multiscale Maxwell–Schroedinger equations. Coupling macroscopic Maxwell's equations with thousands of TDSE's necessitates the use of High-Performance Computers such as mammouth (`http://ccs.usherbrooke.ca`). Typical realistic simulations that will be presented with the actual code require several days on hundreds (up to 512) of processors and hundreds of GBytes of RAM.

BERTRAND MAURY, Laboratoire de Mathématiques, Université Paris-Sud, 91405 Orsay Cedex
Direct simulation of dense suspensions

The modelling fluid particle flows calls for efficient solvers of Poisson-like problems on domains with (possibly many) holes. After a description of the native difficulties of the problem, we will give an overview of the several methods which have been proposed to address this challenge, and present some of them, paying a special attention to numerical efficiency, conditionning aspects, and accuracy. Among the methods we plan to present, let us mention the direct approach, based on a boundary fitted (and therefore unstructured) mesh, and some fictitious domain methods (based on a global mesh which covers the whole region of interest), like the Penalty Method, the Fat Boundary method, and saddle-point approaches.

BIJAN MOHAMMADI, Univ. Montpellier II, I3M – CC51 – 34095 Montpellier, France
Involutive completion for constrained PDE systems

We propose to use the involutive form of the system of PDEs in numerical computations.

We illustrate our approach by applying it to Stokes system. As in case of the solution of differential algebraic equations our approach takes explicitly into account the integrability conditions of the system which are only implicitly present in the original formulation. The extra calculation cost is negligible while the discrete form becomes much simpler to handle. One interesting consequence is that the discretization need not verify the classical LBB stability condition.

The approach is very general and can be useful for a wide variety of systems not as well known as fluid flow equations.

The application of the approach to various PDE systems under constraint will be presented together with numerical examples.

SERGE NICAISE, Université de Valenciennes et du Hainaut Cambrésis, LAMAV, FR CNRS 2956, ISTV, F-59313 Valenciennes Cedex 9, France
Adaptive finite element methods: abstract framework and applications

We consider a general abstract framework of a continuous elliptic problem set on a Hilbert space V that is approximated by a family of (discrete) problems set on a finite-dimensional space of finite dimension not necessarily included into V. We give a series of realistic conditions on an error estimator that allows to conclude that the marking strategy of bulk type leads to the geometric converge of the adaptive algorithm. These conditions are then verified for different concrete problems like convection-reaction-diffusion problems approximated by conforming $\mathbb{P}_1$ finite elements or by a discontinuous Galerkin method with an estimator of residual type or obtained by equilibrated fluxes. Numerical tests that confirm the geometric converge will be presented.

NILIMA NIGAM, McGill University, 805 Sherbrooke West, Montreal
A multigrid preconditioner for an integral equation of the first kind for acoustics

We present a multigrid strategy for an integral equation of the first kind arising in acoustics. Such integral equations arise naturally, for example, in the study of screen scattering problems. Unfortunately, the integral operator involved has a spectrum whose behaviour is not directly conducive to multigrid strategies. We present an extension of ideas to circumvent this problem in the positive-definite case due to Bramble et al., and demonstrate how their use leads to a convergent method. We also present some numerical experiments

STEVE RUUTH, Simon Fraser University, Burnaby, BC

A Simple Technique for Solving Partial Differential Equations on Surfaces

Many applications require the solution of time-dependent partial differential equations (PDEs) on surfaces or more general manifolds. Methods for treating such problems include surface parameterization, methods on triangulated surfaces and embedding techniques. This talk describes an embedding approach based on the closest point representation of the surface and describes some of its advantages over other embedding methods. Noteworthy features of the method are its generality with respect to the underlying surface and its simplicity. In particular, the method requires only minimal changes to the corresponding three-dimensional codes to treat the evolution of PDEs on surfaces.

DOMINIK SCHOETZAU, University of British Columbia

Exactly divergence-free discontinuous Galerkin methods for incompressible fluid flow

We present a class of discontinuous Galerkin methods for the incompressible Navier–Stokes equations yielding exactly divergence-free velocity approximations. Exact incompressibility is achieved by using divergence-conforming velocity spaces for the approximation of the velocities. The resulting methods are also locally conservative and energy-stable. We discuss the numerical analysis of the methods and illustrate their practical performance in a series of numerical experiments.

JOHN STOCKIE, Simon Fraser University, Department of Mathematics, 8888 University Drive, Burnaby, BC V5A 1S6

A new approach for simulating flow through porous immersed boundaries

Porous, deformable boundaries are encountered in a wide range of applications including cell membranes, vesicles, porous wave makers, and parachutes. The *immersed boundary method* has already proven to be a versatile and robust approach for simulating the interaction of an impermeable, elastic structure with an incompressible fluid flow. We show how to extend the method to handle porous boundaries by incorporating an explicit porous slip velocity through use of Darcy's law.

We derive a simple, radially-symmetric exact solution, which is then used to validate numerical simulations of porous membranes in two dimensions.