INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Team Bang

Biomédical, Analyse Numérique et Géophysique

Rocquencourt

THEME 4B

Activity Report

2003

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1. Team

BANG (Biomédical, Analyse Numérique et Géophysique) is a continuation of the former project M3N.

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2. Overall Objectives

BANG (Biomédical, Analyse Numérique et Géophysique) is a continuation of the former project M3N. It aims at developing models and numerical methods for two kinds of problems involving Partial Differential Equations. Firstly problems from life sciences (blood flows, respiratory flows, cancer modeling...) are considered. Secondly models for complex fluid flows are studied (flows with a free surface, flows of holes and electrons in semiconductors, coupling with a magnetic field...).

The common scientific features behind these applications come from models involving coupled systems of PDEs (as Navier-Stokes equations) that are solved (simulated) on computers involving new algorithms.

3. Scientific Foundations

3.1. Introduction

Partial Differential Equations are mathematical tools that allow to represent efficiently the evolution of complex physical phenomena. The most classical PDE is certainly the Navier-Stokes system which describes the evolution of the density $\rho(t,x)$ the velocity $\overrightarrow{u}(t,x)$ and the temperature $T(t,x)$ of a fluid parametrized by time t and space position x.

Since the XIXth century this formalism has shown its efficiency and ability to explain both qualitative and quantitative behaviors of fluids. The knowledge that has been gathered on such physical models, on algorithms for solving them on computers, on industrial implementation, opens the hope for success when dealing with life sciences also. This is one of the main goals of BANG.

3.2. Mathematical Modeling

What are the relevant physical or biological variables, what are the possible dominant effects ruling their dynamics, how to analyse the informations coming out from a mathematical model and interpret them in the real situations under consideration ? these are the questions leading to select a mathematical model, generally also to couple several of them in order to render all physical or biomedical features which are selected by specialist partners (engineers, physicists, medical doctors). These are usually based on Navier-Stokes system for fluids (blood flow, respiration, free surface fluid flows), on parabolic-hyperbolic equations (blood filtration, Saint-Venant system for shallow water, flows of electrons/holes in semiconductors), on fluid-structure interaction (blood flow in vessel, aneurism, respiration).

3.3. Multiscale analysis

The complete physical or biomedical description is usually complex and requires very small scales. Efficiency of computer resolution leads to simplifications using averages of quantities. Methods allowing to achieve that goal are numerous and mathematically deep. Some examples studied in BANG are

- Reduction of fluid flow in a porous medium to a hyperbolic/parabolic equation with applications to blood filtration, using homogeneisation procedure.
- Reduction of full 3d Navier-Stokes system to 2d or 1d hyperbolic equations by a section average (derivation of Saint-Venant system for shallow water, hyperbolic models of blood flow).
- Coupled multiscale modelling (pulmonary airways, cardiovascular system, degenerate semi-conductors).

3.4. Numerical Algorithms

Numerical methods used in BANG are mostly based on finite elements or finite volume methods. Algorithmic improvments are needed in order to take into account the specificity of each model, of their coupling, or their 3D features. Among them we can mention

- Fluid-structure coupling in blood vessels.
- Well-balanced schemes for shallow water system.
- Free-surface Navier-Stokes solvers based on Arbitrary-Lagrangian-Eulerian formulation.
- Mixed finite elements for problems with large density variations (semi-conductors, chemotaxis).

4. Application Domains

4.1. Panorama

BANG has decided to develop new biomedical applications and focusses its know-how in these directions, while keeping more classical industrial relations. These are developed in relation with other INRIA projects: MACS, SOSSO, GAMMA, ESTIME.

4.2. Biofluids

This is the main biomedical application developed in BANG. More specifically our research is oriented to

- Blood flows. The goal is to develop numerical simulation of several aspects of blood circulation thus allowing a better medical understanding of pathologies. This includes the propagation of pressure waves in vessels (fluid-structure interaction), large deformations in aneurisms or artery valvs...
- Respiratory flows. This research is aimed at developing a ventilation simulator. A medical target being aerosols deposition.
- Blood filtration. For human blood transfusion white cells are filtered. A research is developed and aims at undertanding the blood flow in the filters, the filtering mecanism and the filter optimisation.

4.3. Cancer modeling

This research activity aims at studying mathematical models related to tumors developments and their control. Among the many biological aspects let us mention: cell movments (chemotaxis, vasculogenesis, angiogenesis), cell cycle, immune reaction and adaptive dynamics.

4.4. Free surface flows

Several industrial applications require to solve fluid flows with a free surface. BANG develops algorithms in two directions. Firstly flows in rivers and coastal areas using Saint-Venant model with applications to dam break and pollution problems. Secondly, fluid/electromagnetism coupling for free surface flows in aluminium industry.

4.5. Semiconductors

Mathematical models based on drift-diffusion systems or energy transport systems are solved using mixed finite elements methods. BANG has developed a highly sophisticated code which is able to simulate very stiff semiconductor devices.

5. Software

5.1. Introduction

Softwares initiated and developped within former projects (Menusin, M3N) and currently in use in the present project.

5.2. OPTMTR

Generation of metric maps for use with *adapted meshes* generator (with Gamma project)

5.3. EMC2

Interactive 2D mesh generator (with Gamma project)

5.4. MISTRAL

Participants: Jean-Frédéric Gerbeau, Tony Lelièvre [CERMICS].

Research software for the simulation of incompressible MHD flows in presence of free surface. (Déposé à l'Agence pour la protection des Programmes).

5.5. HET_2D

Participants: Americo Marrocco [correspondant], Philippe Montarnal [Former PhD student M3N], Abderrazzak El Boukili [Former PhD student M3N], Frédéric Hecht [LAN, Université Paris 6.], Jean-Christophe Rioual [Former PhD student, CERFACS].

Research software for the numerical simulation of semiconductor devices. Drift-Diffusion and Energy-Transport models are implemented. The mathematical formulation is described using as unknowns the electrostatic potential, the quasi Fermi levels and additionaly the electron temperature. The approximation is carried out via mixed finite elements (Raviart-Thomas element RT_0). Parallel computation via domain decomposition is available for some modules and an interface with the **Bamg** software (Gamma project) has been developped for automatic mesh adaption.

6. New Results

6.1. Biofluids

6.1.1. Numerical methods and modelling for fluids in moving domains

Participants: Jean-Frédéric Gerbeau, Paola Causin, Marina Vidrascu [projet MACS, Rocquencourt], Nuno-Miguel Diniz Dos Santos.

6.1.1.1. Fluid-structure interaction. Blood flows.

The main purpose of these studies is the simulation of the mechanical interaction between the blood and the artery wall.

We have proposed in [27], [22] a numerical method to solve the coupling between the Navier-Stokes equations on moving domains (ALE formulation) and a shell model in large displacements. The core of the algorithm is a quasi-Newton method based on a reduced model which offers a significative gain in robustness and efficiency compared to standard methods commonly used in this field.

In [33], we give, on a simplified model, a theoretical explanation of several empirical facts observed in the simulation of blood flows in compliant vessels. In particular, we show that under certain choices of the physical parameters, typically when the densities of the fluid and of the structure are close or when the domain is a slender geometry, loosely coupled schemes are unstable irrespectively of the time step.

In [34], we propose a nested preconditionner of GMRES and acceleration techniques which improve the efficiency of quasi-Newton methods.

In [32], we try to parallelize in time fluid-structure problems adapting the “parareal” method by Y. Maday, J.L. Lions, G. Turinici (projet Micmac).

6.1.1.2. Cardiovascular system modelling

In a very preliminar work with E. Delavaud (DESS student, Paris 6), in collaboration with J. Sainte-Marie (projet MACS), we have proposed a coupling between a network of several arteries (1D fluid-structure models) and a 1D electromechanical model of the heart proposed in the ICEMA consortium (projets MACS, SOSSO, EPIDAURE).

6.1.2. Collapsed tubes

Participants: Salah Naili [LMP, Université Paris 12], Christian Ribreau [LMP, Université Paris 12], Marc Thiriet.

6.1.2.1. Wall shear stress in a laminar flow through a collapsed tube with wall contact

This work is aimed at studying mainly the wall shearing force of a laminar steady flow of an incompressible Newtonian fluid which is conveyed through a straight collapsed tube. This tube is composed of a tapered segment, a contact region where the opposite walls touch and a reopened segment. The tube geometry and characteristics of the flow are obtained from measurements in a collapsed tube at a steady state, in particular the tube shape mimics a frozen configuration obtained from ultra-sound measurements on a Starling resistor.

The NAVIER-STOKES equations associated with the classical boundary conditions are solved using the finite element method. The tube configuration induces a three-dimensional flow. These flow behaviour is affected by both the tube shape and by the flow conditions (a REYNOLDS number larger than 1000 associated with a maximum velocity of about 1.4 m/s). The three-dimensional flow structure is defined by a set of swirls in the reopened segment downstream from the contact region, in the core behind the wall contact and along the diverging walls, as well as in the exit attachment duct. Two side jets emerging from the two small tear-drop-shaped outer passages of the contact zone of the collapsed tube run centrally and partially merge in the proximal segment of the rigid attachment duct. A lateral high velocity stream is still present far downstream in the exit attachment duct. In order to compute both the streamwise and transverse components of the shearing force on the wall, a local basis is defined in each wall node. The jets exiting from the contact region and the sets of flow reversals explain the variation in wall shear stress characterized by important gradient in both the streamwise and transverse directions.

6.1.2.2. Developing steady laminar flow through uniform straight pipes with varying wall cross curvature

Shear-stress longitudinal gradient are known to trigger important changes in cell shape, density, rate division and biological functions. A coupling between haemodynamics and the vasomotor tone of the vessel wall has been demonstrated, mainly in straight test section of circular cross section. The cell behavior is affected not only by the longitudinal gradient in the flow chambers in which the flow is not fully developed but also by the cross gradients of the axial component of the wall stress when the wall is characterize by a non-constant cross curvature. The straight pipe in its collapsed configuration provides the simplest test section to produce both effects. In order to study the mechanotransduction property of endothelial cells (ECs) under stretch and torsion, straight cell-coated channels with axially uniform cross sections but with varying wall cross curvature have thus been proposed. Numerical computations are thus used to (i) determine the load exerted by the flowing fluid on the tube wall and (ii) the entry length of a laminar steady flow of an incompressible Newtonian fluid in uniformly collapsed channels. This study is performed in order to exhibit the mechanical environment of cultured ECs in collapsed-design flow chamber and to optimize the fabrication cost of the test section. Uniformly collapsed tube might be observed in inclined deformable vessels when viscous effects balance hydrostatic forces.

Five cross section shapes are used. The reference cross section S_0 is slightly elliptic (ellipticity of 1.005). Four cross section shapes, which mimic collapsed vessels in an uniformly frozen state, are defined according to the curvature of their opposite faces (the mid-face is located on the minor axis) S_q (parallel faces), S_t (face folding), S_c (point contact between faces) and S_ℓ (line contact). These four selected cross shapes are characterized by large changes in both the cross sectional shape and area with respect to S_0. The cross shapes are obtained from the computation of the deformation under uniform transmural pressures, without extension, of a thin-walled conduit of infinite length and of homogeneous purely elastic walls of constant thickness. The NAVIER-STOKES equations are solved using the finite element method for the five tubes $\sum_0, \sum_q, \sum_t, \sum_c$ and $\sum_\ell$, which are associated with S_0, S_q, S_t, S_c and S_ℓ respectively. The numerical tests are performed with the same value of the volume flow rate whatever the tube configuration for three REYNOLDS numbers ($\mathcal{R}_{e_0} = 35, 500$ and 1000).

Three indices have been proposed to determine the entry length. (i) the first is based on the axial fluid velocity, (ii) the second on its derived quantity, the wall shear stress, and (iii) the third on the pressure. In contact configuration, the velocity criterion underestimates the entry length. An additional length of about 10 % of the computed entry length must be added to ensure that the wall shear stress corresponds to a fully developed state. The fluid pressure, which depends on the REYNOLDS number, has been shown to vary non-linearly in the entry length. In contact configurations ($\sum_c$, $\sum_\ell$), especially when $\mathcal{R}_{e_0} \leq 500$, the pressure index is a better parameter than the velocity index. It must be taken into account in order to load the cells under a constant pressure gradient. On the contrary, in open configurations ($\sum_0$, $\sum_q$, $\sum_t$), the velocity index must be used to avoid any axial gradient in wall shear stress.

6.1.3. Respiratory flows

Participants: Leonardo Baffico [LJLL, Université Paris 6], Laurence Vial [Air Liquide -bourse Cifre-], Marc Thiriet.

This investigation is aimed at developing a ventilation simulator. The airways are decomposed into a set of compartments in series. (i) the first set is composed of the superior airways with the nose, the pharynx and the larynx. The nose is in relation with paranasal sinuses. The nose has a complexe geometry. The set of conchae increases the exchange surface between the physiological walls and the inhaled air. The ventilation function of the nose are, indeed, air epuration, air humidification and temperature setting. The pharynx is a rather simple conduit made of three compartments in series, the nasopharynx, the oropharynx and the hypopharynx. The larynx is also composed of three segments in series, the supraglottis with the epiglottis, the aryepiglottic folds the false vocal cordsor folds and the ventricle, which manages wrong food administration, the glottis with the true vocal folds and the subglottis. Due to its geometry, the larynx induces a jet. (ii) The proximal airways are constituted by the trachea (generation G0 of the tracheobronchial tree) with its extrathoracic and intrathoracic segments, its division branches, the right and left main bronchi, which give birth to intrapulmonary airways, visible by the usual medical imaging techniques, the lobe and then segmental bronchi. (iii) the distal airways are defined by the bronchus generation lower than G5 down to alveoli.
The flow in the superior and proximal airways has been studied numerically. The computational domains are derived from medical images. The present simulations are performed with a Dirichlet velocity boundary condition either at the pharynx or at the trachea, while the opposite end(s) of the fluid domain are associated with stress-free conditions. The main parameter of interest for the physician is the ventilation distribution. Tab. 1 gives the ratio of the flow rate entering at inhalation or living at exhalation the right ($\frac{q^D}{q_{tot}}$) and left ($\frac{q^G}{q_{tot}}$) parts of the explored tracheobronchial tree (Fig. 1) at different phases of the respiratory cycle (mid decelerating phase of inspiration MDI, mid accelerating phase of expiration MAE, peak expiration PE mid decelerating phase of expiration MDE, mid accelerating phase of inspiration MAI and peak inspiration PI).

Because the boundary conditions are not appropriate, one needs in modelling in small pulmonary airways as well as the thoracic cage as a ventilation motor. Three types of airway models are under investigation. The mid-size bronchi (G6 - G10) are modelled using the method of reduced basis element (MRBE) as proposed by Y. Maday. The modelling of the small bronchi (G10-G19) (*i.e.* the terminal bronchioles (G10-G16), cranially located with respect to the pulmonary lobules, and the respiratory bronchioles (G17-G19), first generatioons of airways inside the lobules) is based on fractal homogeneisation (FH). Multiphysics homogeneisation (MPH) is the modelling technique for the deformable acini which are composed of alveolar ducts (G20-G22), with more and more alveoli on their walls, alveolar sacs and alveoli.

Table 1.

phase	$\frac{q^G}{q_{tot}}$ (%)	$\frac{q^D}{q_{tot}}$ (%)
MDI	44	56
MAE	44	56
PE	44	56
MDE	45	55
MAI	43	57
PI	42	58

Figure 1. Mesh of a tracheobronchial tree.

6.1.4. Aerosols

Participants: Laurent Boudin [LJLL, Univ. Paris 6], Yves Bourgault [Département de mathématiques et de statistiques, Université d'Ottawa, Canada], Pierre-Emmanuel Jabin, Marc Thiriet.

The governing equation describes the distribution function of aerosol particles $f(t, x, v)$ in the phase space, assuming that the single force acting on any particle is the friction with the suspending fluid. This function which gives the probability to find a particle at time t with position x and speed v is described by the following equation

$$\partial_t f + v \cdot \nabla_x f + \lambda \nabla_v \cdot ((u(t, x) - v)f) = 0,$$

where $u(t, x)$ is the flow velocity and λ a numerical coefficient which depends on the physical parameters. The cost of a direct numerical simulation of this is equation far too high. The physical quantities of interest are the f-moments:

$$m_i(t, x) = \int v^i f(t, x, v)\, dv, \quad \forall i \geq 0.$$

In particular, the aerosol- and energy density are given by m_0 and m_2 respectively and the equations we have to solve are:

$$\partial_t m_i + \partial_x m_{i+1} = i\lambda(m_{i-1}u - m_i).$$

with a truncature $m_{N+1} = \sum_{i=0}^{N} \alpha_i m_i$, where α_i are numerical constants.

6.1.5. White blood cells filtration

Participants: Mohamed Belhadj, Eric Cancès [Projet MicMac, INRIA et CERMICS, Ecole Nationale des Ponts et Chaussées], Jean-Frédéric Gerbeau.

We are interested in the modelling of white blood cell filtration. We have proposed and studied a simplified model of this process [17]. In collaboration with A. Mikelic (Univ. Lyon), we have established the expression of the permeability tensor for Darcy equations in a medium made of fibers with varying orientations [31].

6.2. Cancer modeling

6.2.1. Chemotaxis, angiogenesis and cell motion

Participants: Lucilla Corrias, Americo Marrocco, Benoit Perthame, Hatem Zaag.

Key words: *biophysics chemotaxis*, *numerical algorithm*, *finite element*, *numerical software*, *cancer modeling*.

Movement of cells are important in the process of cancer development. We have developed some activity in the understanding of mathematical models of chemotaxis and angiogenesis. Angiogenesis describes the development of capillary blood vessels triggered by a substance emited by a tumor. Models for the vasculature have been proposed by several authors (Chaplain, Levine, Sleeman) as a coupled parabolic/hyperbolic system. We have investigated existence of weak or strong solutions for this system [20].

Models with several similarities were proposed by Keller-Segel several years ago for chemotaxis, as coupled parabolic/elliptic systems. They describe the collective motion of bacteria taking into account the underlying biochemistry. A new formulation of the system of partial differential equations is obtained bys the introduction of a new variable which is similar to the quasi-fermi level in the framework of semiconductor modelling. The discretization of the model is achieved by mixed finite elements [24].

6.2.2. Cell-cycle and circadian rythm

Participants: Jean Clairambault, Béatrice Laroche, Stéphane Mischler, Benoit Perthame.

We consider a mathematical model for the cell-cycle, i.e. the sequence of events that leads to mitosis, at the level of a population of cells. These are structured population Partial Differential Equations that describes the evolution of the population along each phase of the cycle and the transition to the next phase. These models allow several types of controls such as therapeutic control in case of cancer therapy (some chemotherapy are known to act on specific phases of the cycle or on the transitions between phases) or circadian control by the central nervous system. We study the long time behavior of this system of PDEs using an entropy method and exhibit, by numerical simulations, the action of the circadian control [29].

6.3. Free surface flows

6.3.1. Free surface geophysical flows

Participants: Emmanuel Audusse, François Bouchut [ENS], Marie-Odile Bristeau, Astrid Decoene, Jean-Frédéric Gerbeau, Benoit Perthame.

Key words: *Geophysical flows*, *free surface*, *Saint-Venant equations*, *source term*, *multilayer system*, *3D Navier-Stokes*, *debris avalanches*.

We are involved in research concerning the numerical simulation of free surface geophysical flows such as rivers, lakes, coastal areas and also avalanches. Many applications related to environmental problems are concerned : floodings, dam breaks, transport and diffusion of pollutants, debris avalanches ...

In many cases, the shallow water hypothesis is satisfied and these phenomena can be simulated by the Saint-Venant equations, for other cases we have considered a multilayer Saint-Venant system and also the 3D free surface Navier-Stokes equations.

6.3.1.1. Saint-Venant equations

We have developed 1D and 2D solvers for the Saint-Venant equations, the aim is to obtain robust and efficient numerical tools based on theoretical results ensuring the accuracy and the preservation of physical properties of the flow (conservation, positivity of water depth, equilibrium states...).

The solution method is based on a kinetic solver applied on finite volumes. To compute the numerical fluxes at the interfaces, we consider the microscopic behavior of the system and from the discretization of the linear kinetic equation, we deduce the kinetic scheme at the macroscopic level. A useful property of this conservative scheme is the built-in preservation of the water height positivity under a CFL condition.

The equilibria of the 1D Saint-Venant system are easy to describe. But when we are interested in real flow situations and so we use the 2D Saint-Venant system, the situation is much more complex and only one particular equilibrium, the steady state of a lake at rest, reminds really interesting. But even if this equilibrium is very easy to characterized it is well known since Leroux et al. that its numerical treatment is not so obvious. In the context of our development of a numerical treatment of the 2D Saint-Venant system we propose a new method to obtain a *well-balanced scheme* [15], i.e. to preserve this equilibrium. By analogy with atmospheric situations, we base our strategy on a hydrostatic reconstruction of the water heights. Departing from any numerical solver, the point is to derive a new variant that is no more based on the classical conservative quantities (h, hu) but on new conservative quantities (h^*, h^*u) where h^* is a hydrostatic reconstructed water height. This specific reconstruction makes possible to balance the influences of the hydrostatic pressure and of the topographic source term. It follows that departing from any numerical solver which is consistent with the homogeneous Saint-Venant system, we obtain a solver which is consistent with the Saint-Venant system with topographic source term and which exactly preserves the steady state of a lake at rest. Moreover we exhibit two stability properties. First the modified solver preserves the non negativity of the water height if the original one does it. Second the semi-discrete modified scheme ensures an in-cell conservative entropy inequality if it is true for the original one.

In order to improve the accuracy of the above first-order scheme, we have introduced a second-order extension. The interface fluxes are computed from limited reconstructed values on both sides of each interface rather than from cell-centered values. These new values are classically obtained with three ingredients: prediction of the gradients in each cell, linear extrapolation, and limitation procedure. We can show that the second-order reconstruction preserves the important features of the scheme. First, the cell by cell reconstruction preserves the mass conservation property of the finite volume method. Second, the limitation procedure ensures the nonnegativity of the second-order reconstructed water heights and under the constraint of the mass conservation with the reconstructed water heights we can write a CFL condition implying also the water height non negativity. The third important point is that the second-order reconstruction preserves the lake at rest steady state. To ensure this property we reconstruct also the bottom topography $z(x)$ although it is a data. Indeed only two of the three quantities $h, z, h + z$ need be explicitly reconstructed, the last being necessarily a combination of the other two, we show that the only choice which preserves the steady state is to work with the quantities h and $h + z$.

6.3.1.2. Transport of pollutant in shallow water

We have also studied the transport of a passive pollutant by the flow modeled by the shallow water equations using a new time discretization that allows large time steps for the pollutant computation. For the hydrodynamic part we use the previous kinetic solver. The interest of the developed method [16] is to disconnect the hydrodynamic time step - related to a classical CFL condition - and the transport one - related to a new CFL condition based only on the velocity - and further the hydrodynamic calculation and the transport one. The transport computation ensures the conservation of pollutant mass, a nonnegativity property and a maximum principle for the concentration of pollutant and the preservation of discrete steady states associated with the lake at rest equilibrium. Numerical examples have shown the efficiency of this new scheme, the CPU time for the transport equation is very reduced and we can easily solve different transport problems with the same stored hydrodynamic solution.

6.3.1.3. Multilayer Saint-Venant system

For some applications like the transport of tracers of different densities or the effect of wind on a lake, we need to know the vertical profile of the velocity and by definition, we cannot get relevant information from Saint-Venant equations. These questions are also fundamental in ocean models and atmospheric sciences.

In these cases, and in order to avoid the 3D Navier-Stokes system when large scale problems are considered, we introduce a new multilayer Saint-Venant system [14]. Thanks to a precise analysis of the shallow water assumption we propose an approximation of the Navier-Stokes equations which consists in a set of coupled

Saint-Venant systems. It extends the range of validity and gives a precise description of the vertical profile of the horizontal velocity while preserving the computational efficiency of the classical Saint-Venant system. The fluid is divided in a given number of layers, each layer satisfies the Saint-Venant equations and is linked to the others by pressure terms (water height coupling) and viscosity (velocity coupling).

We prove that this multilayer Saint-Venant system satisfies some stability properties : it admits an energy and preserves the positivity of the water height. We discuss of the loss of hyperbolicity of the model and we exhibit a variant of the multilayer model for which the left hand side, i.e. the conservative part, is hyperbolic. We have performed the numerical implementation using a multilayer kinetic scheme which preserves the stability properties of the classical kinetic scheme. We have validated the model through some numerical examples (see Fig. 2).

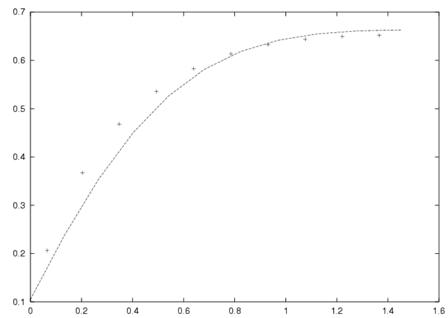


Figure 2. Comparison between the Navier-Stokes equations (dash line) and the multilayer (ten layers) Saint-Venant system (crosses).

6.3.1.4. 3D Free surface Navier-Stokes

For the cases where the 3D effects cannot be neglected, we are studying the 3D incompressible Navier-Stokes equations with free surface. At first, we consider the model with hydrostatic approximation. This work is done in collaboration with EDF/LNHE.

After time discretisation of the equations, the fractional step method can be applied in order to split the non-linear advection terms and the "hydrostatic system" composed by the resulting momentum equation and the depth-integrated continuity equation which is linearised. As the horizontal and vertical diffusion can be splitted as well, we have studied the system with and without the viscous terms. In both cases, we have established a variational formulation leading to a mixed and symmetric problem coupling a 3D variable, the horizontal velocity, and a 2D variable, the free surface.

The Telemac-3D software developed by EDF/LNHE solves the free surface Navier-Stokes equations splitted into 4 parts: advection, horizontal and vertical diffusion, hydrostatic system without diffusion and hydrodynamic correction. Moreover, the hydrostatic system is solved on the averaged horizontal velocity and the water height, by depth-integrating the equations: this leads to a mixed problem which is solved using 2D stable finite elements. Our aim is, on one side, to allow a complete 3D treatment of the equations, and on the other side, take profit of the stabilising property of the diffusion terms in the hydrostatic system. Therefore, we have first implemented a resolution of the 3D hydrostatic system (without depth-integrating), and then included the treatment of the viscous terms. At the moment, we are analysing the stability of this new formulation.

6.3.1.5. Granular flows, debris avalanches

The hypothesis of shallow flow is generally well satisfied by debris avalanche and the most classical models are those of Saint-Venant and Savage-Hutter. They both assume limitations of the basal variations. Our purpose [19] is to explain precisely these limitations, and thus to compare the models, but also to introduce a new model where restrictions on the basal topography are completely dropped and only shallow flow limitations remain. An expansion in the slope variation of our model allows to recover the Savage-Hutter model, while an expansion in the slope itself gives the Saint-Venant equations. Our analysis relies on the explicit computation of the dependence of the fluid velocity in the normal direction when solving exactly the hydrostatic Euler system. Moreover this new model provides an energy dissipation inequality.

Besides this modelisation work, we have begun the simulation of debris avalanches using the Saint-Venant model in which the behaviour of granular media is taken into account by a Coulomb type friction term. A kinetic scheme with a Dirac distribution of particles at the microscopic level has been proposed which allows the simulation of equilibrium states of the granular mass [30].

This work is done in collaboration with the Laboratoire de Modélisation et Tomographie Géophysique (IPGP, Paris 7).

6.3.2. Magnetohydrodynamics of liquid metal

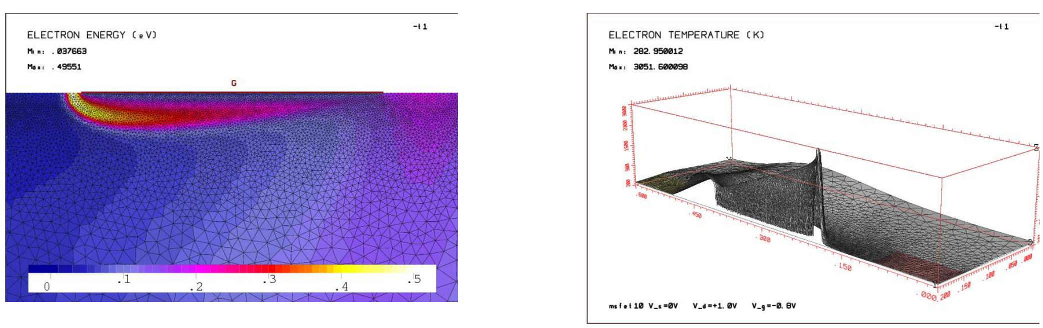
Participants: Jean-Frédéric Gerbeau, Claude Le Bris [Projet MicMac, INRIA et CERMICS, Ecole Nationale des Ponts et Chaussées], Tony Lelièvre [CERMICS, Ecole Nationale des Ponts et Chaussées].

We are interested in the mathematical modelling and the numerical analysis of aluminium electrolysis. The physical system consists of two fluids separated by a free interface and carrying an electrical current which interacts with a magnetic field. Stabilized finite elements techniques and an Arbitrary Lagrangian Eulerian formulation are used in the numerical simulations. Energy stability and properties of conservation of the numerical scheme have been studied [21].

6.4. Semiconductors

Participants: Americo Marrocco, Jean-Michel Sellier [Phd student from Catania university].

Key words: *numerical algorithm*, *domain decomposition*, *finite element*, *numerical software*, *modelling*, *parallel computation*, *semiconductor*.



(a)Contour view of the electron energy (b)3D view of the electron temperature distribution

Figure 3. NUMERICAL SIMULATION OF A SI-MESFET $V_{DS} = 1V$ *and* $V_G = -0.8V$.

In 2003, the collaboration with the professor M. Anile (Catania university) and his team has been continued. The preliminary study related to a new approach in the derivation of the diffusion matrix of the electrons in a semiconductor medium in the framework of energy-transport model [[13]] has been extended to the *Kane's* band approximation. In this model, a linear relation between the electron temperature and electron energy does not exists as in the parabolic band approximation case. A *PhD* student from Catania university spent 6 months of his time at Inria in order to contribute to the implementation of this extension. Typical -small dimensions- MESFET and MOSFET have been used for the numerical simulations. See for example the figure(3) which gives the distribution of the electron energy in a Si-MESFET for a typical polarization point in the case of *Kane's* band approximation.

7. Contracts and Grants with Industry

7.1. Aluminium

Participants: Jean-Frédéric Gerbeau, Claude Le Bris [Projet MicMac, Inria et CERMICS].

Industrial contract with Ecole Nationale des Ponts et Chaussées in the framework of a collaboration with Aluminium Pechiney on the mathematical modelling of aluminium electrolysis cells.

7.2. Free surface flows

Participants: Emmanuel Audusse, Marie-Odile Bristeau, Astrid Decoene, Jean-Frédéric Gerbeau, Benoit Perthame.

The studies concerning the kinetic scheme for Saint-Venant equations and the improvment of the 3D Navier-Stokes solver are supported by a contract with LNHE of EDF. The results are included in the Telemac-2D and Telemac-3D softwares of EDF.

8. Other Grants and Activities

8.1. Actions at region level

Participation to a working group on the debris avalanches with the Laboratoire de Modélisation et Tomographie Géophysique (IPGP, Paris 7). Participation to the ATIP of CNRS "Modélisation des avalanches de débris: prise en compte de la transition fluide/solide" (A. Mangeney, IPGP).

8.2. Actions at nation level

8.2.1. ACI "Prévention des catastrophes naturelles"

The project BANG has participated to the ACI "Prévention des Catastrophes Naturelles" [28] in the project "Modélisation de processus hydrauliques à surface libre en présence de singularités" in collaboration with different laboratories: ENS-DMA, Cemagref Lyon, IMF Toulouse, LMF/INSA Lyon, LMFA Lyon.

8.3. European actions

8.3.1. RTN network on blood flows

Jen-Frédéric Gerbeau is the french coordinator of a european network RTN on blood flows modelling (from october 2002 to september 2006). Participants: INRIA, Université Paris 6, Politecnico di Milano (Italy), Imperial College (UK), Ecole Polytechnique Fédéral de Lausanne (Switzerland), Instituto Superior Técnico de Lisboa (Portugal), Technische Universität Graz (Austria)

8.3.2. RTN network HYKE

Participation to the european network HYKE (Hyperbolic and Kinetic equations). (url http://www.hyke.org).

8.3.3. RTN network M3CS-TuTh

Participation to the european network M3CS-TuTh (Modelling, Mathematical Methods and Computer Simulation of Tumour Growth and Therapy).

8.4. Visit and invitations

- Visit of C. Klaiany, Université Saint-Joseph, Beyrouth (Liban) -2 weeks-
- Invitation of A. Marrocco at Catania University (Italy) feb. 2003 -2 weeks-

9. Dissemination

9.1. Scientific community

Marie-Odile Bristeau is in the editorial comity of the Intenational Journal Computer Methods in Applied Mechanics and Engineering. Benoit Perthame is Editor-in-chief of M2AN and editor in various journals (CALCOLO, CPDE, SIAM J. Math. Analysis, DCDS(B))

9.2. Teaching

1. "Fluid-structure interaction in biological flows", DEA Analyse Numérique, Université Paris 6 (Jean-Frédéric Gerbeau with Y. Maday and M. Thiriet)
2. "Numerical methods in fluid mechanics and MHD", DEA Equations aux dérivées partielles et applications, Université Paris-Dauphine (Jean-Frédéric Gerbeau)
3. Scientific computing and analysis, Ecole Nationale des Ponts et Chaussées (Jean-Frédéric Gerbeau)
4. Finite volume methods, Ecole Polytechnique de Tunisie (Benoit Perthame)
5. Finite element methods for fluid mechanics, Ecole polytechnique de Tunisie (Benoit Perthame)

9.3. Participation to congresses, workshops,...

- Joint workshop on applied mathematics and scientific computing, Jerusalem, january 2003 (M. Thiriet)
- Journée sur le chimiotactisme, Université de Nice, march 2003 (A. Marrocco)
- CANUM, Congrès d'Analyse Numérique, Montpellier, June 2003 (E. Audusse, M. Thiriet)
- Journées Modélisation en Médecine, ENS Lyon, june 2003, (M. Thiriet)
- MACSI-net event Cardio Point (Cardiac and cardiovascular models) Graz, june 2003 (M. Thiriet)
- International Symposium on Modeling of Physiological Flows, EPFL Lausanne, september 2003 (M. Thiriet, invited lecture)
- Telemac Users' Club, Chamrousse, October 2003 (E. Audusse, A. Decoene)
- 26th National Congress in Computational and Applied Mathematics (CNMAC), Brasil (Jean-Frédéric Gerbeau, Invited plenary lecture)
- Second M.I.T. conference on Computational Fluid and Solid Mechanics,USA (Jean-Frédéric Gerbeau)
- Applied Mathematics and Applications of Mathematics, AMAM, France (Jean-Frédéric Gerbeau)
- Prospective sur la Modélisation mathématique en médecine (à l'occasion des 20 ans de la SMAI), 2003 (Jean-Frédéric Gerbeau)
- "Fluid-structure interaction and nonlinear PDE" workshop, Université de Mulhouse. (Jean-Frédéric Gerbeau)
- Seminar, GDR MOMAS, CIRM, Marseille. (Jean-Frédéric Gerbeau)
- Seminar, Ecole Polytechnique de Tunisie. (Jean-Frédéric Gerbeau)
- Seminar in honor of Ivo Babuska, Université Paris 6. (Jean-Frédéric Gerbeau)
- Seminar Collège de France. (Jean-Frédéric Gerbeau)

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