Interface Capture Methods for the Simulation of Compressible Two-Phase Flows with Interfaces

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Abstract

One of the key technical challenges of the Neptune project [7] is to improve and validate the two-phase flow models in order to pave the road for upcoming models and methods of two-phase flow simulation. We develop a methodology which consists in testing these models against series of simulations at finer scales.

The present work deals with the simulation of flows with interfaces that separate two compressible media. One objective of our work consists in preserving a good scalability of the methods in order to enable massive parallel computing. Therefore we chose to update the interface position thanks to an interface capture method which describes the interface as a transition zone between the fluids and we opted for explicit approximate Godunov methods on cartesian meshes. We address here two problems: the design of accurate numerical schemes for advecting the interface thanks to pure convective effects and the modelling of phase change. Dynamic dissipation processes are neglected.

Five-equation model [1, 10]

$$\begin{cases} \partial_t(\rho y) + \operatorname{div}(\rho y \mathbf{u}) = 0 \\ \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}[\rho \mathbf{u} \otimes \mathbf{u} + P(z, y, \rho, \varepsilon)\mathrm{Id}] = \Pi_{\text{tension}} + \rho \mathbf{g} \\ \partial_t \left[\rho\varepsilon + \dfrac{|\mathbf{u}|^2}{2}\right] + \operatorname{div}\left[\left(\rho\varepsilon + \dfrac{|\mathbf{u}|^2}{2} + P\right)\mathbf{u}\right] = (\Pi_{\text{tension}} + \rho \mathbf{g}) \cdot \mathbf{u} \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \end{cases}$$

Variables

- ρ density
- ε internal energy
- $\mathbf{u}$ velocity
- y mass fraction
- z color function
- P pressure
- $\mathbf{g}$ gravity

Capillarity

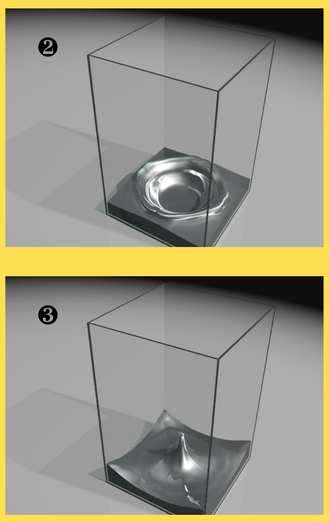
Continuum Surface Force (CSF) approach [3]

$$\Pi_{\text{tension}} = -\sigma \operatorname{div}\left(\frac{\mathbf{grad}\, z}{|\mathbf{grad}\, z|}\right)\frac{\mathbf{grad}\, z}{|\mathbf{grad}\, z|}$$

3D Parallel Simulations & Anti-Diffusive Interface Capture Algorithms

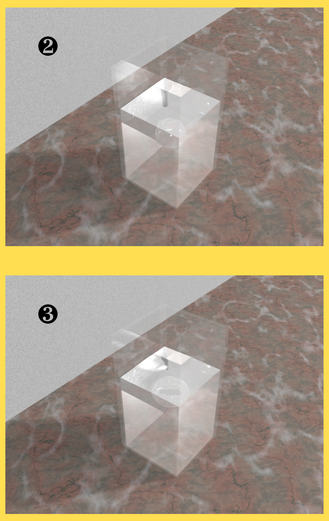
Drop Impact on a Liquid Film

- 3D gravity-driven simulation with surface tension (no phase change, no thermal diffusion)
- parallel solver on a 12 bicores cluster
- $100 \times 100 \times 200$ mesh



Rise of a Bubble towards a Liquid Free Surface

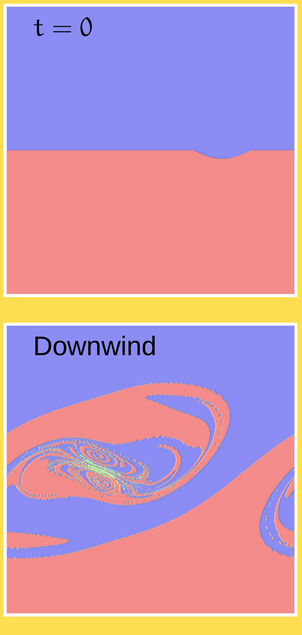
- 3D gravity-driven simulation with surface tension (no phase change, no thermal diffusion)
- parallel solver on a 12 bicores cluster
- $100 \times 100 \times 200$ mesh



Simulation of a 2D Kelvin-Helmoltz instability

Comparison of the standard upwind solver with the new anti-diffusive solver. This solver is a Lagrange-Remap scheme based on the approach of [5, 6]. This simulation does not enable any phase change nor surface tension.

- conservative numerical scheme for $\rho y, \rho$, $\rho \mathbf{u}$ and $\rho\varepsilon + \rho|\mathbf{u}|^2/2$
- anti-diffusive convection of the interface without any interface reconstruction algorithm
- no numerical tuning required
- positivity for y and z



Phase Change

- **Relaxation Approach [8]**

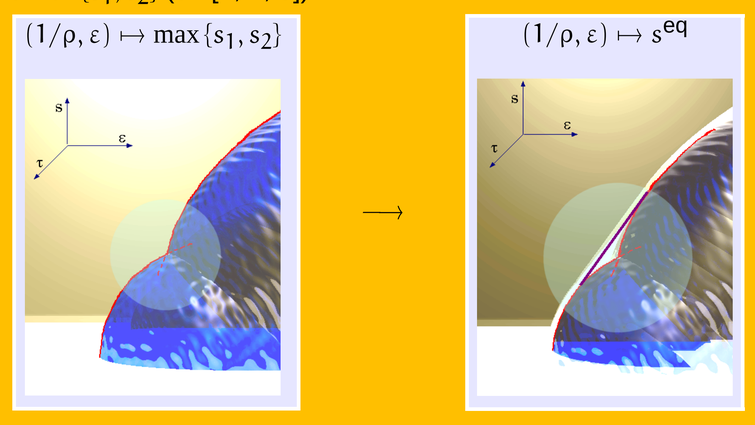
Let $(1/\rho_\alpha, \varepsilon_\alpha) \mapsto s_\alpha$ be the physical entropie for the phase α.

step-I: solve five-equation system [1, 10];

step-II: update the variables z and y by projecting $(y, z, \rho\mathbf{u}, \rho\varepsilon)$ onto the equilibrium manifold defined by

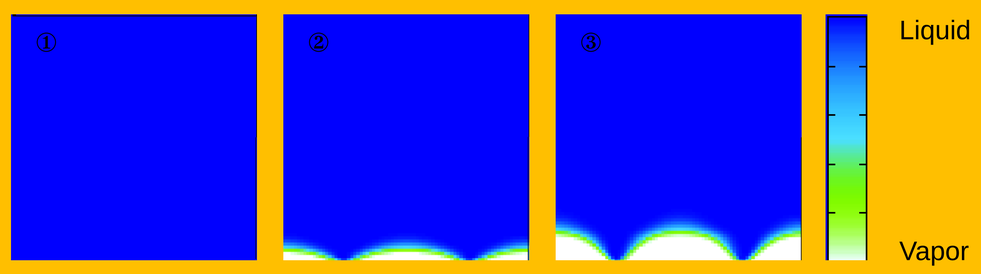
- chemical potential equilibrium
- thermal equilibrium
- pressure equilibrium.

This is equivalent to replace the entropy $\sum_\alpha y_\alpha s_\alpha$ of the five-equation system [1, 10] by a new entropy $(1/\rho, \varepsilon) \mapsto s^{\text{eq}}$ defined with the concave hull of the $\max\{s_1, s_2\}$ (cf. [2, 4, 9]):



Additional-step: implicit implementation of thermal effect.

- **Numerical Example: 2D nucleating bubble**



References

[1] Allaire, G., Clerc, S., and Kokh, S. (2002). A five-equation model for the simulation of interfaces between compressible fluids. *J. Comput. Phys.*, 181(2):577–616.

[2] Allaire, G., Faccanoni, G., and Kokh, S. (2007). A strictly hyperbolic equilibrium phase transition model. *C. R. Acad. Sci. Paris Sér. I*, 344:135–140.

[3] Brackbill, J. U., Kothe, D. B., and Zemach, C. (1992). A continuum method for modeling surface tension. *J. Comput. Phys.*, 100(2):335–354.

[4] Callen, H. B. (1985). *Thermodynamics and an Introduction to Thermostatistics*. John Wiley & sons, second edition.

[5] Després, B. and Lagoutière, F. (1999). Un schéma non-linéaire anti-dissipatif pour l'équation d'advection linéaire. *C. R. Acad. Sci. Paris, Série I*, t. 328:pp. 939–944.

[6] Després, B. and Lagoutière, F. (2006). Numerical resolution of a two-component compressible fluid model with interfaces. *Progress in Computational Fluid Dynamics*.

[7] Guelfi, A., Bestion, D., Boucker, M., Boudier, P., Fillion, P., Grandotto, M., Hérard, J.-M., Hervieu, E., and Péturaud, P. (2007). NEPTUNE - A New Software Platform for Advanced Nuclear Thermal-Hydraulics. *Nuclear Science and Engineering*, to appear.

[8] Helluy, P. and Seguin, N. (2006). Relaxation model of phase transition flows. M2AN, *Math. Model. Numer. Anal.*, (40 (2)):331–352.

[9] Jaouen, S. (2001). *Étude mathématique et numérique de stabilité pour des modèles hydrodynamiques avec transition de phase*. PhD thesis, Université Paris 6.

[10] Kokh, S. (2001). *Aspects numériques et théoriques de la modélisation des écoulements diphasiques compressibles par des méthodes de capture d'interfaces*. PhD thesis, Université Paris 6.

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