



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team SMASH

*Simulation, Modeling and Analysis of
Heterogeneous Systems in continuum
mechanics*

Sophia Antipolis - Méditerranée

Theme : Computational models and simulation

Activity
R *eport*

2010

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SMASH is a common project between INRIA-Sophia Antipolis–Méditerranée and Aix-Marseille University. Its main topic is related to both the mathematical and numerical modelling of heterogeneous and complex flows in heterogeneous media, such as (inert or reactive) granular materials, interface problems or pollutant propagation in urban environments. This project team was previously located at both locations (till 2008) and is now uniquely located at Marseille. While two INRIA members left SMASH to join another INRIA project team PUMAS in 2009, two associated professors have been hired at Marseille both in September 2009: Fabien Petitpas who has got a University-CNES chair, and Nicolas Favrie, who has got an associate professor position at the Civil Engineering Department of Polytech’Marseille School, Aix-Marseille I University.

1. Team

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2. Overall Objectives

2.1. Presentation

SMASH is a common project between INRIA Sophia Antipolis – Méditerranée and Aix-Marseille University. Its main topic is related to both the mathematical and numerical modelling of heterogeneous flows such as multiphase media, granular materials and interface problems.

The first issue deals with the *design* and *improvements* of *theoretical models* for multiphase and interfacial flows. Particular attention is paid to *well posedness* issues and *system’s hyperbolicity*.

The second issue deals with the *design* of *appropriate numerical schemes*. These models are not known as well as conventional single fluid models and pose numerical challenges such as, for example, the numerical approximation of *non-conservative terms*. These numerical issues pose *theoretical* questions such as, *shock wave existence in multiphase mixture*, *cell averages of non-conservative variables*, *Chapman–Jouguet detonation conditions for heterogenous explosives* and so on.

The final aim is to *implement* the resulting algorithms on *parallel machines* for solving *large scale problems* for the design of advanced technology systems in Space, Defense and Nuclear energy, but also in security problems such as the propagation of pollutants in urban atmosphere and environment.

One of the main original features of the SMASH researches on heterogeneous flows lies in the way we deal with multiphase mixtures. Our aim is to solve the *same equations* everywhere with the *same numerical method* :

- in pure fluid,
- in multi-velocity mixtures,
- in artificial smearing zones at material interfaces or in mixture cells,
- in shocks, phase transition fronts, detonation waves,
- in elastic-plastic materials.

An example of such computations is given in the figure 1.

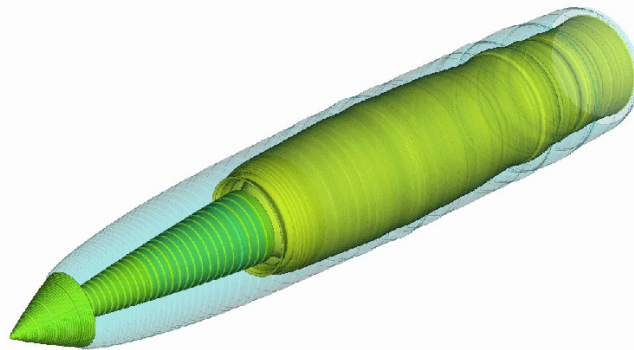


Figure 1. Numerical simulation of an underwater missile flying at 600 m/s. Three fluids are present : liquid water, steam and propulsion gases. Two different types of interfaces are present : a contact interface separates steam and combustion gases while an evaporating interface separates metastable expanded liquid and steam. To deal with metastable phase transition, the novel approach of [9] is used. The numerical approximation of the non-conservative hyperbolic system with stiff relaxation is achieved by the method of [49].

There are some advantages with this approach :

- the most obvious relies in the *coding simplicity* and *robustness* as a *unique algorithm* is used;
- *conservation principles* are guaranteed for the mixture. Conventional algorithms are able to preserve mass conservation only when dealing with interfaces;
- *interface conditions* are perfectly matched even for the coupling of complex media (granular flows, capillary fluids, transition fronts) even in the presence of *shocks*;

- this approach is the *only one able to deal with dynamic appearance of interfaces* (cavitation, spallation);
- our methods allow the *coupling of multi-velocities, multi-temperatures mixtures* to macroscopic interfaces where a single velocity must be present. To illustrate this capability consider the example of a cloud of bubbles rising up in a liquid to the surface, where a free boundary is present. Two velocities have to be considered for the bubbles rising, while a single velocity must be present just after their crossing through the interface. This is also the only method able to deal with such situations.

Our approach rises increasing attention from the *scientific community* as well as *the industry*. As will be detailed further, many projects are currently under development with french oriented research centers (DGA, CNES, SNECMA) as well as foreign ones (Idaho National Laboratory - USA, ADD, Korea).

2.2. Highlights

Richard Saurel has received the Prix Edmond Brun award from the French Academy of Sciences for his research work in multiphase flows in the spatial sciences area, last October 2010.

3. Scientific Foundations

3.1. Modelling of Multiphase Media

Conventional one-dimensional models of two-phase mixtures having two velocities form a system of six partial differential equations: two mass, two momentum and two energy equations. Those models are not hyperbolic and are consequently ill posed. It means that there is no continuous dependance from initial data and boundary conditions to the solution. In other words, wave propagation may have no physical sense.

This issue has been understood by [53] and subtle remedy was given by [29]. They proposed an extended model with seven equations. The extra differential equation replaced the pressure equilibrium assumption in the mixture. Thanks to this new equation, the model was correctly posed, unconditionally hyperbolic.

This model had little diffusion as it was presented in the context of a specific problem of detonation physics. Also, the model was difficult to solve at the numerical level, in particular with modern algorithms based on the Riemann problem solution. In [48] we developed the first Godunov type method for this model and derived accurate approximation formulas for the non-conservative terms. Moreover, a specific relaxation method was built in order to solve these equations in the presence of stiff relaxation terms. This issue was particularly important as,

- this model was involving two pressure and two velocities,
- at an interface the jump condition corresponds to continuous normal velocities and continuous pressures,
- in order to fulfill this condition it was necessary to relax the two pressures and velocities to unique equilibrium variables.

Such an issue was reached by using specific relaxation solvers, with infinite relaxation parameters like in [5]. With this solver, the model was able to solve interface problems (air/water for example) and multiphase mixtures with two velocities. Important applications of fundamental and applied physics were possible to solve. Financial supports from DGA and CEA helped us to pursue the investigations.

Denoting $p_r = p_1 - p_2$, $u_r = u_1 - u_2$, the two-phase flow model presents under the form (1) :

$$\begin{aligned}
\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} &= \mu p_r , \\
\frac{\partial(\alpha_1 \rho_1)}{\partial t} + \frac{\partial(\alpha_1 \rho_1 u_1)}{\partial x} &= 0 , \\
\frac{\partial(\alpha_1 \rho_1 u_1)}{\partial t} + \frac{\partial(\alpha_1 \rho_1 u_1^2 + \alpha_1 p_1)}{\partial x} &= p_I \frac{\partial \alpha_1}{\partial x} - \lambda u_r , \\
\frac{\partial(\alpha_1 \rho_1 E_1)}{\partial t} + \frac{\partial[\alpha_1 (\rho_1 E_1 + p_1) u_1]}{\partial x} &= p_I u_I \frac{\partial \alpha_1}{\partial x} - \mu p_I' p_r - \lambda u_I' u_r .
\end{aligned} \tag{1}$$

Only the equations for phase 1 are written, since those of phase 2 are symmetric. General closure relations for this system need the determination of :

- the interface velocity u_I and pressure p_I that respectively represent the velocity and pressure that exert at the boundary of a cloud of bubbles or droplets,
- the average interface velocity u_I' and pressure p_I' that exert in the bulk of a two-phase control volume,
- the relaxation parameters λ and μ that control the rate at which velocities and pressures relax to mechanical equilibrium respectively.

These relations were unknown, either estimated in limit cases only, or determined by experimental means. In order to determine these closure relations a new homogenization method has been built in [1].

This new averaging method considers the mixture at the discrete level, with a stencil composed of three computational cells. In each cell, at each cell boundary and at each internal boundary separating the phases, the Riemann problem of the pure fluid equations (RP) is solved. The RP solution provides all local interfacial information. These RP solutions are then averaged in the computational cell as done originally with the first version of the Godunov method, derived originally for the Euler equations. In our context, extra difficulties appear, due to the presence of internal material interfaces, material discontinuities at cell boundaries and variable sub-volumes, due to the phase presence in the cells. But the philosophy was the same as with the Godunov method : we are dealing with average RP solutions and not with discretized partial differential equations.

The resulting system of this averaging procedure is a quite complicated discrete system in algebraic form. It corresponds to the result of the Discrete Equations Method (DEM). The closure relations for the various interface variables have been obtained by reaching the continuous limit of these discrete equations [8], [30] that provide information easier to interpret than discrete formulas.

With this strong modelling foundations, it was possible to consider problems with extended physics : turbulence, phase transition, ions and electrons in plasma mixtures, granular materials, chemical reactions, continuum media with elastic-plastic effects. An example is shown in the figures 2-3.

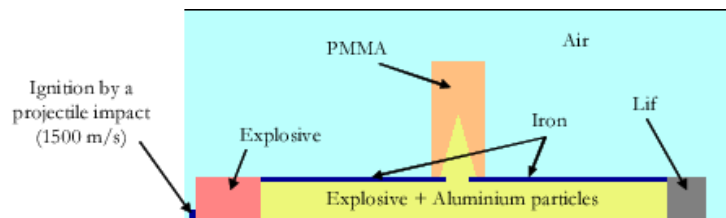


Figure 2. A steel tube is filled with a heterogeneous explosive. A high velocity impactor creates a shock wave passed onto the explosive, that becomes a detonation wave.

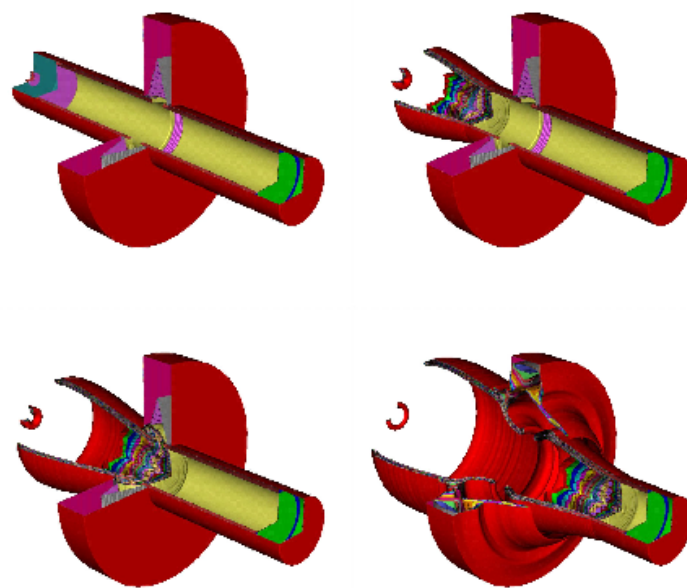


Figure 3. After a short period of time the shock wave becomes a detonation wave that produces gas and solid products at very high pressure. They set into intense motion solid tube walls. Two different types of mixture are present in this type of application : a physical one, corresponding to the mixture of gases and solid particles during the detonation dynamics, and artificial mixtures, corresponding to the ones that appear at material interfaces, here at the gas - steel tube boundary. Both types of mixture are solved by the same equations and the same numerical algorithm [49]. Moreover, the detonation dynamics is checked against generalized CJ solutions [47], specifically determined for this temperature non-equilibrium model.

Most of these extensions are done with the help of the Hamilton principle of least action [52], [3] to develop appropriate single phase material models that are then coupled with the DEM to form a multiphase flow model.

3.2. Modelling of Interface and Multi-Fluid Problems

In order to solve interfaces separating pure fluids or pure materials, two approaches have been developed. The first one has been described previously. It consists in solving a non-equilibrium flow model with two pressures and two velocities, and then in relaxing instantaneously these variables to equilibrium ones. Such a method allows a perfect fulfillment of interface conditions in mixture cells, that appear as a result of numerical diffusion at material interfaces.

The second option consists in determining the *asymptotic model* that results from stiff mechanical relation. In the context of two fluids, it consists in a set of five partial differential equations [41], [38] : two masses, one mixture momentum, one mixture energy and one volume fraction equations. Such a system is obviously less general than the previous non-equilibrium system, but it is particularly interesting in solving interface problems, where a single velocity is present. More precisely, it is more appropriate and simpler, when considering extra physics extensions such as, phase transition, capillary effects, elastic-plastic effects.

Contrarily to conventional methods, there is no need to use a front tracking method, nor level set [34], nor interface reconstruction and so on. The same equations are solved everywhere [42], [43] and the interface is captured with the 5 equation model. This model provides correct thermodynamic variables in artificial mixture zones. Although seemingly artificial, this model can handle huge density ratio, and materials governed by very different equations of state, in multi-dimensions. It is also able to describe multiphase mixtures where stiff mechanical relaxation effects are present, such as, for example, reactive powders, solid alloys, composite materials *etc.*

Several extensions have been done during these recent years by the SMASH team :

- a model involving *capillary, compressibility* and *viscous effects* [46]. This is the first time such effects are introduced in a hyperbolic model. Validations with experiments done at IUSTI (the laboratory where the group of Marseille is located at) have shown its excellent accuracy, as shown in the figure 4;
- *phase transition in metastable liquids* [9]. This is the first time a model solves the ill-posedness problem of spinodal zone in van der Waals fluids.

The combination of capillary and phase transition effects is under study in order to build a model to perform direct numerical simulation (DNS) of phase transition at interfaces, to study explosive evaporation of liquid drops, or bubble growth in severe heat flux conditions. This topic has important applications in *nuclear engineering* and *future reactors* (ITER for example). A collaboration has been started with the Idaho National Laboratory, General Electric, and MIT (USA) in order to build codes and experiments on the basis of our models and numerical methods. In another application domain, several contracts with CNES and SNECMA have been concluded to model phase transition and multiphase flows in the Ariane VI space launcher cryogenic engine.

In the presence of shocks, fundamental difficulties appear with multiphase flow modelling. Indeed, the volume fraction equation (or its variants) cannot be written under divergence form. It is thus necessary to determine appropriate jump relations.

In the limit of *weak* shocks, such relations have been determined by analysing the dispersive character of the shock structure in [50], [36] and [35]. Opposite to single phase shocks, backward information is able to cross over the shock front in multiphase flows. Such phenomenon renders the shocks smooth enough so that analytical integration of the energy equations is possible. Consequently, they provide the missing jump condition.

These shock conditions have been validated against all experimental data available in the various American and Russian databases, for both *weak* and *very strong* shocks.

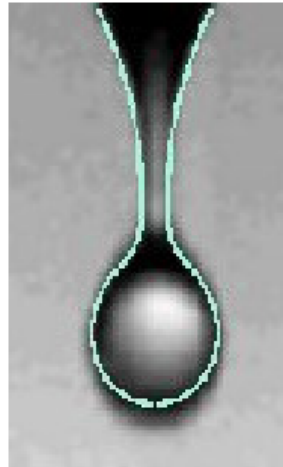


Figure 4. Comparison of the drop shape during formation (experiment in grey area, computations in lines). No interface tracking nor interface reconstruction method are used. The same equations are solved at each mesh point. The model accounts for compressible, viscous and capillary effects. The compressible effects are negligible in the present situation, but they become fundamental in other situations (phase transition for example) where the full thermodynamics of each fluid is mandatory. The method treats in a routinely manner both merging and fragmentation phenomena.

At this point, the theory of multiphase mixtures with single velocity was closed. Thanks to these ingredients we have done important extensions recently :

- *restoration of drift effects* : a dissipative one-pressure, one-velocity model has been studied in [45], and implemented in a parallel, three-dimensional code [44]. This model is able to reproduce phase separation and other complex phenomena [37];
- extending the approach to deal with *fluid-structure interactions*. A non-linear elastic model for compressible materials has been built [2]. It extends the preceding approach of Godunov to describe continuum media with conservative hyperbolic models. When embedded in our multiphase framework, fluid solid interactions are possible to solve in highly non-linear conditions with a single system of partial differential equations and a single algorithm. This was the aim of Nicolas Favrie's PhD thesis [32], that has been pursued last year [33];
- determining the *Chapman-Jouguet conditions* for the detonation of *multiphase explosives*. The single velocity - single pressure model involves several temperatures and can be used to describe the non-equilibrium detonation reaction zone of condensed heterogenous energetic materials. Since the work of Zeldovich-Neumann and Doering (ZND model), the detonation dynamics of gaseous and condensed energetic materials is described by the ZND approach, assuming mixtures in thermal equilibrium. However, in condensed energetic materials, the mixture is not of molecular type and the thermal equilibrium assumption fails. With the help of the same model used for phase transition [9], closed by appropriate shock conditions [50], it is now possible to develop a ZND type model with temperature disequilibrium. This opens a new theory for the detonation of condensed materials. Successful computations of multidimensional detonation waves in heterogenous explosives have been done with an appropriate algorithm in [47].

Obviously, all these models are very different from the well studied gas dynamics equations and hyperbolic systems of conservation laws. The building of numerical schemes requires special attention as detailed hereafter.

3.3. Approximation methods

All the mathematical models considered and studied in SMASH consist in hyperbolic systems of PDE's. Most of the attention is focused on the 7 equation model for non-equilibrium mixtures and the 5 equation model for mechanical equilibrium mixtures. The main difficulty with these models is that they cannot be written under divergence form. Obviously, the conservation principles and the entropy inequality are fulfilled, but some equations (the volume fraction equation in particular) cannot be cast under conservative form. From a theoretical point of view, it is known since the works of Schwartz [51] that the product of two distributions is not defined. Therefore, the question of giving a sense to this product arises and as a consequence, the numerical approximation of non-conservative terms is unclear [31], [40]. Aware of this difficulty, we have developed two specific methods to solve such systems.

The first one is the *discrete equations method* (DEM) presented previously as a new homogenization method. It is moreover a numerical method that solves non-conservative products for the 7 equation model in the presence of shocks. With this method, Riemann problem solutions are averaged in each sub-volume corresponding to the phase volumes in a given computational cell. When a shock propagates inside a cell, each interaction with an interface, corresponds to the location where non-conservative products are undefined. However, at each interaction, a diffraction process appears. The shock discontinuity splits in several waves : a left facing reflected wave, a right facing transmitted wave and a contact wave. The interface position now corresponds to the one of the contact wave. Along its trajectory, the velocity and pressure are now continuous : this is a direct consequence of the diffraction process. The non-conservative products that appear in these equations are precisely those that involve velocity, pressure and characteristic function gradient. The characteristic function gradient remains discontinuous at each interface (it corresponds to the normal) but the other variables are now continuous. Corresponding non-conservative products are consequently perfectly defined : they correspond to the local solution of the Riemann problem with an incoming shock as initial data. This method has been successfully developed and validated in many applications [1], [8], [6], [30].

The second numerical method deals with the numerical approximation of the *five equation model*. Thanks to the shock relations previously determined, there is no difficulty to solve the Riemann problem. However, the next step is to average (or to project) the solution on the computational cell. Such a projection is not trivial when dealing with a non-conservative variable. For example, it is well known that pressure or temperature volume average has no physical meaning. The same remark holds for the *cell average* of volume fraction and internal energy. To circumvent this difficulty a new relaxation method has been built [49]. This method uses *two main ideas*.

The first one is to *transform* one of the *non-conservative products* into a *relaxation term*. This is possible with the volume fraction equation, where the non conservative term corresponds to the asymptotic limit of a pressure relaxation term. Then, a splitting method is used to solve the corresponding volume fraction equation. During the hyperbolic step, there is no difficulty to derive a positivity preserving transport scheme. During the stiff relaxation step, following preceding analysis of pressure relaxation solvers [5], there is no difficulty neither to derive entropy preserving nor positive relaxation solvers.

The second idea deals with the *management of the phase's energy equations*, which are also present under *non-conservative form*. These equations are able to compute regular/smooth solutions, such as expansion waves, but are inaccurate for shocks. Thus they are only used at shocks to predict the solution. With the predicted internal energies, phase's pressures are computed and then *relaxed to equilibrium*. It results in an *approximation* of the volume fraction at shocks. This approximation is then used in the *mixture equation of state*, that is unambiguously determined. This equation of state is based on the *mixture energy*, a supplementary equation. This equation, apparently redundant, has to be fulfilled however. Its numerical approximation is obvious even in the presence of shocks since it is a conservation law. With the help of the mixture energy and predicted volume fraction, the *mixture pressure* is now computed, therefore closing the system. This treatment guarantees *correct, convergent and conservative wave transmission* across material interfaces separating pure media. When the interface separates a fluid and a mixture of materials, the correct partition of energies among phases is fulfilled by replacing at the shock front the internal energy equations by their corresponding jumps

[50]. To ensure the numerical solution strictly follows the phase's Hugoniot curves, the poles of these curves are transported [47]. With this treatment, the method also converges for multiphase shocks.

This method is very *efficient* and *simple to implement*. This also helped us considerably to solve very large systems of hyperbolic equations, like those arising for elastic materials in large deformations. The fluid-solid coupling via diffuse interfaces with extreme density ratios was done efficiently, as shown in figure 5.

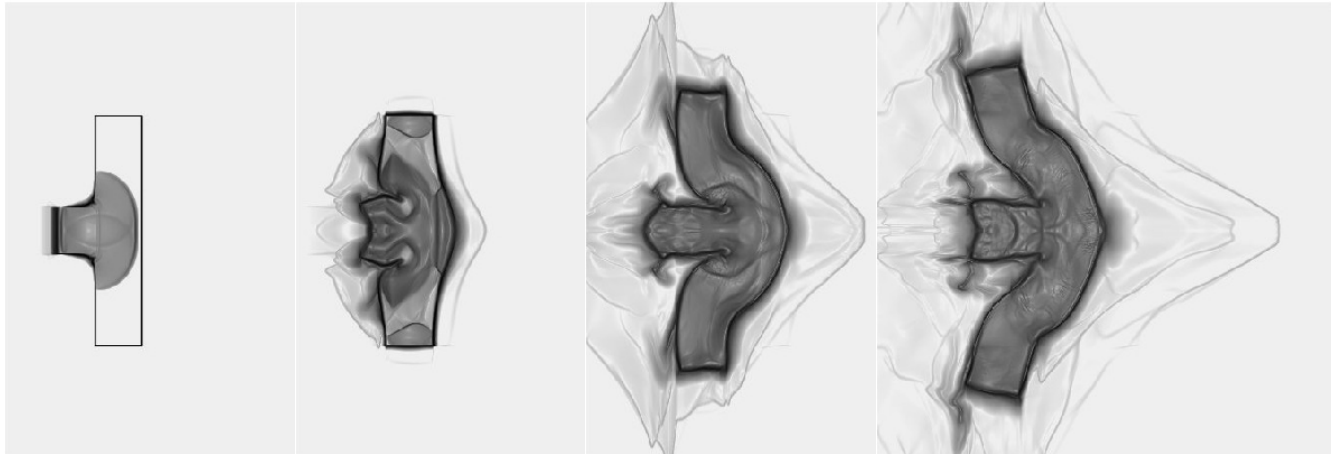


Figure 5. A copper projectile impacts a copper plate at the velocity of 800 m/s. Both materials are considered compressible and elastic, and are surrounded by air at atmospheric pressure.

Another difficulty encountered in solving two-phase flow problems comes from the high disparity between the wave speeds of each existing fluid material. In particular, one of the fluids may be very close to the incompressibility limit. In that case, we face up the problem of very low Mach number flows. The numerical treatment of these flows is still a problem and involves non trivial modifications of the original upwind schemes [39], [38]. Our investigations in that domain concern both acoustic and incompressible aspects in methodologies for setting up suitable numerical methods.

4. Application Domains

4.1. Panorama

About 15 years ago, working on the physics of detonation waves in highly energetic materials, we discovered a domain where flow conditions were extreme. Numerical simulations in detonation conditions were a true challenge. The mathematical models as well as numerical methods must be particularly well built. The presence of material interfaces was posing considerable difficulties.

During the years 90–95, we have investigated open and classified literature in the domain of multimaterial shock-detonation physics codes. We came to the conclusion that nothing was clear regarding *mixture cells*. These *mixture cells* are a consequence of the numerical diffusion or cell projection of flow variables at contact discontinuities.

Thus, we have developed our own approach. On the basis of multiphase flow theory, revisited for a correct treatment of wave dynamics, we have proposed to solve mixture cells as true multiphase mixtures. These mixtures, initially out of equilibrium, were going to relax to mechanical equilibrium with a single pressure and velocity.

From this starting point, many extensions have been done, most times initiated by applications connected to the Defense domain. Collaborations have never stopped with these specialized laboratories since 1993. Applications have also been done with Space, Automotive, Oil, Nuclear engineering domains. International projects have started with the US and Korea.

From the technology developed in the Defense area, important applications are now coming for Space industry (CNES and SNECMA). The aim is to restart the Ariane cryogenic engine several times, for orbit change. Restarting a cryogenic engine is very challenging as the temperature difference between cryogenic liquid and walls is about 300K. Stiff phase change, cavitation, flashing in ducts and turbopumps are expected. These phenomena have to be particularly well computed as it is very important to determine the state of the fluids at the injection chamber. This is crucial for the engine ignition and combustion stability.

From a modelling point of view, our models and methods are aimed to replace the technology owned by space laboratories, taken 10 years ago from nuclear laboratories.

To deal with these industrial relations, the startup RS2N has been created in 2004 on the basis of the Innovation Law of the Minister Claude Allègre.

4.2. Defense Applications

4.2.1. Explosions

Four contracts with the Gramat Research Center (DGA) are under realization for the modelling of explosions with liquid tanks, granular materials, combustion of particle clouds, phase change etc. The total amount is 2M€ for 6 years work. They will end in 2013.

4.2.2. Solid-fluid coupling

A contract with DGA (REI) is under realization for the modelling of solid-fluid coupling in extreme conditions. The diffuse interface theory is under extension to build equations which will be valid in pure solids, pure fluids as well as interfaces. The total amount is 300 K€ for 3 years work. It will end in 2011.

4.2.3. Hypervelocity underwater missile

A contract with Chungnam National University (South Korea) is starting in order to model supercavitation around a high velocity torpedo, propelled by underwater solid rocket motor. The total amount is 100 K\$ for one year work. It will end in 2010, but will possibly continue.

4.3. Space Industry

CNES and SNECMA have joined their support and efforts to ask SMASH for the development of flow solvers to study the restart stage of cryogenic engine under microgravity.

A three year project plan has been validated during 2009 for the total amount of 650 K€. In addition, Richard Saurel has been asked by SNECMA to make different expertise works in other areas, such as cavitation and system codes.

5. New Results

5.1. Mathematical Modelling

5.1.1. A discrete model for compressible flows in heterogeneous media

Participants: Olivier Le Métayer, A. Massol, Nicolas Favrie, Sarah Hank.

This work deals with the building of a discrete model able to describe and to predict the evolution of complex gas flows in heterogeneous media. In many physical applications, large scale numerical simulation is no longer possible because of a lack of computing resources. Indeed the medium topology may be complex due to the presence of many obstacles (walls, pipes, equipments, geometric singularities, ...). Aircraft powerplant compartments are examples where topology is complex due to the presence of pipes, ducts, coolers and other equipments. Other important examples are gas explosions and large scale dispersion of hazardous materials in urban places, cities or undergrounds involving obstacles such as buildings and various infrastructures. In all cases efficient safety responses are required. Then a new discrete model is built and solved in reasonable execution times for large cells volumes including such obstacles. Quantitative comparisons between experimental and numerical results are shown for different significant test cases, showing excellent agreement [17].

5.1.2. A hyperbolic Eulerian model for dilute two-phase suspensions

Participants: Sarah Hank, Richard Saurel, Olivier Le Métayer.

Conventional modelling of two-phase dilute suspensions is achieved with the Euler equations for the gas phase and gas dynamics pressureless equations for the dispersed phase, the two systems being coupled by various relaxation terms. The gas phase equations form a hyperbolic system but the particle phase corresponds to a hyperbolic degenerated one. Numerical difficulties are thus present when dealing with the particles system. In the present work, we consider the addition of turbulent effects in both phases in a thermodynamically consistent manner. It results in two strictly hyperbolic systems describing phases dynamics. Another important feature is that the new model has improved physical capabilities. It is able, for example, to predict particle dispersion, while the conventional approach fails. These features are highlighted on several test problems involving particles jets dispersion and are compared against experimental data. With the help of a single parameter (a turbulent viscosity), excellent agreement is obtained for various experimental configurations studied by different authors [14].

5.1.3. Toward a thermal disequilibrium multiphase model for high explosives containing metallic particles

Participants: Gérard Baudin, Alexandre Lefrançois, Richard Saurel, Fabien Petitpas, Olivier Le Métayer, Jacques Massoni, Vladimir M. Belski, Eugène Zotov.

To investigate the effects of explosive composition on Al combustion, in particular regarding its oxygen balance, several liquid mixtures are experimentally studied with varying oxygen balance. They are then loaded with Al particles and the velocity of detonation (VOD) is recorded. Computational results with the help of conventional Chapman Jouguet (CJ) codes are compared but fail to reproduce experimental observations. A new multiphase flow model out of thermal equilibrium is then considered. Two options are considered as limiting cases : stiff thermal relaxation and vanishing heat exchange between Al and detonation products. With this last option, predictions are in excellent agreement with the experiments. This suggests that temperature disequilibrium plays a major role in heterogeneous explosives detonation dynamics [10].

5.1.4. The discrete equation method (DEM) for fully compressible, two-phase flows in ducts of spatially varying cross-section

Participants: Ray A Berry, Richard Saurel, Olivier Le Métayer.

For the simulation of light water nuclear reactor coolant flows, general two-phase models (valid for all volume fractions) have been generally used which, while allowing for velocity disequilibrium, normally force pressure equilibrium between the phases (see, for example, the numerous models of this type described by H. Städtke in [54]). These equations are not hyperbolic, their physical wave dynamics are incorrect, and their solution algorithms rely on dubious truncation error induced artificial viscosity to render them numerically well posed over a portion of the computational spectrum. The inherent problems of the traditional approach to multiphase modelling, which begins with an averaged system of (ill-posed) partial differential equations (PDEs) which are then discretized to form a numerical scheme, are avoided by employing a new homogenization method

known as the Discrete Equation Method (DEM), [28]. This method results in well-posed hyperbolic systems, this property being important for transient flows. This also allows a clear treatment of non-conservative terms (terms involving interfacial variables and volume fraction gradients) permitting the solution of interface problems without conservation errors, this feature being important for the direct numerical simulation of two-phase flows.

Unlike conventional methods, the averaged system of PDEs for the mixture are not used, and the DEM method directly obtains a well-posed discrete equation system from the single-phase conservation laws, producing a numerical scheme which accurately computes fluxes for arbitrary number of phases and solves non-conservative products. The method effectively uses a sequence of single phase Riemann problem solutions. Phase interactions are accounted for by Riemann solvers at each interface. Non-conservative terms are correctly approximated. Some of the closure relations missing from the traditional approach are automatically obtained. Lastly, the continuous equation system resulting from the discrete equations can be identified by taking the continuous limit with weak-wave assumptions. In this work, this approach is tested by constructing a DEM model for the flow of two compressible phases in one-dimensional ducts of spatially varying cross-section with explicit time integration. An analytical equation of state is included for both water vapor and liquid phases, and a realistic interphase mass transfer model is developed based on interphase heat transfer. A robust complement of boundary conditions are developed and discussed. Though originally conceived as a first step toward implicit time integration of the DEM method (to relieve time step size restrictions due to stiffness and to achieve tighter coupling of equations) in multidimensions, this model offers some unique capabilities for incorporation into next generation light water reactor safety analysis codes. We demonstrate, on a converging-diverging two-phase nozzle, that this well-posed, 2-pressure, 2-velocity DEM model can be integrated to a realistic and meaningful steady-state with both phases treated as compressible [11].

5.1.5. *Shallow water model for lakes with friction and penetration*

Participants: Nikolay V. Chemetov, Fernanda Cipriano, Sergey Gavriluk.

We consider the flow of an ideal fluid in a two-dimensional bounded domain, admitting flows through the boundary of this domain. The flow is described by the Euler equations with *non-homogeneous* Navier slip boundary conditions. We establish the solvability of this problem in the class of solutions with L_p -bounded vorticity, $p \in (1, \infty]$. To prove the solvability we realize the passage to the limit in Navier-Stokes equations with vanishing viscosity [12].

5.1.6. *Propagation of acoustic waves in porous media and their reflection and transmission at a pure fluid/porous medium permeable interface*

Participants: Angela Madeo, Sergey Gavriluk.

We find a sufficient condition of hyperbolicity for a system of partial differential equations governing the motion of a one-dimensional porous medium, so ensuring the well posedness of a solution for the associated Cauchy problem. We study propagation of linear waves in presence of a pure-fluid/porous-medium interface and we deduce novel expressions for the reflection and transmission coefficients in terms of the spectral properties of the governing differential system. We also propose an indirect method for measuring Biot's parameters when the measurement of the reflection and transmission coefficients associated to acoustic waves is possible [18].

5.1.7. *Mathematical and numerical model for nonlinear viscoplasticity*

Participants: Nicolas Favrie, Sergey Gavriluk.

A macroscopic model describing elastic-plastic solids is derived in a special case of the internal specific energy taken in separate form: it is the sum of a hydrodynamic part depending only on the density and entropy, and a shear part depending on other invariants of the Finger tensor. In particular, the relaxation terms are constructed compatible with the von Mises yield criteria. Also, the Maxwell type material behavior is shown up: the deviatoric part of the stress tensor is decaying during plastic deformations. Numerical examples show the ability of this model to deal with real physical phenomena [13].

5.1.8. Modelling dynamic and irreversible powder compaction

Participants: Richard Saurel, Nicolas Favrie, Fabien Petitpas, Marie-Hélène Lallemand, Sergey Gavrilyuk.

A multiphase hyperbolic model for dynamic and irreversible powder compaction is built. Three major issues have to be addressed in this aim. The first one is related to the irreversible character of powder compaction. When a granular media is subjected to a loading-unloading cycle the final volume is lower than the initial one. To deal with this hysteresis phenomenon a multiphase model with relaxation is built. During loading, mechanical equilibrium is assumed corresponding to stiff mechanical relaxation, while during unloading non-equilibrium mechanical transformation is assumed. Consequently, the sound speeds of the limit models are very different during loading and unloading. These differences in acoustic properties are responsible for irreversibility in the compaction process. The second issue is related to dynamic effects where pressure and shock waves play important role. Wave dynamics is guaranteed by the hyperbolic character of the equations. Each phase compressibility is considered, as well as configuration pressure and energy. The third issue is related to multidimensional situations that involve material interfaces. Indeed, most processes with powder compaction entail free surfaces. Consequently the model has to be able to solve interfaces separating pure fluids and granular mixtures. These various issues are solved by a unique model fitting the frame of multiphase theory of diffuse interfaces [48], [41], [49]. Model's ability to deal with these various effects is validated on basic situations, where each phenomenon is considered separately. Special attention is paid to the validation of the hysteresis phenomenon that occurs during powder compaction. Basic experiments on energetic material (granular HMX) and granular NaCl compaction are considered and are perfectly reproduced by the model. Excepting the materials equations of state (hydrodynamic and granular pressures and energies) that are determined on the basis of separate experiments found in the literature, the model is free of adjustable parameter. Its ability to reproduce the hysteresis phenomenon is due to a relaxation parameter that tends either to infinity in the loading regime, or to zero in the unloading stage. Discontinuous evolution of this relaxation parameter is explained [19], [27].

5.2. Approximation Methods

5.2.1. A numerical scheme for the Green-Naghdi model

Participants: Olivier Le Métayer, Sergey Gavrilyuk, Sarah Hank.

For this work, a hybrid numerical method using a Godunov type scheme is proposed to solve the Green-Naghdi model describing dispersive *shallow water* waves. The corresponding equations are rewritten in terms of new variables adapted for numerical studies. In particular, the numerical scheme preserves the dynamics of solitary waves. Some numerical results are shown and compared to exact and/or experimental ones in different and significant configurations. A dam break problem and an impact problem where a liquid cylinder is falling to a rigid wall are solved numerically. This last configuration is also compared with experiments leading to a good qualitative agreement [16].

6. Contracts and Grants with Industry

6.1. DGA

6.1.1. Modelling detonation waves in nano-structured energetic materials

Participants: Richard Saurel, Fabien Petitpas.

This study realized under DGA grant deals with the development of models and computational tools for nano-structured explosives. Comparative experiments are done at Nuclear Federal Center, Sarov, Russia.

6.1.2. Modelling liquid and particle dispersion under explosion phenomena

Participants: Jacques Massoni, Richard Saurel, Olivier Le Métayer, Eric Daniel, Julien Verhaegen.

This study realized under DGA grant, deals with the development of multiphase algorithms to compute the dispersion of a multiphase mixture in air and its interaction with detonation products.

6.1.3. Multiphase modelling of fluid–solid interaction

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

This study realized under DGA grant, deals with the development of a conservative elastic-plastic-fluid flow model to deal with fluid-solid coupling in extreme deformations. A collaboration with Prof. S.K. Godunov is also active in this area.

6.2. CNES and SNECMA : Multiphase flows in cryogenic space launcher engines

Participants: Olivier Le Métayer, Richard Saurel, Jacques Massoni, Fabien Petitpas.

Modelling and simulation of two-phase flows in cryogenic engine of space launchers (Ariane V) is the aim of this contract. A first contract is under realization with CNES. Another one with SNECMA. These two supports are aimed to continue during 4 years.

6.3. International collaboration

Scientific collaboration with the Lavrentyev Institute of Hydrodynamics in Russia: Nikolai Makarenko has been invited for one month staying in 2010.

6.4. Teaching

In the academic year 2009–2010, project members have taught the following courses :

Éric Daniel : Aix-Marseille I University : 138 h (partial discharge of education),

Polytech Engineering School : first and second year in *fluid mechanics* and *numerical methods in fluid dynamics*;

Master M2 : *two-phase dilute flows*.

Nicolas Favrie : Aix-Marseille I University : 192 h,

Polytech Engineering School : First, second and third year in *Mathematics, Structure modelling, Programming languages, Material resistance and concrete structure study in civil engineering*.

Sergey Gavrilyuk : Aix-Marseille III University : 192 h,

Master M1 : *mathematical methods for physicists, continuum mechanics*;

Master M2 : *two-phase flows modelling*.

Olivier Le Métayer : Aix-Marseille I University : 140h (in half delegation at CNRS),

Polytech Engineering School : First and second year in *mathematics, fluid mechanics* and *thermics*.

Jacques Massoni : Aix-Marseille I University : 192 h,

Polytech Engineering School : first, second and third year in *programming languages for scientific computing, fluid mechanics* and *numerical methods for fluid dynamics*;

Master M2 : *high performance computing*.

Fabien Petitpas : Aix-Marseille I University : 64 h,

Polytech Engineering School : First year in *Thermodynamics*.

Richard Saurel : Aix-Marseille I University : 16h (in delegation at INRIA),

Master M2 : *Heterogeneous flows*;

Polytech Engineering School : Fifth year in *Heterogeneous flows*.

6.5. Responsibilities

Éric Daniel : is still this year the Director of the Mechanical Engineering Department of Polytech Engineering School of Marseille with a partial discharge of education (96 hours).

Sergey Gavriluk : is Director of the Master M2 *Diphasic flows, Energetics and Combustion*.

Richard Saurel : is Director of the Doctoral School in Engineering Sciences, including all research units of Marseilles, Aix and Toulon in *Mechanics, Acoustics, Energetics, Macroscopic Physics, Micro and Nanoelectronics*. The laboratories are CNRS UMR and UPR units: LMA, IUSTI, IRPHE, M2P2, IM2NP. The doctoral school involves more than 300 researchers and 200 PhD students.

6.6. Ph.D thesis

This year, the project has harbored the following Ph. D Students :

Gregory Huber : Aix-Marseille University, RS2N-Région PACA grant ,
Modelling irreversible and dynamic compaction of powders, since 2008.

Laurent Munier : Aix-Marseille University and DGA Gramat, DGA financial support,
Experimental and numerical study of liquid and solid dispersion under explosion conditions.

Julien Verhaegen : Aix-Marseille University, DGA grant ,
Modelling multiphase explosions and dispersion phenomena, since 2007.

Sarah Hank : Aix-Marseille University, MRE support,
Modélisation et simulation numérique de la dispersion de fluides dans un milieu fortement hétérogène, since 2009.

Gaël Richard : Aix-Marseille University, salaried, (professor at the CPGE of "Lycée Notre Dame de Sion", Marseille,
Écoulements des eaux peu profondes avec effet de cisaillement, since 2009.

Sébastien Le Martelot : Aix-Marseille University, CNES-SNECMA support,
Simulation numérique directe de la crise d'ébullition dans les systèmes spatiaux , since November 1st 2010.

6.7. Invited Conferences

Members of the project team SMASH have delivered invited lectures and/or have been coorganizers in the following conferences , schools and/or seminars :

Sergey Gavriluk, Nicolas Favrie and Richard Saurel

- *ICMS, Mathematical challenges and modelling in hydroelasticity*, Edinburgh, United Kingdom, 21-24 Juin, 2010, [21];
(<http://www.icms.org.uk/downloads/hydro/Gavriluk.pdf>)
- *CANUM 2010*, Carcans-Maubuisson, May 31–June 4,2010 (S. Gavriluk only), [22];
(http://smai.emath.fr/canum2010/sql_conferenciers.php)
- *Advances in Continuum Mechanics*, Bohum, Germany, June 30–July 2, 2010 (S. Gavriluk only), [23];
(http://www.ruhr-uni-bochum.de/lam/ACMT_2010/downloads/ACMT-program.pdf)
- *International school "Variational methods in solid and fluid mechanics"*, CISM, July 2010 , Udine, Italy (S. Gavriluk has also co-organized that school), [24];

(http://www.unina2.it/doc/2010/avvisi/ateneo/cirm/dell_isola-gavriluk2_22.pdf)

- CIRM Workshop "Méthodes de domaine fictif pour des conditions aux limites immergées", August 30–September 3, Marseille, 2010;
- École d'été franco-allemande de l'UFA (Université Franco-Allemande) 2010 : Modélisation, simulation numérique et optimisation en mécanique des fluides : théorie et pratique, September 6–9 2010 (Nicolas Favrie has given an invited lecture on *Solid-fluid elasto-plastic diffuse interface model in cases of extreme deformations*, [20]); (<http://numhpc.math.kit.edu/schule.php>)

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Major publications by the team in recent years

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Publications of the year

Articles in International Peer-Reviewed Journal

- [10] G. BAUDIN, A. LEFRANÇOIS, R. SAUREL, F. PETITPAS, O. LE MÉTAYER, J. MASSONI, VLADIMIR M. BELSKI, E. ZOTOV. *Toward a thermal disequilibrium multiphase model for high explosives containing metallic particles*, in "Journal of Energetic Materials", 2010, vol. 18, p. 154–179, <http://www.informaworld.com/10.1080/07370651003776983>.
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- [20] N. FAVRIE. *Solid-fluid elasto-plastic diffuse interface model in cases of extreme deformations*, in "French-German UFA Summer School on Modelling, Numerical Simulation and Optimization in Fluid Mechanics", Karlsruhe, Germany, 2010, <http://numhpc.math.kit.edu/schule.php>.

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