INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Bang

Biophysique, Analyse Numérique et Géophysique

Rocquencourt

THEME NUM

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1. Team

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

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Vincent Calvez [Elève ENS]
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2. Overall Objectives

2.1. Overall Objectives

BANG (Biophysique, 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 (cell movement, tissue growth, cancer modeling...) are considered. Secondly models for complex fluid flows are studied (flows with a free surface, flows of holes and electrons in semiconductors).

The common scientific features behind these applications come from models involving coupled systems of PDEs (as Keller-Segel or Saint-Venant systems) 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 XIX$^{\text{th}}$ 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 information 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 (as in free surface fluid flows), on parabolic-hyperbolic equations (Saint-Venant system for shallow water, flows of electrons/holes in semiconductors, Keller-Segel model of chemotaxis).

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 full 3d Navier-Stokes system to 2d or 1d hyperbolic equations by a section average (derivation of Saint-Venant system for shallow water).
- Coupled multiscale modelling (degenerate semi-conductors, description of tumor from the cell level to the organ scale).
- Description of cell movement from the individual to the collective scales.

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

- Well-balanced schemes for shallow water system.
- Free-surface Navier-Stokes solvers based on a multilayer St-Venant approach.
- 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: GAMMA, REO.

4.2. Tissue growth and cell movment

This research activity aims at studying mathematical models related to tumors developments and the control of therapy. Among the many biological aspects let us mention

- cell movments (chemotaxis, vasculogenesis, angiogenesis),
- cell cycle, immune reaction and adaptive dynamics (structured population dynamics),
- modelling and optimization of chemotherapy through differential systems.

4.3. 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 in averaged shallow water systems. Secondly, 3D hydrostatic flows by a multilayer Saint-Venant approach and 3D Navier-Stokes flows.

4.4. 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. 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. Tissue growth and cell movment

Keywords: *cancer chronotherapy*, *cancer modeling*, *cell population*, *differential equations*, *numerical algorithm*, *optimal control*.

6.1.1. Dynamics of structured cell populations; applications to cell cycle modelling:

Participants: Fadia Bekkal-Brikci, Jean Clairambault, Piotr Gwiazda [Université de Varsovie], Philippe Michel, Benoit Perthame, Melina Rapacioli [CONICET], Edmundo Rofman [CONICET], Emilio Seijo Solis, Romain Yvinec.

- **Circadian rhythm and tumour growth.** A model of the cell cycle of the Von Foerster-McKendrick type (first developed in 2003, INRIA Res. Report # 4892) has been used in a simplified version (2 phases) to test in a theoretical setting the influence of circadian rhythms on tumour growth, following experimental observations by E. Filipski et al. at F. Lévi's INSERM lab in Villejuif. The first eigenvalue of a linear PDE system is evaluated with respect to different types of control, constant or periodic, on apoptosis and phase transition rates [17]. The theoretical results show that, contrarily to what was expected on the basis of experimental evidence, periodic control on the sole apoptosis rates enhance tumour growth, whereas periodic control on phase transition rates has variable effects, slowing down or accelerating tumour growth according to phase durations. This subject has been the theme of Romain Yvinec's report at ENS-Lyon on the 2-phase model, and is presently under study by Emilio Seijo Solis (INRIA internship 2006-07) in a 1-phase model with variable duration and different periodic controls at the cell division step.
- **4-phase cell cycle model.** A 4-phase cell cycle model with two main phase transitions, G_1/S and G_2/M, and the synchronisation between these two mechanisms, is currently under study. Parametrizing the minimal and maximal durations of the phases is an issue, as has been shown with a 2-phase model used for circadian rhythm and tumour growth, and it is the object of discussions with our biologist partners.
- **Quiescent and proliferative cell cycle models for healthy and tumoral tissues**

  A cell population model structured in age and cyclin content with proliferation and quiescence for healthy and tumoral tissues has been developed. The necessity to add a quiescent (or G_0) phase to a model of cell and tissue proliferation, with nonlinear terms describing exchanges between G_0 and G_1 phases, is clear if one is to take account of not always exponential growth behaviour observed in experimental tumour growth curves and tissue homeostasis (i.e., conservation of tissue volume in the mean) in the case of healthy fast renewing tissues. The chosen exchange functions are the same in each case, but with different parameters according to the nature of the tissue, healthy with saturation or tumoral with exponential or subpolynomial growth. This distinction aims at giving a rationale for the simultaneous action of drugs on both types of tissues, which is always the case (toxicity versus anti-tumour efficacy) in the clinic. This proliferative/quiescent cell cycle model has been the main work of Fadia Bekkal Brikci's postdoctoral year at INRIA [10][27].
- **Mathematical analysis of age or size stable dynamics**

  We consider the renewal equation (also called McKendrick-VonFoerster) equation that arises as a simple model for structured population dynamics and the size structured population equation which does not have representation formula. We prove the exponential convergence in long time to the steady state, after renormalization by a damping factor to compensate for the system growth.

Our approach, by opposition with the original method of Feller based on Laplace transform, uses the direct variable and the specific strucutre of the equations under consideration. In the case of age structure it uses an entropy approach and new invariants of the equation, to which we systematically associate a condition for the exponential convergence. See [19].

- **Modelling neural tube development in the Chicken embryo.** Stimulated by observations coming from a team of Argentinian biologists, pointed to Benoit Perthame and Jean Clairambault by Edmundo Rofman, we are currently developing a space-and-age-structured model of the spatial growth of a population of neuroepithelial cells along the neural tube of the Chicken embryo. This is the main theme of a beginning collaboration between INRIA and CONICET, in which are involved Argentinian biologists and mathematicians and which will see the visit at INRIA of Melina Rapacioli, an Argentinian biologist, in the first weeks of January 2006 (other themes involve modelling of colorectal cancer proliferation and invasion).

6.1.2. Pharmacokinetic-pharmacodynamic (PK-PD) modelling for anticancer therapy

Participants: Jean Clairambault, Francis Levi [INSERM U776, Hospital Paul-Brousse, Villejuif].

An ODE model of the action of cytototoxic drugs at the molecular level is currently being developed in order to take into account drugs which are of everyday clinical use in the treatment of colorectal cancer, namely oxaliplatin and 5-fluorouracil, in association. Oxaliplatin (an alkylating agent) is not cell cycle phase-specific, whereas 5-fluorouracil is S-phase specific. The aim of this approach is to provide clinicians with a rationale to optimise the combination of such anti-cancer drugs; this makes it necessary not only to develop the abovementioned model of the cell cycle, but also to represent at the molecular level the action of drugs and their activation or inhibition by enzymes which are regulated with circadian rhythmicity and show genetic polymorphism. Together with the following topic (optimisation), these modelling pharmacological approaches are intended to help clinicians design optimised patient-tailored therapeutics. New anti-cancer drugs are presently the object of PK-PD modelling, in particular Irinotecan (S-phase specific) and Seliciclib (acting on G_1/S and G_2/M phase transitions), that are the main anti-cancer drugs investigated within a European FP6 STREP which has started on October 1st, 2006. The connection between these ODE models, from the drug infusion flow as an external control input to the action on cell cycle phase transitions and secondary apoptosis, and age-structured PDE models of the cell cycle is under development, with the aim to obtain a full mechanistic PK-PD model involving cell cycle representation for different anti-cancer drugs.

6.1.3. Optimisation of anticancer drug infusion by using chronobiology concepts

Participants: Jean Clairambault, Francis Levi [INSERM U776, Hospital Paul-Brousse, Villejuif], Jean-Charles Gilbert [Estime project], Souad Mezouar, Jan Stuchly.

M2 Master or last year engineering school research stay students: Houssem Eddine Miled (EPT Tunis for Bang); Souad Mezouar (M2 Paris VI for Estime and Bang) have developed and tested, in the existing frame of an ODE system dedicated to modelling anticancer drug therapeutics by continuous infusion [16], other optimisation methods than the Uzawa-like algorithm firstly designed and implemented by C. Basdevant: augmented lagrangian (HEM) and SQPAL (SM). The results confirm the suboptimal solutions found by the Uzawa algorithm, but with faster convergence, especially for SQPAL.

The identification of the parameters of a simplified macroscopic population dynamics PK-PD model used to define optimised chronotherapeutic strategies has been the object of Jan Stuchly's internship between the Bang and Estime projects (report to appear).

6.1.4. Chemotaxis and cell movment

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

Participants: Vincent Calvez, Americo Marrocco, Neijla Nouaili, Benoit Perthame, Hatem Zaag.

Movment of cells are important in various aspects of medical sciences and biology such as cancer development. We have developed some activity in the understanding of mathematical models of chemotaxis and in numerical simulation of bacterial colony growth (see [5] for a general presentation). Several new theoretical results are presented in [13][23][18][11] concerning blow-up and existence of solutions.

Models of cell movement were proposed by Keller-Segel several years ago, as coupled parabolic/elliptic systems. They describe the collective motion of bacteria taking into account the underlying biochemistry (chemotaxis). These models are defined by two partial differential equations, one for the bacterial density and one for the attractant concentration.

This system of equations is very similar to the drift-diffusion model for the (unipolar) semiconductor devices, so for the numerical simulation of bacteria aggregation, we derive a new formulation by introducing an unknown variable which is called quasi-Fermi level in semiconductor framework. By this way we can use and extend discretization approach and numerical schemes developped for the semiconductors.

This year we have continued with our experiments on the extended model which takes into account the stimulants concentration (food) i.e. a Keller-Segel system with three coupled equations. The figure 1 gives a partial result of a numerical simulation. The initial conditions are an inoculum of bacteria at the center of the circular domain (localized high bacterial density), no chemoattractants and a uniform repartition of food. The solution (isovalues of the bacterial density, chemoattractant and stimulant concentrations) is represented for two different moments of the evolution process, at $t = 4.53$ and $t = 13.3$ (adimensionned values).

We have also investigated a new model in which two type of bacteria are considered in the development of patterns: active bacteria and inactive ones. The Mimura model is specially well adapted for the colonial branching patterns by the *Bacillus Subtilis* type of bacteria. We can see on figure 2 the kind of pattern that can be obtained with the mimura's model. We have also improved the efficiency of our numerical simulator by the implementation of the PARDISO solver [34] [33] which allows us to solve now huge linear systems with relatively small amount of computer time. Extended numerical results are given in [28]

The theoretical study of this extended Keller-Segel system has also been initiated. The main technical difficulty is that the extended system does not have an energy structure. Several scales of initial data can be treated using modified energy fnctional.

This is a long term program because several levels of modelling lead to different energy structures.

6.2. Free surface geophysical flows

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

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 if, in addition, the bottom slope is small, these phenomena can be simulated by the Saint-Venant equations. However we have developed two useful extensions:

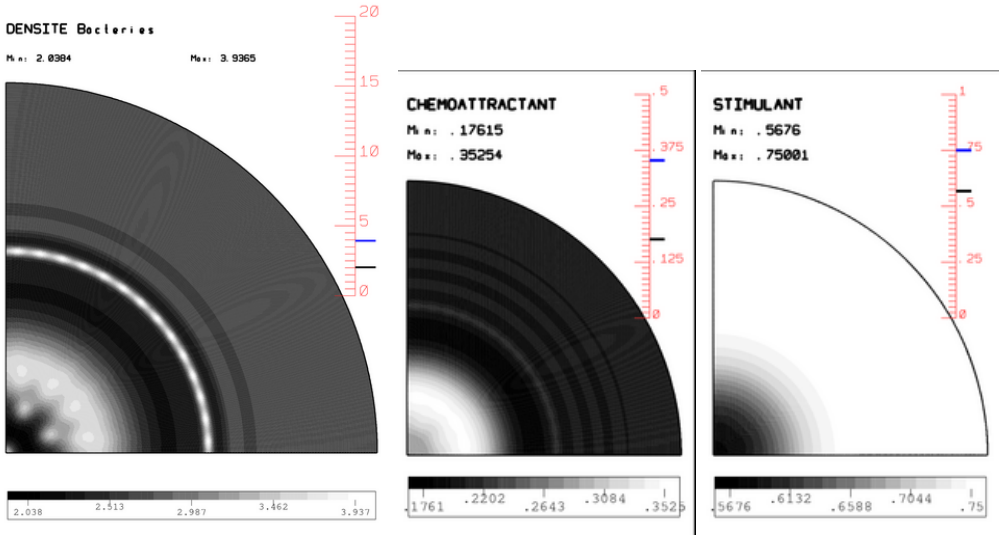
- the Bouchut-Westdickenberg models valid for small slope variations or for arbitrary topographies,

- a multilayer Saint-Venant system which gives a precise description of the vertical profile of the horizontal velocity.

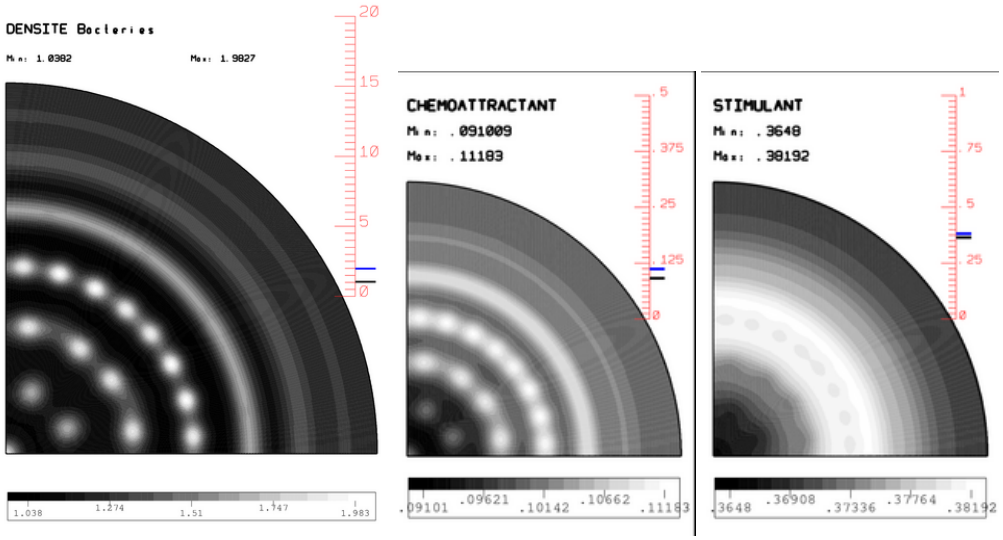
A 3D free surface Navier-Stokes solver has also been studied.

6.2.1. Saint-Venant equations

Participants: Emmanuel Audusse [Université Paris 13], François Bouchut, Marie-Odile Bristeau, Tomas Morales, Benoit Perthame.



(a) $T = 4.53$



(b) $T = 13.33$

Figure 1. NUMERICAL SIMULATION OF BACTERIA AGGREGATION (CHEMOTAXIS).

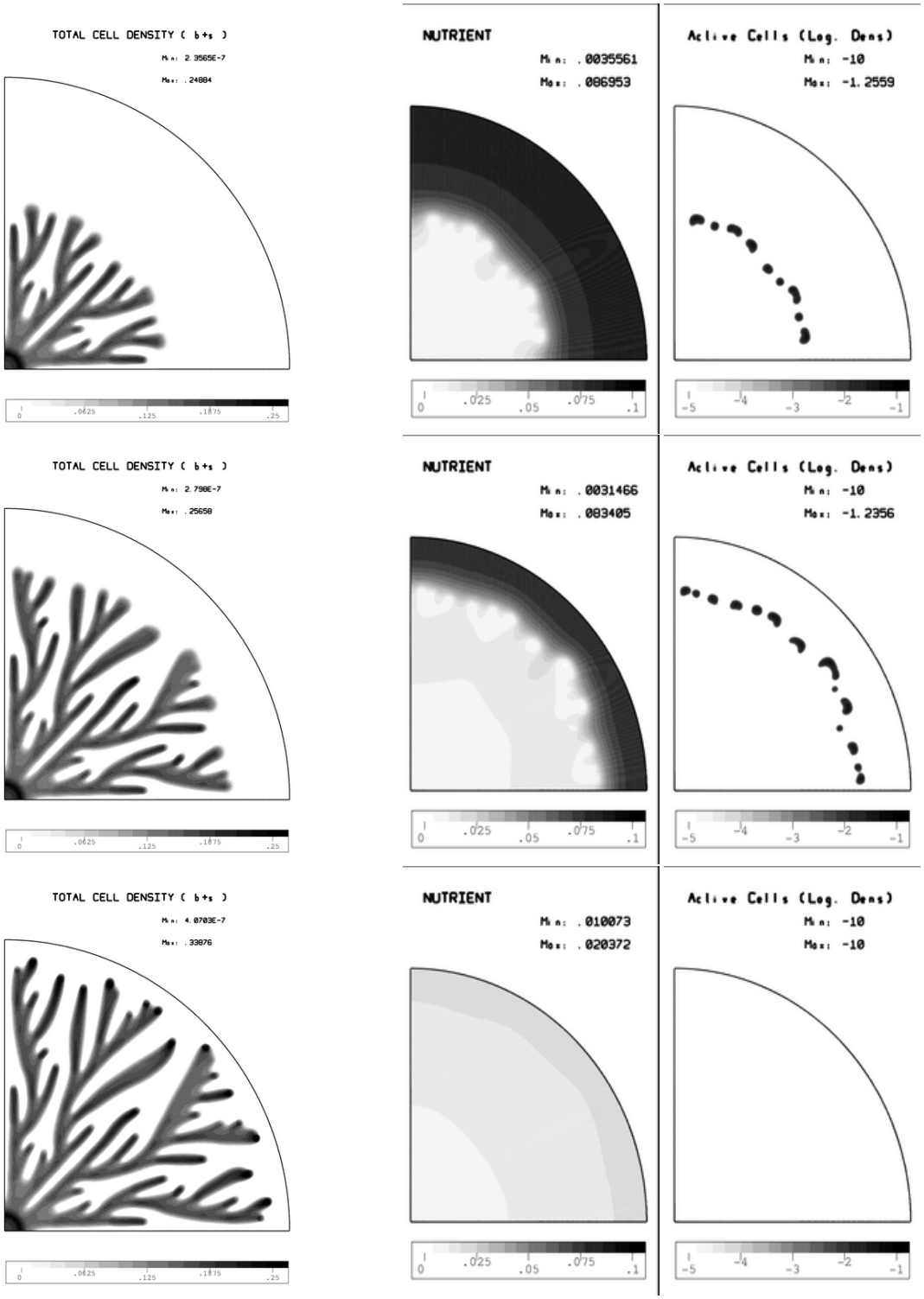


Figure 2. BACILLUS SUBTILIS BRANCHING PATTERNS.

We recall the main features of the Saint-Venant solvers developed the previous years and which are the basic tools of the different generalisations.

We have developed 1D and 2D solvers for the Saint-Venant equations with source terms. The aim was 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...). Our method is based on a kinetic solver and a hydrostatic reconstruction procedure [31].

First considering the homogeneous Saint-Venant equations we introduce their kinetic interpretation and deduce a macroscopic finite volume kinetic solver. The solver has good stability properties as the inherent preservation of the water depth positivity even when applications with dry areas are considered.

Second we consider the Saint-Venant system with source terms and a hydrostatic reconstruction strategy [30] allows us to extend any positivity preserving homogeneous scheme to a positivity preserving well-balanced scheme.

Finally we use a conservative and positivity preserving formally second-order extension based on linear reconstruction procedures. By introducing an enriched discretization of the source terms we construct a stable and well-balanced "second-order" scheme [31].

A recent application of this method concerns the overland flow on agricultural soils. On this subject, we are participating to a working group (url http://www.univ-orleans.fr/mapmo/methode) initiated by S. Cordier (Mapmo, Université d'Orléans) and F. Darboux (Inra, Orléans). The problem is motivated by environment resources preservation (decrease of soil thickness by erosion, nutrient losses, decrease in water quality). More precisely, we are interested by the effect of the surface morphology (topography, ditches, furrows) on a small agricultural watershed.

6.2.2. Granular flows, debris avalanches

Participants: François Bouchut, Marie-Odile Bristeau.

This work is done in collaboration with A. Mangeney, J.P. Vilotte (Laboratoire de Modélisation et Tomographie Géophysique, IPGP, Paris 7) and M. Pirulli, C. Scavia (Department of Structural and Geotechnical Engineering, Politecnico di Torino, Italy).

Simulation of geophysical granular flows is a useful tool for risk assessment and for understanding the erosion processes at the surface of the Earth and other telluric planets [21].

For avalanches, the topographic effects are important, and the classical Saint-Venant system developed for small slopes is no more valid. F. Bouchut and M. Westdickenberg [32] using the shallowness assumption have deduced two models of the free surface Navier-Stokes system, the first one is valid for small slope variations and the second one for arbitrary topography. The variables are the material thickness in the direction normal to the topography and the tangential velocity. A Coulomb friction term is added to deal with the behaviour of dry granular flows.

A finite volume code on structured grids has been developed by F. Bouchut [20], and now a finite volume scheme on unstructured meshes is under development. We are interested by unstructured meshes, since the topography can be accurately depicted through local refinement without significantly increasing the number of nodes.

6.2.2.1. Multilayer Saint-Venant system

Participants: Emmanuel Audusse [Université Paris 13], Marie-Odile Bristeau.

For some applications, we need to know the vertical profile of the velocity and by definition, we cannot get relevant information from Saint-Venant equations. In this case, and in order to avoid the 3D Navier-Stokes system when large scale problems are considered, we have introduced a multilayer Saint-Venant system [29]. Thanks to a precise analysis of the shallow water assumption we propose an approximation of the hydrostatic 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). This approach is a transition step towards 3D simulations with the Navier-Stokes system with two main advantages: we have not to deal with a moving mesh and the vertical velocity is only an output variable, it is not a variable of the system since the kinematic boundary condition is applied at each interface.

We have continued the improvement and the validation of the multilayer Saint-Venant solver [8],[22],[9] based on the Saint-Venant kinetic scheme described in Sec.6.2.1. Comparisons of the results obtained with the 2D multilayer solver with solutions of the 3D hydrostatic Navier-Stokes solver presented in the next section and also with the non-hydrostatic version of Telemac 3D (LNHE/EDF) have shown on one side, the good agreement of the solutions of the multilayer and hydrostatic Navier-Stokes models and on the other side, the effect of the hydrostatic assumption.

6.2.2.2. 3D Free surface Navier-Stokes

Participants: Astrid Decoene, Jean-Frédéric Gerbeau [Reo project].

This is the subject of the Ph.D thesis of A. Decoene [6] prepared in collaboration with LNHE/EDF and defended in May 2006.

This PhD thesis aims to deepen the analysis of the equations governing the three-dimensional free surface flows. On one hand we present a new weak formulation of the hydrostatic problem leading to a well-posed time-discrete problem. This problem is analysed mathematically and its resolution is implemented into the Telemac-3D system, developed at the Laboratoire National d'Hydraulique et Environnement (LNHE), EDF. Some numerical results are shown. On the other hand, we study the ALE interpretation of the sigma transformation method for the vertical discretization of three-dimensional domains. Especially we propose a generalization allowing to improve the representation of stratifications in a flow. Finally, we introduce an ALE-MURD scheme [26] for the linear advection problem posed on moving domains. A particular constraint must be satisfied for the scheme to be conservative when the domain moves. We show how to ensure this constraint in the particular case where the domain is three-dimensional and only moves in the vertical direction. This result is illustrated numerically in the framework of the three-dimensional free surface flow problem.

7. Other Grants and Activities

7.1. Actions at region level

Participation to the GDR-CNRS "CHANT"(équations Cinétiques et Hyperboliques : Aspects Numériques, Théoriques, et de modélisation).(url http://chant.univ-rennes1.fr)

ENS-DMA and Bang project take part to the ANR project *MACBAC* (Analyse multidisciplinaire du processus de colonisation de surface par les bactéries: surfactine, migration, formation des profils) managed by S. Seror at the *Institut de génétique et microbiologie* -Université de Paris Sud.

7.2. European actions

7.2.1. RTN network HYKE

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

7.2.2. RTN network M3CS-TuTh

Participation to the european network M3CS-TuTh (Modelling, Mathematical Methods and Computer Simulation of Tumour Growth and Therapy). (url http://calvino.polito.it/~mcrtn).

7.2.3. NoE Biosim

Biosimulation,a new tool in drug development. J. Clairambault takes part with F. Lévi (INSERM U 776) in workpackage 13, *Modeling circadian drug effects in anti-cancer treatment*.

7.2.4. Strep Tempo

Temporal genomics for tailored chronotherapeutics. J. Clairambault is head of workpackage 2 *Integration and modeling*, which involves the Bang and Contraintes projects at Inria and also two SMEs, Helios Biosciences (Créteil) and Physiomics PLC (Oxford).

8. Dissemination

8.1. Scientific community

Benoit Perthame is Editor-in-chief of M2AN and editor in various journals (CALCOLO, CPDE, SIAM J. Math. Analysis, DCDS(B))

8.2. Participation to congresses, workshops,...

- PSMN day, Lyon jan. 2006 (J. Clairambault)
- Workshop on mathematical methods and modeling of biophysical phenomena, Angra dos Reis, Brazil, march 2006 (F. Bekkal-Brikci, J. Clairambault, B. Perthame)
- Reaction-Diffusion Systems in the Life Sciences, Orsay, march 2006 (A. Marrocco)
- Congress of the "Société Francophone de Chronobiologie", Lyon may 2006 (J. Clairambault)
- Congrès d'analyse numérique (CANUM), Guidel, may 2006 (A. Decoene)
- Euroconference in Mathematics:*Which Mathematics for Biology?*, Anogia, Crete july 2006 (F. Bekkal-Brikci, J. Clairambault, B. Perthame, Jan Stuchly)
- Summer School of the EU-Marie-Curie network:*Modelling, Mathematical Methods and Computer Simulation of Tumour Growth and Therapy* Kolymbari, Crete july 2006 (F. Bekkal-Brikci, J. Clairambault, B. Perthame, Jan Stuchly)
- Co-organisation of the minisymposium:*Coordination of Physiological Rhythms* in the annual IEEE-EMBS Conference, New-York, Aug. 2006 (J. Clairambault
- European Conference on Computational Fluid Dynamics (ECCOMAS), Egmond aan Zee, The Netherlands, sept 2006 (A. Decoene)
- Congrès scientifique sur les Environnements Côtiers, Vannes, sept. 2006 (M.-O. Bristeau)
- Co-organisation of the Workshop on Cancer *Modelling and Therapeutic Innovation: from Theory to Clinic*, Lyon sept. 2006 (J. Clairambault)
- 2nd Conference of the European network Biosim, Mallorca, oct. 2006 (J.Clairambault)
- Participation in the European exhibition Eurobio, Paris oct. 2006 (J. Clairambault)

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Year Publications

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