Modélisation numérique des interfaces liquide-vapeur dans les écoulements

Numerical Modeling of Liquid-Vapor Interfaces in Fluid Flows

Atelier scientifique
Lundi 12 et mardi 13 décembre 2016
Institut Henri Poincaré, Amphi Hermite, Paris

Conférenciers invités

- Marie Béchereau (Ecole normale supérieure Paris-Saclay)
- Guillaume Bois (CEA, Paris-Saclay)
- Hélène Mathis (Université de Nantes)
- Gérard Liger-Belair (Université de Reims Champagne-Ardenne)
- Richard Saurel (Université d'Aix-Marseille)
- Arthur Talpaert (CEA et Ecole Polytechnique, Paris-Saclay)
- Laurette Tuckerman (ESPCI, Paris)
- Stéphane Zaleski (Université Pierre et Marie Curie, Paris)

Organisation

- Stéphane Dellacherie (CEA Saclay et Polytechnique Montréal)
- François Dubois (CNAM Paris et Université Paris Sud)
- Stéphan Fauve (Ecole normale supérieure, Paris)
- Renée Gatignol (Université Pierre et Marie Curie, Paris)

Workshop on Numerical Modeling of Liquid-Vapor Interfaces in Fluid Flows
Institut Henri Poincaré, 12 - 13 december 2016
Amphi Hermite
Sponsors : ***SMAI, GDR Turbulence***

Monday 12 december

8h30 – 9h00	**Welcome**
9h00 – 9h45	Gérard Liger-Belair
	Effervescence in champagne and sparkling wines: Recent advances and future prospects
9h45 – 10h30	Arthur Talpaert
	Direct Numerical Simulation of Bubbles with Adaptive Mesh Refinement with Distributed Algorithms
10h30 – 11h00	**Pause**
11h00 – 11h30	Daniel Fuster
	Numerical simulations of gas/vapor bubble oscillations
11h30 – 12h00	Dena Kazerani
	Simulation of free surface fluids in incompressible dynamics
12h00 – 12h30	Sébastien Tanguy
	Direct Numerical Simulation of Liquid-Vapor Phase Change. Applications to Leidenfrost Droplet and Nucleate Boiling
12h30 – 14h15	**Lunch**
14h15 – 15h00	Stéphane Zaleski
	Numerical simulation of flows with sharp interfaces by the Volume-Of-Fluid method
15h00 – 15h45	Guillaume Bois
	Applications of the Front-Tracking algorithm of TrioCFD to turbulent bubbly flows in plane channels
15h45 – 16h30	**Pause**
16h30 – 17h00	Elie Hachem
	High fidelity anisotropic adaptive FEM towards physical couplings occurring in turbulent boiling
17h00 – 17h30	Francois-Xavier Demoulin

Modelling atomization with phase change

17h30 – 18h00 Rémi Abgrall

Locally conservative approximation of (conservative) systems written in non conservation form: application to Lagrangian hydrodynamics and multifluid problems

18h00 End of Day 1

Tuesday 13 december

9h00 – 9h45 Hélène Mathis

Modelling liquid-vapor phase change with metastable states

9h45 – 10h30 Richard Saurel

Diffuse interfaces with compressible fluids, phase transition and capillarity

10h30 – 11h00 Pause

11h00 – 11h45 Laurette Tuckerman

Numerical simulation of Faraday wave patterns

11h45 – 12h30 Marie Béchereau

Lagrange-Euler Lattice-Boltzmann Method And Its Application to Two-Fluid Flows Dynamics With Possibly High Density Ratio

12h30 – 14h30 **Lunch**

14h30 – 15h00 Laurent Martin Witkowski

Benchmarking rotating flow with free surface deformation

15h00 – 15h30 Saira Pineda

Numerical simulation of a gas bubble collapse using the SPH-ALE method

15h30 – 16h00 Bérénice Grec

Simulations of a heated fluid at low Mach number: modelling of phase transition and numerical strategies

16h00 – 16h30 **Pause**

16h30 – 17h00 End of Day 2

Locally conservative approximation of (conservative) systems written in non conservation form: application to Lagrangian hydrodynamics and multifluid problems

R. Abgrall and S. Tokareva
Institute of Mathematics, University of Zurich, Switzerland

Since the celebrated Lax Wendroff theorem, it is known that the right way of discretising systems of hyperbolic equations written in conservation form is to use a flux formulation. However, in many occasions, the relevant formulation, from an engineering point of view, is not to consider this conservative formulation but one non conservative form. For example, with standard notations, a one fluid model writes

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\mathbf{u}\\ E\end{pmatrix} + \text{ div }\begin{pmatrix}\rho\mathbf{u}\\ \rho\mathbf{u}\otimes\mathbf{u}+p\text{Id}\\ (E+p)\mathbf{u}\end{pmatrix} = 0, \tag{1}$$

but the interesting quantities are the mass, velocity and pressure, which evolution is described by:

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho\mathbf{u}\\ p\end{pmatrix} + \begin{pmatrix}\text{div }\rho\mathbf{u}\\ \text{div }(\rho\mathbf{u}\otimes\mathbf{u}+p\text{Id})\\ \mathbf{u}\cdot\nabla p+\rho c^2\text{ div }\mathbf{u}\end{pmatrix} = 0 \tag{2}$$

Unfortunately this form is not suitable to approximation. In the case of a multi-fluid system, the same problem occurs.

In this talk, we will describe a method to overcome this issue. It does not use any flux formulation *per se*, but can be shown to provide the right solutions. In order to illustrate the method, we will consider several examples in Eulerian and Lagrangian hydrodynamics

We will first start from the Residual Distribution (RD) (re-)interpretation of the Dobrev et al. scheme [1] for the numerical solution of the Euler equations in Lagrangian form. The first ingredient of the original scheme is the staggered grid formulation which uses continuous node-based finite element approximations for the kinematic variables and cell-centered discontinuous finite elements for the thermodynamic parameters. The second ingredient of the Dobrev et al. scheme is an artificial viscosity technique applied in order to make possible the computation of strong discontinuities. Using a reformulation in term of RD scheme, we can show that the scheme is indeed locally conservative while the formulation is *stricto sensu* non conservative. Using this, we can generalise the construction and develop locally conservative artificial viscosity free schemes. To demonstrate the robustness of the proposed RD scheme, we solve several one-dimensional shock tube problems from rather mild to very strong ones: we go from the classical Sod problem, to TNT explosions (with JWL EOS) via the Collela-Woodward blast wave problem.

In a second part, we show how to extend this method to the Eulerian framework and give applications on single fluid and multiphase problems via the five equation model.

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[1] V. Dobrev, T. Kolev, and R. Rieben. High order curvilinear finite element methods for Lagrangian hydrodynamics. *SIAM J. Sci. Comput*, 34:B606–B641, 2012.

Lagrange-Euler Lattice-Boltzmann Method and its application to two-fluid flows dynamics with possibly high density ratio

Marie Béchereau, Florian De Vuyst
CMLA CNRS UMR 8536, ENS Cachan*
bechereau@cmla.ens-cachan.fr

Two-fluid extensions of Lattice Boltzmann methods with free boundaries usually consider "microscopic" pseudopotential interface models. In this paper, we rather propose an interface-capturing Lattice Boltzmann approach where the mass fraction variable is considered as an unknown and is advected. Several works have reported the difficulties of LBM methods to deal with such two-fluid systems especially for high-density ratio configurations. This is due to the mixing nature of LBM, as with Flux vector splitting approaches for Finite Volume methods. We here give another explanation of the lack of numerical diffusion of Lattice Boltzmann approaches to accurately capture contact discontinuities. To fix the problem, we propose an arbitrary Lagrangian-Eulerian (ALE) formulation of Lattice-Boltzmann methods. In the Lagrangian limit, it allows for a proper separated treatment of pressure waves and advection phenomenon. After the ALE solution, a remapping (advection) procedure is necessary to project the variables onto the Eulerian Lattice-Boltzmann grid.

We explain how to derive this remapping procedure in order to get second-order accuracy and achieve sharp stable oscillation-free interfaces. It that be shown that mass fractions variables satisfy a local discrete maximum principle and thus stay in the range $[0, 1]$. The theory is supported by numerical computations of rising bubbles (without taking into account surface tension at this current state of development).

Even if our methods are currently used for inviscid flows (Euler equations) by projecting the discrete distributions onto equilibrium ones at each time step, we believe that it is possible to extend the framework formulation for multifluid viscous problems. This will be at the aim of a next work.

Acknowledgements

This work is supported by the Grant RDM IdF program, and is part of the ENS Cachan CUDA Research Center project.

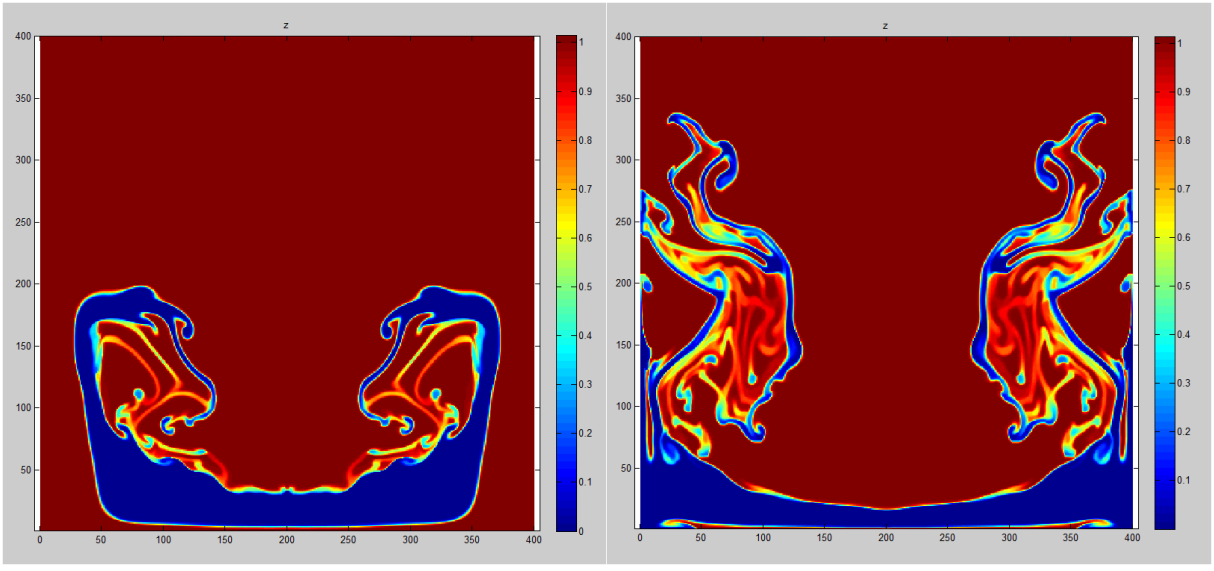

Figure 1: Free fall of an initial square block of a dense fluid surrounded by a lighter fluid into a box

*61, avenue du Président Wilson 94235 Cachan cedex France

Applications of the Front-Tracking algorithm of TrioCFD to turbulent bubbly flows in plane channels.

Guillaume BOIS

DEN-Service de thermo-hydraulique et de mécanique des fluides (STMF)

CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France

Description:

The Front-Tracking method has been implemented in TrioCFD and improved over the last decade. It has been widely used on large parallel architectures to study incompressible two-phase flows. The permanent increase in computing capabilities allows to perform simulations of fully turbulent bubbly flows in relatively small periodic domains. This talk will be organized in two parts. The numerical method used to perform Front-Tracking simulations will be presented. The code is capable to deal with phase change and specific Ghost-Fluid Methods have been implemented to guarantee a great accuracy of the solution, even in the presence of large jumps and phase change.

Then, recent calculations on adiabatic two-phase turbulent bubbly flows will be presented. Averaged results are analyzed in great details in order to better understand the dominant processes in the exchange mechanisms at the interface and in the modulation of turbulence by the vapor inclusions and their wakes. Preliminary results and suggestions for the two-fluid model will conclude the presentation.

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Modelling atomization with phase change

DNS[1], LES [2] and RANS [3] modelling of atomization have been developed for the last decade in our laboratory with a particular attention devoted on the behavior of the interface. In particular model equations for the liquid-gas surface density have been proposed based on the pioneering work of Borghi and Vallet [4]. The purpose of this approach is to determine the surface density that we believe is the first order parameter to determine the mass transfer rate, a key future of fuel injection system. In addition to well-developed procedures usually used to evaluate the vaporization rate for dispersed spray based on the resolution of Boltzmann-Williams kinetic equation, our focus has been to determine the phase change rate for any kind of interface geometry not only spherical droplet. To do so the interface capturing DNS code Archer has been extended to handle heat and mass transfer at the interface based on the method proposed by Tanguy et al. [5], [6]. From this work the turbulent mixing of a scalar quantity issued from an interface such has the vapor concentration has been studied showing the importance of interface boundary layer zone on the global statistic of the scalar field [7]. Further works concern the extension of interface capturing method generally based on incompressible scheme to fully compressible code to handle other phenomena occurring during the injection process such as cavitation.

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Numerical simulations of gas/vapor bubble oscillations

D. Fuster and L. Bergamasco

Institut Jean Le Rond d'Alembert (∂'Alembert), CNRS UMR 7190,
Sorbonne Universités, UPMC Paris 6, 4 Place Jussieu, 75005 Paris, France

In this work we numerically investigate the effect of heat and mass transfer on the dynamic response of gas-vapor bubbles. The numerical solution of the full non-linear 1D equations is compared with the analytical solution of the equations obtained for the oscillation of an spherical gas/vapor bubble in response of a weak pressure perturbation (linear solution). For a system with known gas/vapor/liquid properties, we identify various oscillation regimes as a function of an nondimensional oscillation frequency (e.g. the bubble's Peclet number) and the vapor content. Even at very low frequencies, there exist regimes where transient diffusion effects arise due to heat diffusion in the surrounding liquid and also due to vapor mass diffusion inside the bubble. These phenomena restrict the applicability of the commonly-adopted assumption of full-equilibrium conditions inside the bubble. Simulations of the oscillation of bubbles for strong perturbations shows that non-linear effects restrict even further the range of applicability of the isothermal equilibrium model when the vapor content becomes larger than a critical value.

Simulations of a heated fluid at low Mach number: modelling of phase transition and numerical strategies

Bérénice GREC, MAP5 - Université Paris Descartes

Stéphane DELLACHERIE, DEN/DANS/DM2S/STMF, CEA & Polytechnique Montréal

Gloria FACCANONI, IMATH - Université de Toulon

Yohan PENEL, CEREMA, Inria (team ANGE) & LJLL, UPMC

Thermohydraulic codes used in industry are based on the resolution of compressible Navier-Stokes equations in which acoustic waves are taken into account. This allows to describe fluid flows at any Mach number. However, many difficulties may arise in terms of CPU time, robustness and accuracy in the low Mach number regime. In this regime, an asymptotic expansion with respect to the Mach number leads to simpler models.

Thus, the strategy of our work is to derive, investigate and simulate a system of PDE taking into account phase transition in the low Mach number regime but with possible high heat transfers. More precisely, we focus on the choice of the equation of state and its parameters, with emphasis on the gain due to the low Mach number hypothesis, and we present preliminary 2D numerical simulations with FreeFem++ showing the robustness of the approach.

Bérénice GREC, MAP5 UMR 8145 - Université Paris Descartes, 45 rue des Saints Pères, 75270 Paris Cedex 06, France
berenice.grec@parisdescartes.fr

High fidelity anisotropic adaptive FEM towards physical couplings occurring in turbulent boiling

Elie Hachem, Mehdi Khalloufi, Rudy Valette

Computing and Fluids Research Group
MINES ParisTech, PSL - Research University
CEMEF - Centre for material forming, CNRS UMR 7635
CS 10207 rue Claude Daunesse, 06904 Sophia-Antipolis Cedex, France

We propose in this work an adaptive variational multiscale method for complex multiphase flows with surface tension: applications to 3D bubble dynamics, turbulent boiling and solid quenching with experimental comparisons will be presented. A new conservative level-set method is used to provide a precise position of the interfaces. An implicit implementation of the surface tension in the context of the Continuum Surface Force is proposed to circumvent the capillary time step restriction. The obtained system is then solved using a unified compressible-incompressible variational multiscale stabilized finite element method designed to handle the abrupt changes at the interface and large density and viscosity ratios. Combined with an a posteriori error estimator, we show that anisotropic mesh adaptation yields an accurate 3D modeling framework for turbulent multiphase flows with phase change.

Modelling liquid-vapor phase change with metastable states.

Hélène Mathis
Laboratoire de Mathématiques Jean Leray, Université de Nantes
helene.mathis@univ-nantes.fr

Joint work with Hala Ghazi and François James

We propose a model of liquid-vapor phase transition including metastable states of the van der Waals Equation of State. The first part of the talk concerns the thermodynamics model. Following the second principle, the problem boils down to a minimization problem with constraints of the mixture energy. This "static" description allows to recover the classical equilibria: pure liquid/vapor states and a coexistence state (given by the Maxwell equal area rule). Then, when assuming a dependency with respect to time, we define a dynamical system with long time equilibria which are either the classical equilibria or the metastable states. In a second part of the talk, we use the dynamical system as a source term of a two-phase isothermal model. The homogeneous model is hyperbolic under condition. However for smooth solutions, we manage to prove that the regions of hyperbolically are invariant domains. We finish with some numerical experiments, obtained by a finite volume scheme and a splitting technique to handle the source term.

Simulation of free surface fluids in incompressible dynamique

Dena Kazerani, Laboratoire Jaques-Louis Lions

Pascal FREY, Laboratoire Jaques-Louis Lions

In this work, we present a numerical scheme for solving free surface flows. The free surface is modeled using the level-set formulation. Besides, the mesh is anisotropic and adapted at each iteration. This adaptation allows us to obtain a precise approximation for the free- surface location. In addition, it enables us to solve the time-discretized fluid equation only on the fluid domain. The fluid here is considered incompressible. Therefore, its motion is described by the incompressible Navier–Stokes equation which is temporally discretized using the method of characteristics and is solved at each time iteration by a first order Lagrange–Galerkin method. The level-set function representing the free surface satisfies an advection equation which is also solved using the method of characteristics. The algorithm is completed by some intermediate steps like the construction of a convenient initial level-set function (redistancing) as well as the construction of a convenient flow for the level-set advection equation. Finally, some numerical results are presented.

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Dena Kazerani, 4, Place Jussieu, Université Pierre et Marie Curie
kazerani@ljll.math.upmc.fr

Effervescence in champagne and sparkling wines: Recent advances and future prospects

Gérard Liger-Belair[1], and Thomas Séon[2]

1 : Equipe Effervescence Champagne et Applications, Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA), UMR CNRS 7331, UFR Sciences Exactes et Naturelles, BP 1039, 51687 Reims Cedex 2, France.

2 : Institut Jean Le Rond d'Alembert, UMR CNRS 7190, Université Pierre et Marie Curie, 4 Place Jussieu, F-75005 Paris, France.

Bubbles in a glass of champagne may seem like the acme of frivolity to most of people, but in fact they may rather be considered as a fantastic playground for any fluid physicist. In a glass of champagne, about a million bubbles will nucleate and rise if you resist drinking from your flute. The so-called *effervescence* process, which enlivens champagne and sparkling wines tasting, is the result of the complex interplay between carbon dioxide (CO_2) dissolved in the liquid phase, tiny air pockets trapped within microscopic particles during the pouring process, and some both glass and liquid properties. The journey of yeast-fermented CO_2 is reviewed (from its progressive dissolution in the liquid phase during the fermentation process, to its progressive release in the headspace above glasses). The physicochemical processes behind the nucleation, and rise of gaseous CO_2 bubbles, under standard tasting conditions, have been gathered hereafter. Moreover, when a bubble reaches the air-champagne interface, it ruptures, projecting a multitude of tiny droplets in the air. Based on the model experiment of a single bubble bursting in simple liquids, we depict each step of this process, from bubble bursting to droplet evaporation. In particular, we demonstrate how damping action of viscosity produces

faster and smaller droplets and more generally how liquid properties enable to control the bubble bursting aerosol characteristics. We demonstrate that compared to a still wine, champagne fizz drastically enhances the transfer of liquid into the atmosphere. Conditions on bubble radius and wine viscosity that optimize aerosol evaporation are provided. These results pave the way towards the fine tuning of aerosol characteristics and flavor release during sparkling wine tasting, a major issue of the sparkling wine industry.

Benchmarking rotating flow with free surface deformation

Wen Yang, Guangyang Cui, Jalel Chergui, Yann Fraigneau, Ivan Delbende, Laurent Martin Witkowski

Limsi-Cnrs, Orsay and UPMC, Paris.

The free surface deformation generated by a disk rotating at the bottom of a container partially filled with fluid is an exciting challenge for numerical simulations. The shape of the free surface has shown surprising patterns in experiments performed by different research groups. However, for many regimes (non axisymmetric, dewetted disk, sloshing), an accurate comparison with numerical simulations is clearly missing. We will present the different existing regimes of such flow and show results of comparison between different numerical codes on few selected regimes. Some preliminary measurements on a recent experimental set up will also be presented and we will discuss the relevance of a benchmark on such flow.

NUMERICAL SIMULATION OF A GAS BUBBLE COLLAPSE USING THE SPH-ALE METHOD

Saira PINEDA, Stephane AUBERT, *Ecole centrale de Lyon, LMFA, 69134 Ecully, France*; Jean Christophe MARONGIU, *ANDRITZ Hydro SAS, 69100 Villeurbanne, France.*

A multiphase model developed in SPH-ALE is used to simulate the collapse of a gas bubble in water. This model does not diffuse the interface and guarantees the continuity of normal velocity and pressure at the interface between both fluids. This scheme is able to deal with interfaces of simple contact where normal velocity is continuous.

The model solves the mass, momentum and energy conservation equations of Euler system using a non-isentropic equation of state for each phase, the Stiffened Gas EOS for water and the ideal gas EOS for the gas bubble. Both phases are compressible and the phase change is not modeled.

A multiphase shock tube is presented for validation purpose, with satisfactory results in comparison with reference solutions. The dynamics of the Rayleigh collapse of a bubble in a free-field and near a planar rigid wall are analyzed. Collapse behavior, interfacial velocities and surface pressure as a function of time are analyzed for the free-field collapse case, and in addition, as a function of the initial bubble stand-off distance from the wall for the case of the bubble collapse near the wall.

For the case of the bubble collapse near a wall, a re-entrant jet directed towards the surface is observed due to the non-symmetry initial configuration. The potential damage to the surface wall is estimated by measuring the wall pressure.

Diffuse interfaces with compressible fluids, phase transition and capillarity

Richard Saurel
Aix Marseille University and IUF

Conventional models of capillary fluids with phase transition consider linked thermodynamics and capillarity. Such coupling has serious consequences, such as:

- sound propagation, undefined in some critical regions,

- very thin interfaces, causing serious issues in practical computations.

In the present talk an approached based on hyperbolic systems with relaxation is promoted to solve interfaces with phase transition and surface tension. The method deals with arbitrary pressure and density jumps.

The diffuse interface model consists in a set of balance equations of mass for each phase and momentum and energy for the mixture. When simple contact is considered (in the absence of heat diffusion), a volume fraction equation is needed as well. In this frame each phase is compressible and governed by its own (convex) equation of state, preserving sound propagation. The two equations of state are rendered compatible through appropriate constants determined from the phase diagram. Phase change is modeled through Gibbs free energy relaxation terms. Capillarity is modelled through mass fraction gradients at interfaces and is consequently decoupled of thermodynamics.

Examples of cavitating, flashing and boiling flows with and without shocks are shown.

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Direct Numerical Simulation of Bubbles with Adaptive Mesh Refinement with Distributed Algorithms

Arthur Talpaert, CEA and École polytechnique
Grégoire Allaire, École polytechnique
Stéphane Dellacherie, Polytechnique Montréal
Samuel Kokh, CEA
Anouar Mekkas, CEA

This talk presents the implementation of the simulation of two-phase flows in conditions of water-cooled nuclear reactors, at the scale of individual bubbles. To achieve that, we study several models for Thermal-Hydraulic flows and we focus on a technique for the capture of the thin interface between liquid and vapour phases. We thus review some possible techniques for Adaptive Mesh Refinement (AMR) and provide algorithmic and computational tools adapted to patch-based AMR, which aim is to locally improve the precision in regions of interest. More precisely, we introduce a patch-covering algorithm designed with balanced parallel computing in mind. This approach lets us finely capture changes located at the interface, as we show for advection test cases as well as for models with hyperbolic-elliptic coupling. The computations we present also include the simulation of the incompressible Navier-Stokes system, which models the shape changes of the interface between two non-miscible fluids. We highlight two canonical test cases: the (one-phase) lid-driven cavity as well as the Rayleigh-Taylor instability.

Direct Numerical Simulation of Liquid-Vapor Phase Change. Applications to Leidenfrost Droplet and Nucleate Boiling.

Sébastien Tanguy,

Institut de Mécanique des Fluides de Toulouse

Studies on two-phase flows are of interest in many fundamental problems and industrial applications, as the spray formation in internal combustion engine, the bubble formation in heat exchangers, the fluid management in satellites or space launcher tanks, the spray cooling or the interaction of bubbles with acoustic waves. The Direct Numerical Simulation is a powerful tool, which is complementary to experimental measurements, to provide accurate results in complex situations. However, unlike single-phase flows, currently the direct numerical simulation of two-phase flows cannot be considered as a fully mature field, especially in most configurations involving strong coupling between the interface motion with heat and mass transfer, acoustic or shock waves, and/or a solid boundary where a contact line can be formed. This presentation will emphasize on the development of new numerical methods [1,2,3,4,5] to perform accurate Direct Numerical Simulations of two-phase flows with phase change in the framework of sharp interface capturing numerical methods. The presentation will focus mainly on two specific configurations involving liquid vapor phase change, i.e. Leidenfrost droplets and nucleate boiling. We will discuss about suited numerical strategy to succeed numerical simulations in these configurations. Accurate comparison between experiments and fully-resolved numerical simulations will be presented in order to bring out the relevance of the proposed algorithms.

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Laurette Tuckermann

Workshop NMLVIFF, IHP december 2016.

Numerical simulation of Faraday wave patterns

In 1831, Faraday described the standing wave patterns that form on the surface of a layer of fluid subjected to periodic vertical vibration. These waves usually take the form of stripes, squares, or hexagons. However, other phenomena have been observed numerically, such as quasipatterns, supersquares, heteroclinic cycles, and oscillons.

Until recently, numerical simulation of Faraday waves was out of reach. Since 2009, however, we have simulated not only simple wave patterns but also patterns which involve large-scale modulation. To do so, we have developed a massively parallel multiphase code, BLUE, whose treatment of the free surface uses a hybrid Front-Tracking/Level-Set technique, defining the interface both by a discontinuous density field on the Eulerian grid and by triangles on the Lagrangian interface mesh.

We will discuss the various Faraday wave configurations we have studied: regular square and hexagonal lattices, patterns composed of spherical harmonics on a vibrated drop, and supersquares consisting of a four-by-four array of smaller squares.

25 september 2016.

Numerical simulation of flows with sharp interfaces by the Volume-Of-Fluid method

Stéphane Zaleski
Institut Jean Le Rond d'Alembert, UPMC & CNRS UMR 7190
Paris, France

We discuss recent developments in the Volume-Of-Fluid (VOF) methods, such as the height function method for the approximation of the geometry of the interface, the balanced-force surface tension method, and the methods that conserve mass and momentum at machine accuracy. Applications at high Reynolds number,such as high speed liquid-gas flows, and low Reynolds and low Capillary numbers, are discussed.

Problems of engineering and physical interest, such as jet atomisation or flow in porous media are investigated with these methods as will be shown.