



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Team Bang

*Biomédical, Analyse Numérique et
Géophysique*

Rocquencourt

THEME SYM

Activity
R *eport*

2004

Table of contents

1. Team	1
2. Overall Objectives	1
3. Scientific Foundations	1
3.1. Introduction	1
3.2. Mathematical Modeling	2
3.3. Multiscale analysis	2
3.4. Numerical Algorithms	2
4. Application Domains	2
4.1. Panorama	2
4.2. Cancer modeling	2
4.3. Free surface flows	3
4.4. Semiconductors	3
5. Software	3
5.1. Introduction	3
5.2. OPTMTR	3
5.3. EMC2	3
5.4. HET_2D	3
6. New Results	3
6.1. Cancer modeling	3
6.1.1. Optimising cancer chemotherapy with the help of chronobiology	3
6.1.2. Chemotaxis, angiogenesis and cell motion	4
6.1.3. Structured population dynamics	6
6.2. Free surface geophysical flows	6
6.2.1. Discontinuous Fluxes	6
6.2.2. Saint-Venant equations	7
6.2.3. Transport of pollutant in shallow water	7
6.2.4. Granular flows, debris avalanches	9
6.2.5. Multilayer Saint-Venant system	9
6.2.6. 3D Free surface Navier-Stokes	9
6.3. Semiconductors	10
6.4. Homogenization approach to filtration through a fibrous medium	10
7. Contracts and Grants with Industry	10
7.1. Free surface flows	10
8. Other Grants and Activities	11
8.1. Actions at region level	11
8.2. European actions	11
8.2.1. RTN network HYKE	11
8.2.2. RTN network M3CS-TuTh	11
8.3. Visit and invitations	11
9. Dissemination	11
9.1. Scientific community	11
9.2. Teaching	11
9.3. Participation to congresses, workshops,...	12
10. Bibliography	13

1. Team

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

Head of project-team

Benoit Perthame [université Paris 6 & ENS]

Vice-head of project team

Americo Marrocco [DR]

Administrative assistant

Maryse Desnous [TR, partial time]

Staff member Inria

Marie-Odile Bristeau [DR, partial time 4/5]

Research scientists (partner)

François Bouchut [CNRS]

Hatem Zaag [CNRS,ENS]

Ph. D. students

Emmanuel Audusse [Inria, until sept. 2004]

Mohamed Belhadj [Inria]

Astrid Decoene [Inria]

Haythem Ounaissa [E.P. Tunisie]

Vincent Calvez [Elève ENS]

Philippe Michel [Paris 9]

Tomas Morales [Seville]

Post-doctoral fellow

Piotr Gwazda [Université de Varsovie, since oct. 2004]

Civil servant (on partial secondment)

Jean Clairembault [Université Paris 12]

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 (cell movement, 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 $\vec{u}(t, x)$ 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 (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 improvements 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. Cancer modeling

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 movements (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 developed 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 additionally 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 **Bang** software (Gamma project) has been developed for automatic mesh adaption.

6. New Results

6.1. Cancer modeling

6.1.1. Optimising cancer chemotherapy with the help of chronobiology

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

Participants: Jean Clairembault, Claude Basdevant [LAGA, Université Paris-Nord, Villetaneuse], Francis Levi [INSERM E 0354, Hospital Paul-Brousse, Villejuif].

The chronotherapy concept takes advantage of the circadian rhythm of cells physiology in maximising a treatment efficacy on its target while minimising its toxicity on healthy organs. The object of the present work is to investigate mathematically and numerically optimal strategies in cancer chronotherapy. To this end

a mathematical model describing the time evolution of efficiency and toxicity of an oxaliplatin anti-tumour treatment has been derived. We then applied an optimal control technique to obtain the best drug infusion law.

The mathematical model is a set of six coupled differential equations governing the time evolution of both the target tumour cell population (cells of a Glasgow osteosarcoma, a murine tumour) and the mature enterocyte population, to be shielded from unwanted side effects during a treatment by oxaliplatin. Starting from known tumour and villi populations, and a time dependent drug infusion law being given, the mathematical model allows to compute the time evolution of both tumour and villi populations. The tumour population growth is based on Gompertz law and the drug anti-tumour efficacy takes into account the circadian rhythm. Similarly the enterocyte population is subject to a circadian toxicity rhythm. The model has been derived using as far as possible experimental data.

We choose as an objective function to obtain, after the end of the treatment, the smallest possible tumoral population. However we impose as a toxicity limiting constraint that the villi population does not fall below a given acceptable level. The gradient of the objective function and of the villi population constraint are obtained using the adjoint technique, this allows to derive a minimisation procedure based on a non-linear conjugate gradient algorithm with projection, and an Uzawa-like saddle-point research. The procedure controls both the infusion rate $i(t)$ and the end of treatment time t_i . As the problem is strongly non-linear and not convex we cannot assert that the procedure converges toward the global minimum, however it proves experimentally to be at least almost optimal.

6.1.2. Chemotaxis, angiogenesis and cell motion

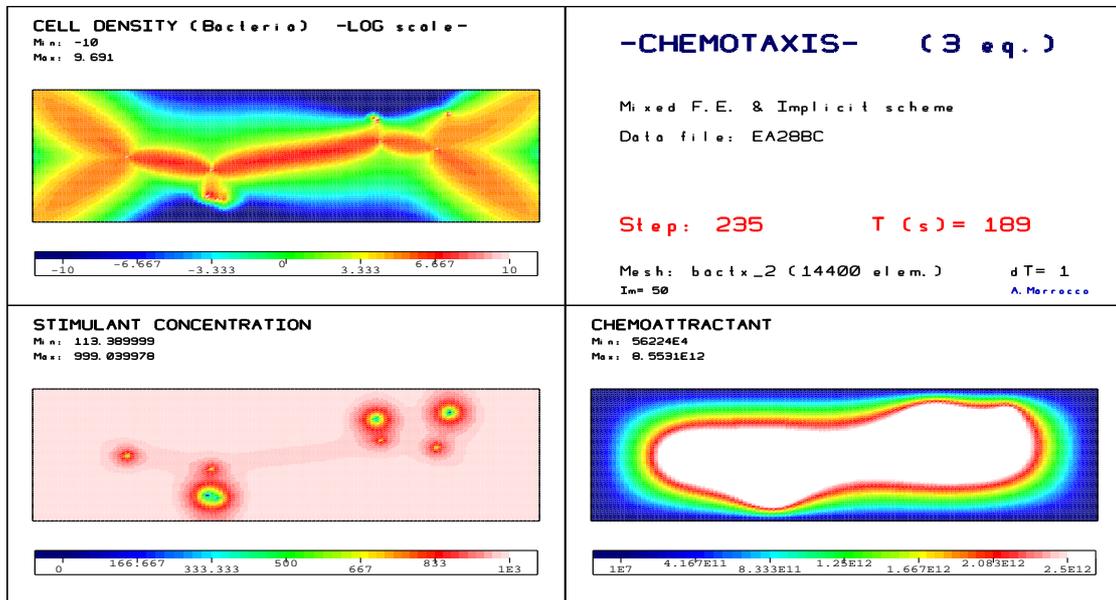
Keywords: *biophysics, cancer modeling, chemotaxis, finite element, numerical algorithm, numerical software.*

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

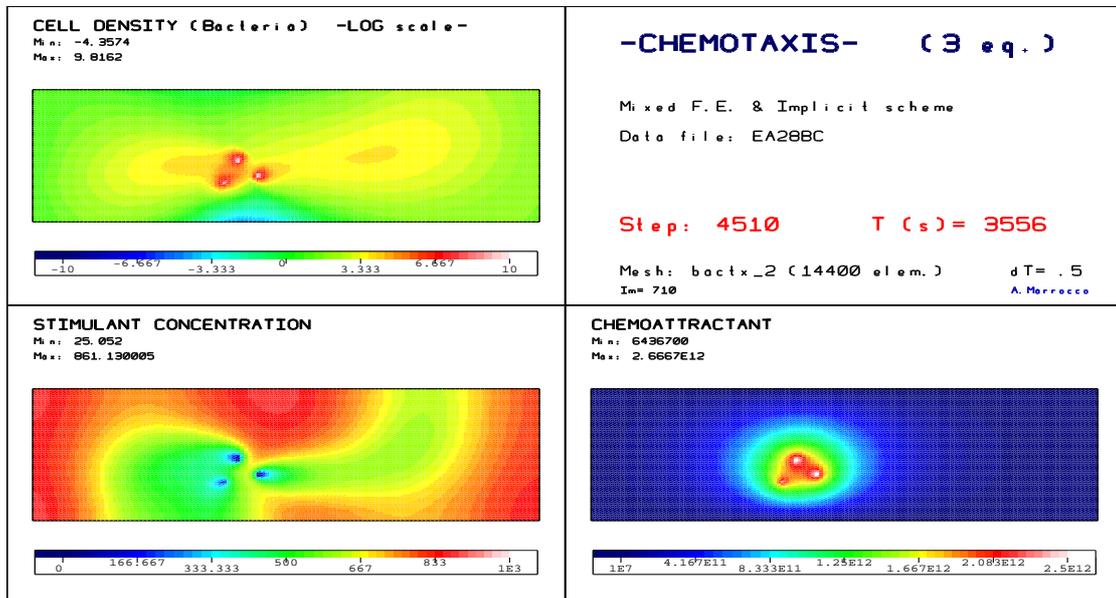
Movement of cells are important in the process of cancer development. We have developed some activity in the understanding of mathematical models of chemotaxis and angiogenesis. Angiogenesis describes the development of capillary blood vessels triggered by a substance emitted by a tumor. Models for the 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 [31].

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. A new formulation of the system of partial differential equations is obtained by 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. The mathematical model has been extended by several authors [30] [28] [32] by adding a third equation related to stimulant concentration. This year, a numerical model with 3 equations and several parameters has been implemented, using the same techniques, ie mixed finite elements for space approximation, fully implicit scheme for time discretization and Newton algorithm for solving (discrete) non linear problems. Various numerical tests have been carried out and we have also obtained numerical results previously obtained (using the model with 2 equations) as particular cases. The numerical results presented in fig 1 are obtained with a chemotaxis model very close to the one given in [30]. The initial state is defined by:

- a quasi-uniform distribution of bacterial density ($10^6 \text{ bact.cm}^{-3}$) in the simulation domain $L \times h = [1.5\text{cm}] \times [0.5\text{cm}]$, except 3 regions where
 - density ($= 1.25 \cdot 10^7 \text{ bact.cm}^{-3}$) in $[0.4L, 0.6L] \times [0.2h, 0.4h]$
 - density ($= 1.25 \cdot 10^7 \text{ bact.cm}^{-3}$) in $[0.65L, 0.75L] \times [0.7h, 0.9h]$
 - density ($= 2 \cdot 10^7 \text{ bact.cm}^{-3}$) in $[0.8L, 0.9L] \times [0.7h, 0.9h]$



(a) Isovalues at the beginning of the evolution process



(b) Results after approximately 1 hour

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

- uniform distribution of stimulants (concentration value 10^3)
- No chemo-attractants present (concentration value 0)

At the beginning of the evolution process (see fig. 1-a) regions with high concentration of bacteria appear together with spots (7 in the present simulation) at very high concentration values ($10^9, 10^{10}$). During the evolution process the number of spots decreases (3 after approximately 1 hour see fig. 1-b) and finally only one spot remains (continuing to travel through the simulation domain. As no renewal of stimulants is assumed, a trivial stationary state (uniform bacterial density distribution, 0-concentrations of stimulants and attractants) is reached when all the stimulants are consumed.

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 functional.

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

6.1.3. Structured population dynamics

Participants: Philippe Michel, Stéphane Mischler, Benoit Perthame.

In biology, it is usual to consider population models structured by a significant parameter (age structured, size structured, maturity structured). These models which can describe mitosis (cell division), growth using a nutrient, death of cells for instance, are not conservation laws. Nevertheless we show that they admit a common relative entropy structure which uses the first eigenelements of the problem. In case of scattering, it is more general than the usual "detailed balance principle". Four types of consequences are deduced from this entropy structure : a priori bounds, large time convergence to the steady state, in some cases, exponential rates of convergence and attraction of orbits by an periodic external forcing (this last is motivated by chronotherapy)

6.2. Free surface geophysical flows

Keywords: 3D Navier-Stokes, Geophysical flows, Saint-Venant equations, debris avalanches, free surface, multilayer system, source term, transport of pollutants.

Participants: Emmanuel Audusse, François Bouchut, Marie-Odile Bristeau, Astrid Decoene, Jean-Frédéric Gerbeau [REO], Tomas Morales, Haythem Ounaissa, Benoit Perthame.

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.

These applications have induced some theoretical works as the study of the uniqueness of the solutions of a scalar conservation law with discontinuous fluxes.

6.2.1. Discontinuous Fluxes

We consider the Cauchy problem associated with a scalar conservation law where the flux depends discontinuously on space - transport equation with discontinuous velocity, sedimentation process, shallow water equations for blood flow, traffic simulation...

$$\begin{cases} \partial_t u + \partial_x [A(x, u)] = 0 & x \in \mathbb{R}, \quad t \in \mathbb{R}_+, \\ u(0, x) = u_0(x) \in L^\infty(\mathbb{R}). \end{cases}$$

We propose a new method [10] to prove a L^1 contraction principle for a class of solutions to this equation when the space dependence of the flux is discontinuous. As in most of the recent papers that deal with this subject, our proof is based on Kruzkov's framework. But our idea is to adapt the definition of Kruzkov entropies to the discontinuous case instead of to adapt the proof.

When the space dependence of the flux is sufficiently smooth, this scalar equation is quite well known. In particular, Kruzkov's theory applies and provides existence and uniqueness of a weak solution that satisfies Kruzkov entropy inequalities.

The problem of the uniqueness of solutions when the flux is discontinuous in space has been investigated for ten years (Diehl, Klingenberg and Risebro, Greenberg and Leroux, Ostrov, Towers). Uptoday the more general results were due to Karlsen, Risebro and Towers (2003), to Seguin and Vovelle (2003) and to Adimurthi, Jaffre and Veerappa Gowda (2004). These three last works use classical Kruzkov entropies coupled with some interface conditions on the discontinuity of the flux and they all exhibit a L^1 contraction principle for a class of solutions. But they must suppose some regularity on the discontinuities of the flux. Moreover it can be shown that, even for very simple convex fluxes, two different interface conditions can selected two different solutions. Here we propose a new way which is to adapt the definition of Kruzkov entropies : we construct the entropies starting from the stationary solutions of the problem, which are no more constant functions. Then the proof is very similar to the classical Kruzkov one and the interface does not need a special attention. Thus we can avoid to impose some regularity requirements or to apply some interface conditions. As an application we present an example for which our method allows to selected the right entropy solution and then the right interface condition.

We are now working on a proof of the existence.

6.2.2. Saint-Venant equations

The Saint-Venant equations are the basis tool of the following developments concerning the transport of pollutants, the debris avalanches and the multilayer system. So we recall the important points of the solvers developed the previous years and which continue to be validated through different applications.

We have developed 1D and 2D solvers for the Saint-Venant equations with source terms, 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...). Our method is based on a *kinetic solver* and a *hydrostatic reconstruction* procedure.

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 [8] allows us to extend any positivity preserving homogeneous scheme to a positivity preserving *well-balanced* scheme. The idea is to use the relation associated to the equilibrium to define new interface values that are used in the definition of the finite volume fluxes and of the source terms.

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 [9][22]. The Figure 2 illustrates the accuracy improvement due to the second-order scheme, even for a problem with complex 2D interactions.

This solver is one of the options of the Telemac-2D code of EDF/LNHE.

6.2.3. 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 [29]. For the hydrodynamic part we use the previous kinetic solver. The interest of the developed method 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. This method has been introduced in the industrial code Telemac-2D of EDF.

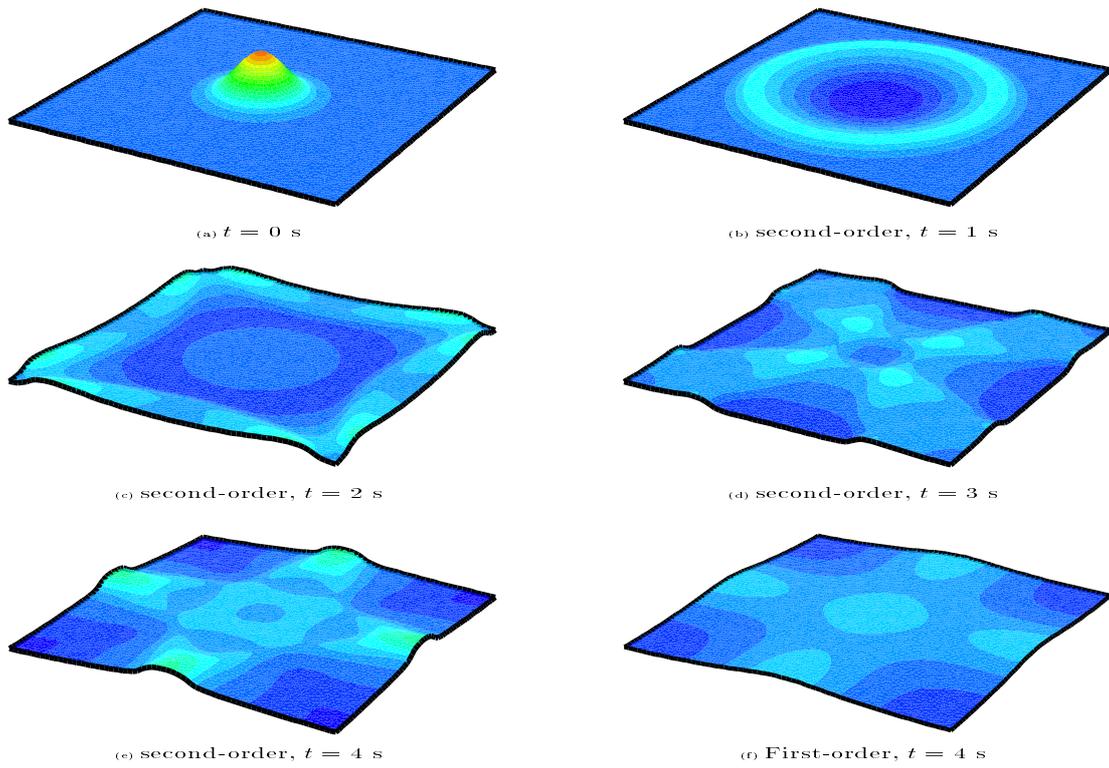


Figure 2.

WATER DROP IN A BASIN (TEST PROBLEM OF TELEMAT CODE).
(e)-(f) COMPARISON OF FIRST-ORDER AND SECOND-ORDER SOLUTIONS.

6.2.4. Granular flows, debris avalanches

The hypothesis of shallow flow is generally well satisfied by debris avalanches. In collaboration with the Laboratoire de Modélisation et Tomographie Géophysique (IPGP, Paris 7), we have considered 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 [16]. We are now studying the case where the earth pressure coefficient is not constant but depends whether the downslope flow is expanding or contracting.

6.2.5. 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 [7]. 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.

The Saint-Venant kinetic solver has been extended to this multilayer model and we have performed a numerical implementation which preserves the stability properties of the kinetic scheme. The 1D multilayer solver has been tested and validated [7][21] by comparisons with a 2D Navier-Stokes solver and we show that we obtain with the multilayer, a good approximation of the vertical profile of the horizontal velocity. The 2D multilayer solver has been developed and we begin the comparisons with 3D Navier-Stokes solutions.

6.2.6. 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. These equations are solved by the Telemac-3D software developed by EDF/LNHE, and our aim is to apply our results to this software in order to improve it.

We have first considered the model with hydrostatic approximation [26]. After time discretisation of the equations, the fractional step method can be applied in order to split the non-linear advection terms and the system - that we call "hydrostatic system" - composed by the resulting momentum equation and the depth-integrated continuity equation which is linearised. We have established a variational formulation leading to a mixed and symmetric problem coupling the 3D horizontal velocity and the 2D free surface. We have analysed this formulation and proved that the problem is generally well posed, provided the time step is not too big. When this is the case, the "INF-SUP condition" has to be verified by the discrete problem, therefore we have proposed a couple of stable finite elements to approximate the 3D horizontal velocity and the 2D free surface. In the actual version of Telemac-3D, the diffusion terms are also split and treated separately, and the hydrostatic system without diffusion 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 was, on one side, to allow a complete 3D treatment of the equations and, on the other side, take advantage of the stabilising property of the diffusion terms in the hydrostatic system. Therefore, we have implemented a resolution of the 3D hydrostatic system, without depth-integrating and including the viscous terms. We have validated the method through many numerical examples and the results are very accurate, but we are still working on optimising the program and illustrating the stabilising effect of the diffusion.

We have also worked on a new way to discretise the 3D domain on the vertical. The moving boundaries are treated using an ALE method : a transformation is defined between the real mesh and a fixed rectangular mesh which layers are all horizontal. The time differentials, as well as some other terms, can then be written in this fixed mesh in order to simplify their treatment. Up to now, the transformation used in Telemac-3D is the so-called "sigma transformation", which consists in transforming only the vertical coordinate from the fixed mesh

to the real one by multiplying it by the water height. This leads to a spatial discretization in which the layers follow the bottom and the free surface at each time step : no layer can therefore be forced to be horizontal, which is an important drawback, especially when stratifications are present in the studied flow that can only be preserved by using horizontal layers. We have generalised the classical sigma transformation in order to allow any position of the intermediate planes : from now on a different sigma transformation is defined on each layer, it has no longer to be constant on the vertical. This modification has required a development of the different numerical methods used in the software. Especially, the mass-conservation was no longer ensured, because the treatment of certain terms written in the fixed mesh had become erroneous with the new transformation. After this work, the mass-conservation of water as well as the mass-conservation and monotonicity of tracers is ensured and even improved with

6.3. Semiconductors

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

Participant: Americo Marrocco.

The collaboration with the university of Catania (Prof. M. Anile and his team) was finalized with the publication of two research reports [24][27], the first one considering only the classical parabolic band approximation and the second one taking into account more accurately the energy bands via the Kane's model. A synthetised paper has also been submitted for publication in Journal of Computational Electronics [6]. The parallel version of the drift-diffusion module (via domain decomposition techniques) has been tested on our "local" network of HP-workstations running HP-UX (about 30 processors available) and on a cluster of Intel-PC running Linux (16 bi-processors). On the network of HP-worstations no specific difficulties were encountered and if we except (perhaps) efficiency, we found similar algorithmic behaviour tha the one obtained on parallel machines like HP-V2250 (at Inria) or SGI-Origin 2000 (at CERFACS). On the Linux cluster, some difficulties related to inter-process communications suddenly arised when the (total) number of elements (finite element approximation) became larger than approximatively 40000 elements. A possible explanation of this trouble could be a "non totally correct" implementation of the MPI library in an environment using F77, C and F90 compilers.

6.4. Homgenization approach to filtration through a fibrous medium

Keywords: *Darcy Equation, Fibrous Porous Media, Filtration, Homogenization, Low Solid Fraction, Permeability, Quasi-periodic.*

Participants: Mohamed Belhadj, Eric Cancès [1], Jean-Frédéric Gerbeau [2], Andro Mikelić [3].

We study the flow through fibrous media using homogenization techniques. The fiber network under study is the one already used by M. Briane in the context of heat conduction of biological tissues. We derive and justify the effective Darcy equation and the permeability tensor for such fibrous media. Finally, the low solid fraction limit is considered. Applying results by G. Allaire to our setting, we justify rigorously the leading order term in the empirical formulas for the effective permeability used in engineering. The results are also confirmed by a direct numerical calculation of the permeability, in which the small diameter of the fibers requires high accuracy approximations [25].

7. Contracts and Grants with Industry

7.1. Free surface flows

Participants: Emmanuel Audusse, Marie-Odile Bristeau, Astrid Decoene, Jean-Frédéric Gerbeau [REO pre-project], Benoit Perthame.

¹MICMAC project

²REO pre-project

³Univ. Lyon1

The studies concerning the kinetic scheme for Saint-Venant equations, the transport of a pollutant and the improvement 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).

Participation to the ACI “Nouvelles Interfaces des Mathématiques”, Maths-Géophysique (Coordinator F. Bouchut [ENS]).

8.2. European actions

8.2.1. RTN network HYKE

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

8.2.2. 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>).

8.3. Visit and invitations

- Invitation of M.O. Bristeau at University of Malaga (Spain), sept. 2004

9. Dissemination

9.1. Scientific community

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. Cours de Java, DEUG MAS, Université Paris-Dauphine (A. Decoene)
2. Systèmes hyperboliques, Ecole Polytechnique de Tunisie (Benoit Perthame)
3. Geophysical flows, Lisbon, july 2004 (Benoit Perthame)
4. Math. bio. DGR Grip, Dourdan (Benoit Perthame)
5. Math. bio. DGR EQAP, Roscoff (Benoit Perthame)

9.3. Participation to congresses, workshops,...

- Plenary conf. at Workshop on Numerical Analysis of Partial Differential Equations (WON-APDE), Conception (Chile), january 2004 (B. Perthame)
- Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE), Conception, Chile, january 2004 (E. Audusse)
- “Di Perna memorial conference”, Berkeley, february 2004 (B. Perthame)
- “Aziz lecture”, University of Maryland, may 2004 (B. Perthame)
- 36 ème Congrès National d’Analyse Numérique, may 2004 (M. Belhadj)
- 4th European Congress on Comput. Meth. in Appl. Sc. and Eng.(ECCOMAS), Jyväskylä, Finland, july 2004, (E. Audusse, M.O. Bristeau)
- Mathematics and Applications in Biology and Medicine, Cemracs, Marseille, august 2004 (A. Decoene, M. Belhadj)
- Invited conf. Copenhagen, august 2004 (B. Perthame)
- Seminar, Berlin Free University, september 2004 (E. Audusse)
- Seminars, Malaga University, september 2004 (M.O. Bristeau)
- Telemac Users’ Club, Toulouse, october 2004 (A. Decoene)
- Dispersive effects in wave propagation, Oberwolfach, october 2004 (B. Perthame)
- Conf. math. model for cell motion, Wien, november 2004, scientific commity (B. Perthame)
- Workshop: Fluide et Structure, Mulhouse, november 2004 (M. Belhadj)
- Colloquium INRIA Calcul scientifique, december 2004 (B. Perthame)

10. Bibliography

Major publications by the team in recent years

- [1] F. HECHT, A. MARROCCO. *Mixed finite element simulation of heterojunction structures including a boundary layer model for the quasi-Fermi levels*, in "NASECODE X Conference, Dublin", Boole Press, june 1994, p. 50-51.
- [2] A. MARROCCO, P. MONTARNAL. *Simulation des modèles energy-transport à l'aide des éléments finis mixtes*, in "C.R. Acad. Sci. Paris", vol. 323, n° Série I, 1996, p. 535-541.
- [3] B. PERTHAME. *Kinetic formulations of conservation laws*, Oxford University Press, 2002.
- [4] B. PERTHAME, M. THIRIET. *Special issue on biological and biomedical applications*, Vol 37, number 4, july/August 2003, M2AN.

Doctoral dissertations and Habilitation theses

- [5] E. AUDUSSE. *Modélisation hyperbolique et analyse numérique pour les écoulements en eaux peu profondes*, Thèse, Université Pierre et Marie Curie, Paris 6, september 2004.

Articles in referred journals and book chapters

- [6] A. M. ANILE, A. MARROCCO, V. ROMANO, J.-M. SELLIER. *Numerical simulation of 2D Silicon MESFET and MOSFET described by the MEP based energy-transport model with a mixed finite element scheme*, in "Journal of Computational Electronics", submitted (april 2004), to appear.
- [7] E. AUDUSSE. *A Multilayer Saint-Venant Model*, in "Discrete and Continuous Dynamical Systems-Serie B", to appear.
- [8] E. AUDUSSE, F. BOUCHUT, M.-O. BRISTEAU, R. KLEIN, B. PERTHAME. *A fast and stable well-balanced scheme with hydrostatic reconstruction for shallow water flows*, in "SIAM J. Sc. Comp.", vol. 25, n° 6, 2004, p. 2050-2065.
- [9] E. AUDUSSE, M.-O. BRISTEAU. *A well-balanced positivity preserving second order scheme for shallow water flows on unstructured meshes*, in "X", to appear.
- [10] E. AUDUSSE, B. PERTHAME. *Uniqueness for a scalar conservation law with discontinuous flux via adapted entropies*, in "submitted", to appear.
- [11] F. CHALUB, P. MARKOWICH, B. PERTHAME, C. SCHMEISER. *Kinetic Models for Chemotaxis and their Drift-Diffusion Limits*, in "Monatshefte fuer Mathematik", vol. 142, n° 1-2, 2004, p. 123-141.
- [12] L. CORRIAS, B. PERTHAME, H. ZAAG. *Global Solutions of some Chemotaxis and Angiogenesis Systems in high space dimensions*, in "Milano J. of Math", vol. 72, 2004, p. 1-29.

- [13] O. DIEKMANN, P.-E. JABIN, S. MISCHLER, B. PERTHAME. *The dynamics of adaptation : an illuminating example and a Hamilton-Jacobi approach*, in "Th. Pop. Biol.", to appear.
- [14] F. FILBET, P. LAURENCOT, B. PERTHAME. *Derivation of Hyperbolic Models for Chemosensitive Movement*, in "J. Math. Biology", to appear.
- [15] T. KATSAOUNIS, B. PERTHAME, C. SIMEONI. *Upwinding Sources at Interfaces in conservation laws*, in "Applied Math. Letters", n° 3940, 2004.
- [16] A. MANGENEY-CASTELNAU, J. P. VILOTTE, M.-O. BRISTEAU, B. PERTHAME, F. BOUCHUT, C. SIMEONI, S. YERNINI. *Numerical modeling of avalanches based on Saint-Venant equations using a kinetic scheme*, in "J. Geophys. Res.", vol. 108, n° B11, 2003, p. 2527-2542.
- [17] P. MICHEL, S. MISCHLER, B. PERTHAME. *General entropy equations for structured population models and scattering*, in "C.R. Acad. Sc. Paris," , vol. Série I, n° 338, 2004, p. 697–702.
- [18] B. PERTHAME. *Mathematical Tools for Kinetic Equations*, in "Bull. A.M.S.", 2004.
- [19] B. PERTHAME. *PDE models for chemotactic movements, Parabolic, hyperbolic and kinetic*, in "Appl. Math", vol. 49, n° 6, 2004.
- [20] B. PERTHAME. *Quelques équations de transport apparaissant en biologie*, in "Bol. Soc. Esp. Mat. Apl.", vol. 28, 2004.

Publications in Conferences and Workshops

- [21] E. AUDUSSE. *A Multilayer Saint-Venant Model*, in "Proceedings of 4th European Congress on Comput. Meth. in Appl. Sc. and Eng., Jyväskylä", P. NEITTAANMÄKI, T. ROSSI, S. KOROTOV, E. OÑATE, J. PÉRIAUX, D. KNÖRZER (editors)., Vol.I, July 2004.
- [22] E. AUDUSSE, M.-O. BRISTEAU, B. PERTHAME. *Second Order Kinetic Scheme for Saint-Venant Equations with Source Terms*, in "Proceedings of 4th European Congress on Comput. Meth. in Appl. Sc. and Eng., Jyväskylä", P. NEITTAANMÄKI, T. ROSSI, S. KOROTOV, E. OÑATE, J. PÉRIAUX, D. KNÖRZER (editors)., Vol.II, July 2004.
- [23] M. BELHADJ, E. CANCÈS, J.-F. GERBEAU, A. MIKELĆ, B. PERTHAME. *Analyse d'un modèle de filtration à travers un milieu fibreux*, in "36 ème Congrès National d'Analyse Numérique", (Best posters award), Université de Strasbourg, 2004.

Internal Reports

- [24] A. M. ANILE, A. MARROCCO, V. ROMANO, J.-M. SELLIER. *Numerical simulation of 2D Silicon MESFET and MOSFET described by the MEP based energy-transport model with a mixed finite elements scheme*, Rapport de recherche, Inria, january 2004, <http://www.inria.fr/rrrt/rr-5095.html>.
- [25] M. BELHADJ, E. CANCÈS, J.-F. GERBEAU, A. MIKELĆ. *Homogenization approach to filtration through a fibrous medium*, Rapport de recherche, Inria, 2004, <http://www.inria.fr/rrrt/rr-5277.html>.

- [26] A. DECOENE. *Equations de Navier-Stokes à surface libre en dimension 3 avec hypothèse hydrostatique*, Rapport Interne, n° HP-75/04/020/A, EDF R&D, LNHE, April 2004.
- [27] A. MARROCCO, V. ROMANO, J.-M. SELLIER. *Numerical simulation of the 2D non-parabolic MEP energy-transport model with a mixed finite elements scheme*, Rapport de recherche, Inria, february 2004, <http://www.inria.fr/rrrt/rr-5103.html>.

Bibliography in notes

- [28] P. K. MAINI, H. G. OTHMER (editors). *Mathematical models for biological pattern formation*, Springer-Verlag, New-York, 2000.
- [29] E. AUDUSSE, M.-O. BRISTEAU. *Transport of Pollutant in Shallow Water. A Two Time Steps Kinetic Method*, in "M2AN", vol. 37, n° 2, 2003, p. 389-416.
- [30] M. P. BRENNER, L. S. LEVITOV, E. O. BUDRENE. *Physical mechanisms for chemotactic pattern formation by bacteria*, in "Biophysical Journal", vol. 74, april 1998, p. 1677-1693.
- [31] L. CORRIAS, B. PERTHAME, H. ZAAG. *A chemotaxis model motivated by angiogenesis*, in "C.R. Acad. Sc. Paris, Série I", vol. 336, n° 2, 2003, p. 141-146.
- [32] J. D. MURRAY. *Mathematical Biology*, Third, vol. I and II, Springer-Verlag, 2002.