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Project-Team SMASH

Simulation, modeling and analysis of heterogeneous systems

IN COLLABORATION WITH: Institut universitaire des systèmes thermiques industriels (IUSTI)

RESEARCH CENTER
Sophia Antipolis - Méditerranée

THEME
Computational models and simulation

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Project-Team SMASH

Keywords: Scientific Computation, Fluid Dynamics, Finite Elements

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 polluant 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 and Nicolas Favrie.*

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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 polluants 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.

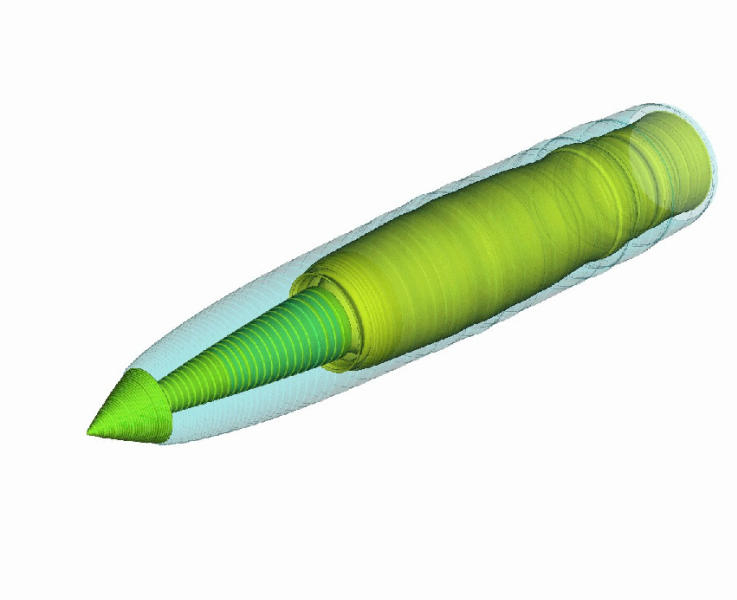

Figure 1. Numerical simulation of an underwater missile flying at 600 m/s. Three fluids are present : liquid water, steam and propulsion gases. Two different types of interfaces are present : a contact interface separates steam and combustion gases while an evaporating interface separates metastable 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 [43].

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 guarantied *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).

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 [47] and subtle remedy was given by [23]. 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 [42] 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], [24] that provide information easier to interprete 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.

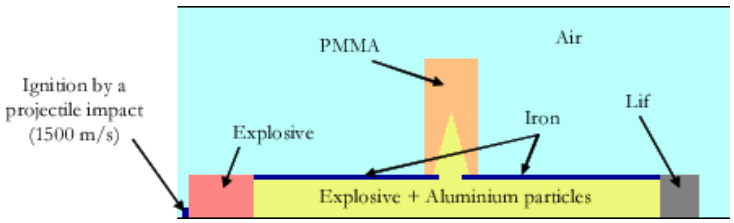

Figure 2. A steel tube is filled with a heterogeneous explosive. A high velocity impactor creates a shock wave passed onto the explosive, that becomes a detonation wave.

Most of these extensions are done with the help of the Hamilton principle of least action [46], [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 consits 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.

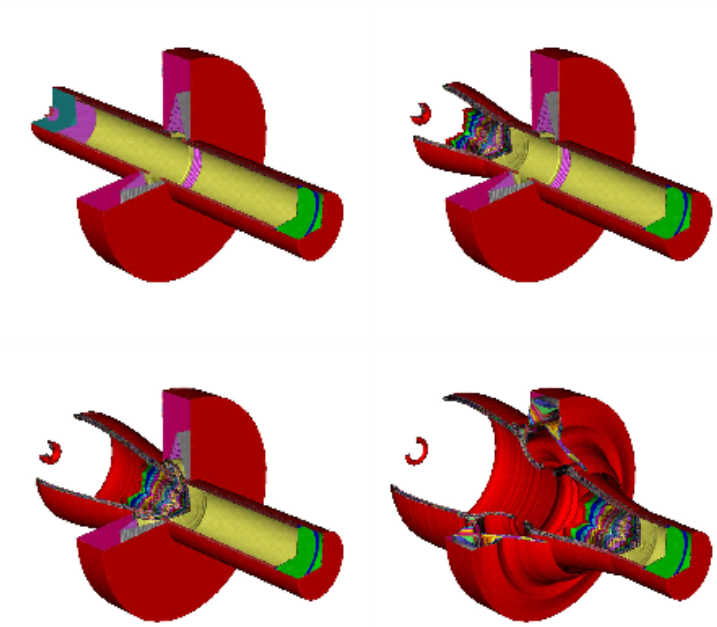

Figure 3. After a short period of time the shock wave becomes a detonation wave that produces gas and solid products at very high pressure. They set into intense motion solid tube walls. Two different types of mixture are present in this type of application : a physical one, corresponding to the mixture 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 [43]. Moreover, the detonation dynamics is checked against generalized CJ solutions [41], specifically determined for this temperature non-equilibrium model.

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 [35], [32] : 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 [28], nor interface reconstruction and so on. The same equations are solved everywhere [36], [37] 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 extentions have been done during these recent years by the SMASH team :

- a model involving *capillary*, *compressibility* and *viscous effects* [40]. 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;

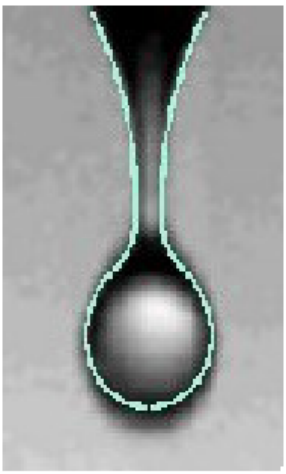

Figure 4. Comparison of the drop shape during formation (experiment in grey area, computations in lines). No interface tracking nor interface reconstruction method are used. The same equations are solved at each mesh point. The model accounts for compressible, viscous and capillary effects. The compressible 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.

- *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 Electrics, 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 [44], [30] and [29]. 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.

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 [39], and implemented in a parallel, three-dimensional code [38]. This model is able to reproduce phase separation and other complex phenomena [31];
- 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 [26], that has been persued last year [27];
- 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 [44], 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 [41].

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 [45] 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 [25], [34]. 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], [24].

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 [43]. 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 fulfiled 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 fulfiled by replacing at the shock front the internal energy equations by their corresponding jumps [44]. To ensure the numerical solution strictly follows the phase's Hugoniot curves, the poles of these curves are transported [41]. 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.

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

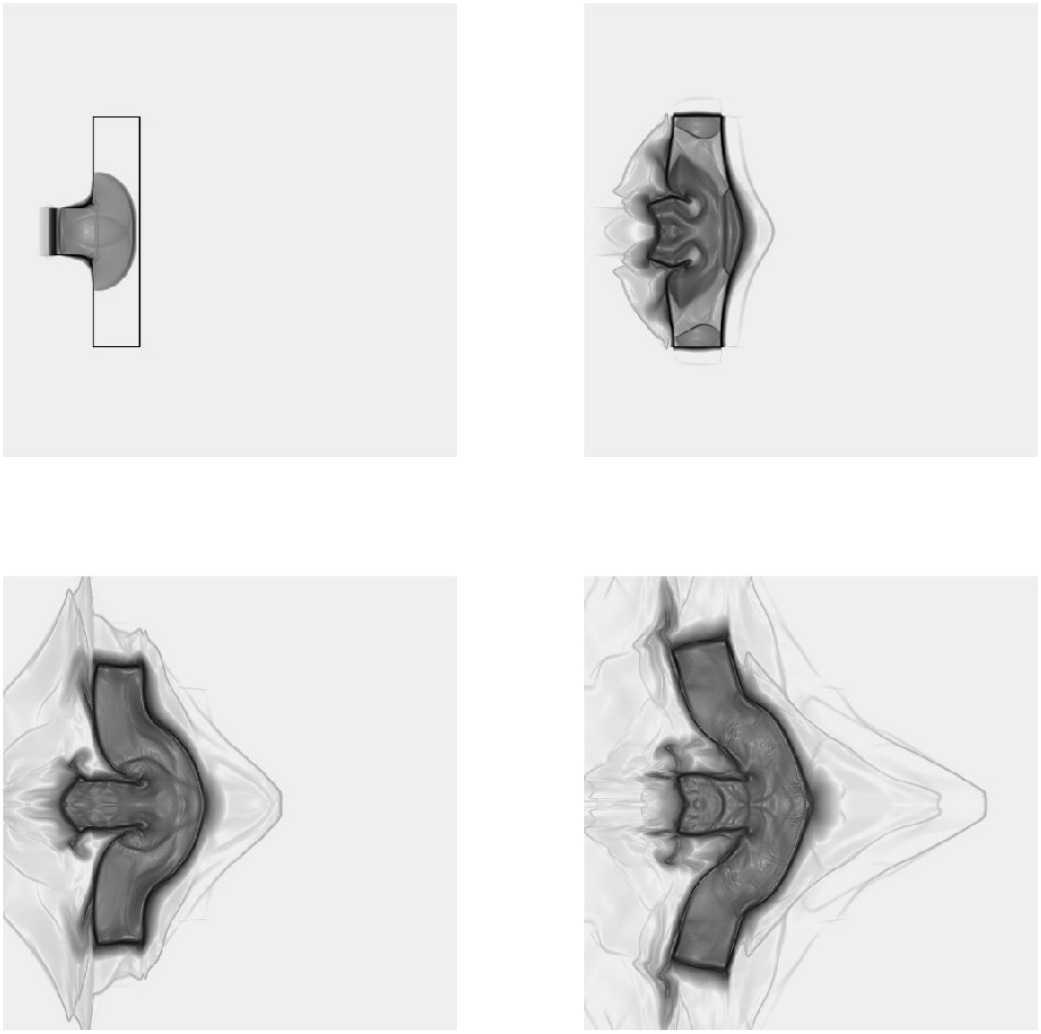

Figure 5. A copper projectile impacts a copper plate at the velocity of 800 m/s. Both materials are considered compressible and elastic, and are surrounded by air at atmospheric pressure.

schemes [33], [32]. 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 litterature 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 discontinuites.

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.

5. New Results

5.1. Mathematical Modelling

5.1.1. Mathematical and numerical model for nonlinear viscoplasticity

Participants: Nicolas Favrie, Sergey Gavrilyuk.

A macroscopic model describing elastic plastic solids is derived in a special case of the internal specificc energy taken in separable 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. In addition, Maxwell-type material behaviour is shown up: the deviatoric part of the stress tensor decays during plastic deformations. Numerical examples show the ability of this model to deal with real physical phenomena [15] .

5.1.2. A discrete model for compressible flows in heterogeneous media

Participants: Olivier Le Métayer, Alexandre 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 scales 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 etc.). Aircraft powerplant compartments are examples where topology is complex due to the presence of pipes, ducts, coolers and other equipment. Other important examples are gas explosions and large scale dispersion of hazardous materials in urban places, cities or underground 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 cell volumes including such obstacles. Quantitative comparisons between experimental and numerical results are shown for different significant test cases, showing excellent agreement [18].

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

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

Conventional modeling 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 dilute phase system. In the present work, we consider the addition of turbulent effects in both phases in a thermodynamically consistent way. It results in two strictly hyperbolic systems describing phase's 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 [17].

5.1.4. Diffuse interface model for compressible fluid - Compressible elastic-plastic solid interaction

Participants: Nicolas Favrie, Sergey Gavrilyuk.

An Eulerian hyperbolic diffuse interface model for elastic plastic solid fluid interaction is constructed. The system of governing equations couples Euler equations of compressible fluids and a visco-plastic model of Maxwell type materials (the deviatoric part of the stress tensor decreases during plastic deformations) in the same manner as models of multicomponent fluids. In particular, the model is able to create interfaces which were not present initially.

The model is thermodynamically compatible: it verifies the entropy inequality. However, a numerical treatment of the model is particularly challenging. Indeed, the model is non-conservative, so a special numerical splitting is proposed to overcome this difficulty. The numerical algorithm contains two relaxation procedures. One of them is physical and is related to the plastic relaxation mechanism (relaxation toward the yield surface). The second one is numerical. It consists in replacing the algebraic equation expressing a mechanical equilibrium between components by a partial differential equation with a short relaxation time. The numerical method was tested in one dimensional case (Wilkins' flying plate problem), two-dimensional plane case (impact of a projectile on a plate) and axisymmetrical case (Taylor test problem, impact with penetration effects, etc.). Numerical examples show the ability of the model to deal with real physical phenomena [13].

5.1.5. Criterion of hyperbolicity for non-conservative quasilinear systems admitting a partially convex conservation law

Participants: Alain Forestier, Sergey Gavrilyuk.

A system of conservation laws admitting an additional convex conservation law can be written as a symmetric t-hyperbolic in the sense of Friedrichs system. However, in mathematical modeling of complex physical phenomena, it is customary to use non-conservative hyperbolic models. We generalize the Godunov Friedrichs Lax approach to this new class of models [16].

5.1.6. A new model of roll waves: comparison with Brock's experiments

Participants: Gaël Richard, Sergey Gavrilyuk.

We derive a mathematical model of shear flows of shallow water down an inclined plane. Periodic stationary solutions to this model describing roll waves were obtained. The solutions are in good agreement with experimental profiles of roll waves measured in Brock's experiments (1967). In particular, the height of the vertical front of the waves, the shock thickness and the wave amplitude are well captured by the model [21].

5.1.7. Modelling gas dynamics in one-dimensional ducts with abrupt area change

Participants: R Menina, Richard Saurel, M Zereg, Lazhar Houas.

Most gas dynamic computations in industrial ducts are done in one dimension with cross-section-averaged Euler equations. This poses a fundamental difficulty as soon as geometrical discontinuities are present. The momentum equation contains a non-conservative term involving a surface pressure integral, responsible for momentum loss. Definition of this integral is very difficult from a mathematical standpoint as the flow may contain other discontinuities (shocks, contact discontinuities). From a physical standpoint, geometrical discontinuities induce multidimensional vortices that modify the surface pressure integral. In the present paper, an improved one-dimensional flow model is proposed. An extra energy (or entropy) equation is added to the Euler equations expressing the energy and turbulent pressure stored in the vortices generated by the abrupt area variation. The turbulent energy created by the flow area change interaction is determined by a specific estimate of the surface pressure integral. Model's predictions are compared with two-dimensional averaged results from numerical solution of the Euler equations. Comparison with shock tube experiments is also presented. The new one dimensional averaged model improves the conventional cross-section-averaged Euler equations and is able to reproduce the main flow features [19].

5.2. Applications for specific flow problems

5.2.1. Modelling cavitating flow around underwater missiles

Participants: Fabien Petitpas, Richard Saurel, B.K. Ahn, S. Ko.

The diffuse interface model of Saurel et al. [9] is used for the computation of compressible cavitating flows around underwater missiles. Such systems use gas injection and natural cavitation to reduce drag effects. Consequently material interfaces appear, separating liquid and gas. These interfaces may have a really complex dynamics such that only a few formulations are able to predict their evolution. Contrarily to front tracking or interface reconstruction method the interfaces are computed as diffused numerical zones, that are captured in a routinely manner, as is done usually with gas dynamics solvers for shocks and contact discontinuity. With the present approach, a single set of partial differential equations is solved everywhere, with a single numerical scheme. This leads to very efficient solvers. The algorithm derived in Saurel et al. [43] is used to compute cavitation pockets around solid bodies. It is first validated against experiments done in cavitation tunnel at CNU. Then it is used to compute flows around high speed underwater systems (Shkval-like missile). Performance data are then computed showing method ability to predict forces acting on the system [20].

5.2.2. Propagation of a planar shock wave through a two-phase gas-liquid medium

Participants: Alain Chauvin, Georges Jourdan, Éric Daniel, Lazhar Houas, R Tosello.

We conducted a series of shock tube experiments to study the influence of a cloud of water droplets on the propagation of a planar shock wave. In a vertically oriented shock tube, the cloud of droplets was released downwards into the air at atmospheric pressure while the shock wave propagated upwards. Two shock wave Mach numbers, 1.3 and 1.5, and three different heights of clouds, 150 mm, 400 mm, and 700 mm, were tested with an air-water volume fraction and a droplet diameter fixed at 1.2 % and 500 μm, respectively. From high-speed visualization and pressure measurements, we analyzed the effect of water clouds on the propagation of the shock wave. It was shown that the pressure histories recorded in the two-phase gas-liquid mixture are different from those previously obtained in the gas-solid case. This different behavior is attributed to the process of atomization of the droplets, which is absent in the gas-solid medium. Finally, it was observed that the shock wave attenuation was dependent on the exchange surface crossed by the shock combined with the breakup criterion [12].

6. Contracts and Grants with Industry

6.1. Contracts with Industry

6.1.1. DGA - Multiphase modelling of fluid–solid interaction

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

The aim of this study, supported by a DGA grant, is to get a conservative elastic-plastic-fluid flow model to deal with fluid-fluid coupling in extreme deformations. An active collaboration with Prof. S.K. Godunov is still active in this area.

6.1.2. CNES-SNECMA grants - Multiphase flows in cryogenic space launcher engines

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

The aim of 4-years grant (3 years remaining), supported by CNES and SNECMA, is concerned with both modelling and simulation of two-phase flows in cryogenic engine of space launchers (Ariane V).

7. Partnerships and Cooperations

7.1. International Initiatives

7.1.1. INRIA International Partners

Scientific collaboration with the Lavrentyev Institute of Hydrodynamics in Russia.

8. Dissemination

8.1. Animation of the scientific community

Reviewing activities in the following international journals :

- Journal of Fluid Mechanics
- Physics of Fluids
- Journal of Computational Physics
- International Journal of Multiphase Flows
- International Journal of Shock Waves
- International Journal of Numerical Methods in Fluids
- Combustion Theory and Modelling
- FUEL
- Journal of Scientific Computing
- European Journal European of Mechanics B/Fluids
- Continuum Mechanics and Thermodynamics
- Journal of Engineering Mathematics
- Mathematical Reviews

8.2. Teaching

1. ÉRIC DANIEL :

   Polytech Engineering school: *Fluid Mechanics (perfect gas)*, *Compressible Fluid Mechanics*, *Numerical Methods for for the engineer* and *Two-phase gas-particle flows*, 144 h, respectively first, second, first and second year, Aix-Marseille University, France.

2. NICOLAS FAVRIE :

   Polytech Engineering school and Licence: *Structure modelling*, *Programming languages*, *Material resistance and concrete structure study in civil engineering* and *Engineering science initiation*, 240 h, first, second and third year and L1, Aix-Marseille University, France.

3. SERGEY GAVRILYUK :

   Master: *Mathematical methods for physicists*, *Continuum mechanics* and *Two-phase flow modelling*, 192 h, M1 and M2, Aix-Marseille University, France.

4. OLIVIER LE MÉTAYER :

   Polytech Engineering School: *Mathematics*, *Fluid mechanics* and *Thermics*, 192 h, first and second year, Aix-Marseille University, France.

5. JACQUES MASSONI :

   Polytech Engineering school, Master: *Programming languages for scientific computing*, *Fluid mechanics*, *Numerical methods for fluid dynamics* and *High performance computing*, 192 h, first, second and third year and M2, Aix-Marseille University, France.

6. FABIEN PETITPAS :

   Polytech Engineering school: *Thermodynamics*, *C programming language* and *Supervision of final study internship*, first, third and fifth year, Aix-Marseille University, France.

7. RICHARD SAUREL :

   Polytech Engineering school, Master: *Heterogeneous flows*,fifth year and M2, Aix-Marseille University, France.

PhD & HdR :

PhD : Julien Verhaegen, *Modélisation multiphasique d'écoulements et de phénomènes de dispersion issus d'explosion*, Université d'Aix-Marseille, April 15th 2011, Éric Daniel [11].

PhD : Laurent Munier, *Simulations expérimentales et numériques des effets retardés d'une explosion en milieu clos et en présence de produits liquides*, Université d'Aix-Marseille, December 11th 2011, Richard Saurel [10].

PhD in progress : Gregory Huber, *Modelling irreversible and dynamic compaction of powders*, 2008, Richard Saurel.

PhD in progress : Sarah Hank, *Modélisation et simulation numérique de la dispersion de fluides dans un milieu fortement hétérogène*, 2009, Olivier Le Métayer.

PhD in progress : Gaël Richard, *Écoulements des eaux peu profondes avec effet de cisaillement*, 2009, Sergey Gavrilyuk.

PhD in progress : Sébastien Le Martelot, *Simulation numérique directe de la crise d'ébullition dans les systèmes spatiaux*, 2010, Richard Saurel.

PhD in progress : Serge Ndanou, *Interface problems between fluids and elastic-plastic media*, 2011, Sergey Gavrilyuk and Philippe Angot.

8.3. Responsabilities

Éric Daniel: Director of the Mechanical Engineering Department of the Polytech Engineering School of Marseille with a partial discharge of eduaction.

Nicolas Favrie: Head teacher of international relations for the Civil Engineering Department.

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

Richard Saurel: Director of the Doctoral School in Engineering Sciences (which includes all research units of Marseille, Aix en Provence and Toulon, in *Mechanics, Acoustics, Energetics, Macroscopic Physics, Micro and Nanoelectronics*). The laboratories involved are CNRS UMR and UPR units (LMA, IUSTI, IRPHE, M2P2, IM2NP), with a total of more than 300 researchers and about 200 PhD students.

9. Bibliography

Major publications by the team in recent years

[1] R. ABGRALL, R. SAUREL. *Discrete equations for physical and numerical compressible multiphase mixtures*, in "Journal of Computational Physics", 2003, vol. 186, n^{o} 2, p. 361–396, http://dx.doi.org/10.1016/S0021-9991(03)00011-1.

[2] S. GAVRILYUK, N. FAVRIE, R. SAUREL. *Modeling wave dynamics of compressible elastic materials*, in "Journal of Computational Physics", 2008, vol. 227, p. 2941–2969, http://dx.doi.org/10.1016/j.jcp.2007.11.030.

[3] S. GAVRILYUK, R. SAUREL. *Mathematical and numerical modeling of two-phase compressible flows with micro-inertia*, in "Journal of Computational Physics", 2002, vol. 175, n^{o} 1, p. 326–360, http://dx.doi.org/10.1006/jcph.2001.6951.

[4] H. GUILLARD, F. DUVAL. *A Darcy law for the drift velocity in a two-phase model*, in "J. Comput. Phys.", 2007, vol. 224, p. 288–313, http://dx.doi.org/10.1016/j.jcp.2007.02.025.

[5] M.-H. LALLEMAND, A. CHINNAYYA, O. LE MÉTAYER. *Pressure relaxation procedures for multiphase compressible flows*, in "Int. J. Numer. Meth. Fluids", 2005, vol. 49, n^{o} 1, p. 1–56, http://dx.doi.org/10.1002/fld.967.

[6] O. LE MÉTAYER, J. MASSONI, R. SAUREL. *Modelling evaporation fronts with reactive Riemann solvers*, in "Journal of Computational Physics", 2005, vol. 205, n^{o} 2, p. 567–610, http://dx.doi.org/10.1016/j.jcp.2004.11.021.

[7] R. SAUREL, R. ABGRALL. *A Multiphase Godunov method for compressible Multifluid and Multiphase flows*, in "Journal of Computational Physics", 1999, vol. 150, p. 425–467, http://dx.doi.org/10.1006/jcph.1999.6187.

[8] R. SAUREL, S. GAVRILYUK, F. RENAUD. *A multiphase model with internal degree of freedom : Application to shock bubble interaction*, in "Journal of Fluid Mechanics", 2003, vol. 495, p. 283-321, http://dx.doi.org/10.1017/S002211200300630X.

[9] R. SAUREL, F. PETITPAS, RÉMI. ABGRALL. *Modeling phase transition in metastable liquids. Application to flashing and cavitating flows*, in "Journal of Fluid Mechanics", 2008, vol. 607, p. 313–350, http://dx.doi.org/10.1017/S0022112008002061.

Publications of the year

Doctoral Dissertations and Habilitation Theses

[10] L. MUNIER. *Simulations expérimentales et numériques des effets retardés d'une explosion en milieu clos et en présence de produits liquides*, Aix-Marseille University, December 11th 2011.

[11] J. VERHAEGEN. *Modélisation multiphasique d'écoulements et de phénomènes de dispersion issus d'explosion*, Aix-Marseille University, April 15th 2011.

Articles in International Peer-Reviewed Journal

[12] A. CHAUVIN, G. JOURDAN, É. DANIEL, L. HOUAS, R. TOSELLO. *Experimental investigation of the propagation of a planar shock wave through a two-phase gas-liquid medium*, in "Physics Of Fluids", 2011, vol. 23, http://dx.doi.org/10.1063/1.3657083.

[13] N. FAVRIE, S. GAVRILYUK. *Diffuse interface model for compressible fluid - compressible elastic-plastic solid interaction*, in "Journal of Computational Physics", 2011, accepted, http://dx.doi.org/10.1016/j.jcp.2011.11.027.

[14] N. FAVRIE, S. GAVRILYUK. *Dynamics of shock waves in elastic-plastic solids*, in "ESAIM Proceedings", 2011, vol. 33, p. 50–67, to appear.

[15] N. FAVRIE, S. GAVRILYUK. *Mathematical and numerical model for nonlinear viscoplasticity*, in "Philosophical Transactions of the Royal Society A", 2011, vol. 369, p. 2864–2880, http://dx.doi.org/10.1098/rsta.2011.0099.

[16] A. FORESTIER, S. GAVRILYUK. *Criterion of hyperbolicity for non-conservative quasilinear systems admitting a partially convex conservation law*, in "Mathematical Methods in the Applied Sciences", 2011, vol. 34, p. 2148–2158, http://dx.doi.org/10.1002/mma.1512.

[17] S. HANK, R. SAUREL, O. LE MÉTAYER. *A hyperbolic Eulerian model for dilute two-phase suspensions*, in "Journal of Modern Physics", 2011, vol. 2, p. 997–1011, http://dx.doi.org/10.4236/jmp.2011.29120.

[18] O. LE MÉTAYER, A. MASSOL, N. FAVRIE, S. HANK. *A discrete model for compressible flows in heterogeneous media*, in "Journal of Computational Physics", 2011, vol. 230, p. 2470–2495, http://dx.doi.org/10.1016/j.jcp.2010.12.020.

[19] R. MENINA, R. SAUREL, M. ZEREG, L. HOUAS. *Modelling gas dynamics in 1D ducts with abrupt area change*, in "International Journal of Shock Waves", 2011, vol. 21, p. 451–466, http://dx.doi.org/10.1007/s00193-011-0321-3.

[20] F. PETITPAS, R. SAUREL, B.K. AHN, S. KO. *Modelling cavitating flow around underwater missiles*, in "International Journal of Naval Architecture and Ocean Engineering", 2011, accepted.

[21] G. RICHARD, S. GAVRILYUK. *A new model of roll waves: comparison with Brock's experiments*, in "Journal of Fuid Mechanics", 2011, submitted.

Scientific Books (or Scientific Book chapters)

[22] F. DELL'ISOLA, S. GAVRILYUK. *Variational Models and Methods in Solid and Fluid Mechanics*, CISM Courses and Lectures, Springer, Wien, New York, 2012, vol. 535.

References in notes

[23] M. BAER, J. NUNZIATO. *A two-phase mixture theory for the deflagration-to-detonation transition* (DDT) *in reactive granular materials.*, in "Int. J. of Multiphase Flows", 1986, vol. 12, p. 861–889.

[24] A. CHINNAYYA, É. DANIEL, R. SAUREL. *Modelling detonation waves in heterogeneous energetic materials*, in "Journal of Computational Physics", 2004, vol. 196, p. 490–538, http://dx.doi.org/10.1016/j.jcp.2003.11.015.

[25] G. DALMASO, P. LEFLOCH, F. MURAT. *Definition and weak stability of non-conservative products*, in "Journal de Mathématiques Pures et Appliquées", 1995, vol. 74, n^{o} 6, p. 483–548.

[26] N. FAVRIE. *Un modèle d'interfaces diffuses pour l'interaction solide–fluide dans le cas des grandes déformations*, Université de Provence, December 1rst, 2008.

[27] N. FAVRIE, S. GAVRILYUK, R. SAUREL. *Solid-fluid diffuse interface model in cases of extreme deformations*, in "Journal of Computational Physics", 2009, vol. 228, n^{o} 16, p. 6037–6077, http://dx.doi.org/10.1016/j.jcp.2009.05.015.

[28] R.P. FEDKIW, T. ASLAM, B. MERRIMAN, S. OSHER. *A Non-oscillatory Eulerian Approach to Interfaces in Multimaterial Flows (the Ghost-Fluid Method)*, in "Journal of Computational Physics", 1999, vol. 152, p. 457–492(36), http://www.ingentaconnect.com/content/ap/cp/1999/00000152/00000002/art06236.

[29] S. GAVRILYUK, R. SAUREL. *Estimation of the turbulent energy production across a shock wave*, in "Journal of Fluid Mechanics", 2006, vol. 549, p. 131–139, http://dx.doi.org/10.1017/S0022112005008062.

[30] S. GAVRILYUK, R. SAUREL. *Rankine-Hugoniot relations for shocks in heterogeneous mixtures*, in "Journal of Fluid Mechanics", 2007, vol. 575, p. 495–507, http://dx.doi.org/10.1017/S0022112006004496.

[31] H. GUILLARD, M. LABOIS, M. GRANDOTTO. *A five-equation dissipative model for two-phase flows*, in "5th International Symposium on Finite Volumes for Complex Applications. - Problems and Perspectives", HERMES, 2008.

[32] H. GUILLARD, A. MURRONE. *On the behavior of upwind schemes in the low Mach number limit : II. Godunov type schemes*, in "Computers and Fluids", 2004, vol. 33, n^{o} 4, p. 655–675.

[33] H. GUILLARD, C. VIOZAT. *On the behaviour of upwind schemes in the low Mach number limit*, in "Computers and Fluids", 1999, vol. 28, n^{o} 1, p. 63–86, http://dx.doi.org/10.1016/S0045-7930(98)00017-6.

[34] T.Y. HOU, P. LEFLOCH. *Why non-conservative schemes converge to the wrong solution: Error analysis*, in "Math. of Comput.", 1994, vol. 62, p. 497–530.

[35] A. KAPILA, R. MENIKOFF, J. BDZIL, S. SON, D. S. STEWART. *Two-phase modeling of* DDT *in granular materials : reduced equations.*, in "Physics of Fluids", 2001, vol. 13, n^{o} 10, p. 3002–3024, http://dx.doi.org/10.1063/1.1398042.

[36] S. KARNI. *Multicomponent Flow Calculations by a Consistent Primitive Algorithm*, in "Journal of Computational Physics", 1994, vol. 112, p. 31–43, http://dx.doi.org/10.1006/jcph.1994.1080.

[37] S. KARNI. *Hybrid Multifluid Algorithms*, in "SIAM Journal of Scientific Computing", 1996, vol. 17, n^{o} 5, p. 1019–1039, http://dx.doi.org/10.1137/S1064827595280003X.

[38] T. KLOCZKO. *Concept, architecture and performance study for a parallel code in CFD*, in "20th International Conference on Parallel Computational Fluid Dynamics", Lyon (France), May 19–22 2008.

[39] M. LABOIS. *Modélisation des déséquilibres mécaniques dans les écoulements diphasiques : approches par relaxation et par modèle réduit*, Université de Provence, October 31rst, 2008, http://tel.archives-ouvertes.fr/docs/00/33/88/18/PDF/these_Mathieu_Labois_2008.pdf.

[40] G. PERIGAUD, R. SAUREL. *A compressible flow model with capillary effects*, in "Journal of Computational Physics", 2005, vol. 209, p. 139–178, http://dx.doi.org/10.1016/j.jcp.2005.03.018.

[41] F. PETITPAS, R. SAUREL, E. FRANQUET, A. CHINNAYYA. *Modelling detonation waves in condensed energetic materials : Multiphase CJ conditions and multidimensional computations*, in "Shock Waves", 2009, vol. 19, n^{o} 5, p. 377–401, http://dx.doi.org/10.1007/s00193-009-0217-7.

[42] R. SAUREL, R. ABGRALL. *A simple method for compressible multifluid flows*, in "SIAM J. Sci. Comp.", 1999, vol. 21, n^{o} 3, p. 1115–1145.

[43] R. SAUREL, F. PETITPAS, R. A. BERRY. *Simple and efficient relaxation methods for interfaces separating compressible fluids, cavitating flows and shocks in multiphase mixtures*, in "Journal of Computational Physics", 2009, vol. 228, n^{o} 5, p. 1678–1712, http://dx.doi.org/10.1016/j.jcp.2008.11.002.

[44] R. SAUREL, O. LE MÉTAYER, J. MASSONI, S. GAVRILYUK. *Shock jump relations for multiphase mixtures with stiff mechanical relaxation*, in "International Journal of Shock Waves", 2007, vol. 16, n^{o} 3, p. 209–232, http://dx.doi.org/10.1007/s00193-006-0065-7.

[45] L. SCHWARTZ. *Sur l'impossibilité de la multiplication des distributions*, in "C.R.A.S. Paris", 1954, vol. I-239, p. 847–848.

[46] D. SERRE. *Sur le principe variationnel des équations de la mécanique des fluides compressibles*, in "M2AN", 1993, vol. 27, n^{o} 6, p. 739–758.

[47] H. STEWART, B. WENDROFF. *Two-phase flow : Models and methods*, in "Journal of Computational Physics", 1984, vol. 56, p. 363–409.