New numerical paradigm for efficient GPU-accelerated multiphase gas-liquid flow solver

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Abstract

Numerical simulations of compressible multiphase gas-liquid flows are still challenging, especially from the computational time point of view. For gas-liquid flows, the ratio between speeds of sound and material velocity makes the flow evolution quite slow on standard CPUs. For that reason, we are looking for new paradigms of mathematical modelling, numerical solution and parallel computation. We investigate into two complementary ways: i) a more conventional numerical solver, namely a remapped Lagrange scheme, but showing some performance issues on GPU processors; ii) an attempt to derive a Lattice Boltzmann-like solver (LB) for such kind of fluids. LB methods are known to provide strong GPU acceleration. As preliminary results, we get reasonable GPU speedups for remapped Lagrange solvers, and it was able to derive compressible LB solver with interesting features. We are confident into achieving runtime multiphase dynamics, which would be of high industrial interest.

Objectives

Solving the inviscid Euler equations for immiscible air-liquid flows:

$$\begin{cases} \partial_t(\alpha\rho_g) & + \vec{\nabla}\cdot(\alpha\rho_g\vec{u}) & = 0,\\ \partial_t((1-\alpha)\rho_\ell) & + \vec{\nabla}\cdot((1-\alpha)\rho_\ell\vec{u}) & = 0,\\ \partial_t(\rho\vec{u}) & + \vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u}+p\mathbf{I}) & = 0 \end{cases}$$

with

- α, mass fraction of gas ($\in \{0,1\}$)
- ρ_g (and ρ_ℓ), gas (and liquid) density
- speed u and pressure $p = \begin{cases} p_g(\rho_g) & \text{if } \alpha = 0 \\ p_\ell(\rho_\ell) & \text{if } \alpha = 1 \end{cases}$

From the numerical point of view, mixed finite volume cells may occur, involving α to be between 0 and 1, and an additional closure is needed.
Foreseen applications are industrial processes and naval applications like Liquid Natural Gas (LNG) sloshing into tankers.

Equation of state (EOS)

Closure = pressure equilibrium within a mixed gas-liquid cell. Simplified EOS are used in such a way that α can be derived easily. For liquid, we use

$$\boxed{\rho_g c_g^2 = p_g(\rho_g) = p = p_\ell(\rho_\ell) = \frac{p_\ell^0}{1 - \frac{\rho_\ell^0 c_\ell^2}{p_\ell^0}\left(1 - \frac{\rho_\ell^0}{\rho_\ell}\right)}}$$

where

- c_g (and c_ℓ), constant reference gas (and liquid) speed of sound
- p_ℓ^0, reference pressure

We get a closed form for both α and p:

$$\boxed{\alpha = 1 - \frac{(K-1)m_g + \rho_g^0}{\rho_g^0 m_\ell + K\rho_\ell^0 m_g} m_\ell, \quad p = \frac{m_g c_g^2 + K^{-2} m_\ell c_\ell^2}{1 - (1-K^{-1})\frac{m_\ell}{\rho_\ell^0}}}$$

where $m_g = \alpha\rho_g$, $m_\ell = (1-\alpha)\rho_\ell$ and $K = \frac{\rho_\ell^0 c_\ell^2}{p_\ell^0}$.

For the free-surface moving boundary, we have developed an innovative antidiffusive interface capturing scheme that provides strong GPU performance, unlike standard Volume-Of-Fluid (VOF) methods that usually topple the parallel performance because of multiple array indirections.

Mathematical and numerical setting

Compressible Lattice Boltzmann method (LBM)

LBM (ref [2]) solves the transport-reaction Boltzmann equation instead of the Euler system (written in 1D for simplicity)

$$\partial_t f_i + v_i \partial_x f_i = \frac{f_i^{eq} - f_i}{\tau}$$

To link this equation to the ones we want to solve, we need these constraints :

$$\sum_i \left(1, v_i, v_i^2\right) f_i^{eq} = \left(\rho, \rho u, \rho u^2 + p(\rho)\right)$$

In the simplified case where the pressure equation of state is the same in both phases ($p = p(\rho) = C\rho^\gamma$), it gives us

$$\begin{cases} f_-^{eq} = -\frac{1}{2}\rho m + \frac{1}{2}\rho m^2 + \frac{p}{2s^2},\\ f_0^{eq} = \rho - \rho m^2 - \frac{p}{s^2},\\ f_+^{eq} = \frac{1}{2}\rho m + \frac{1}{2}\rho m^2 + \frac{p}{2s^2}. \end{cases}$$

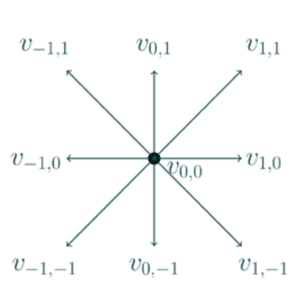
Introducing both physical speed of sound $c = \sqrt{\gamma p/\rho}$ and numerical speed of sound $s = \Delta x/\Delta t$, we set

- the numerical Mach number $m = u/s$
- the physical Mach number $M = u/c$
- $m < M$ (subcharacteristic constraint)

In two dimensions, if we choose a D2Q9 lattice, this gives us nine unknowns for only six equations. Choosing a lattice with less velocities implies other issues, like unstabilty because of the lack of symmetry in the lattice. So we need a trick to close the system and find a solution. We proceed by space tensorization.

We get $\mathbf{f_{ij} = g_i h_j}$ with $\mathbf{i, j \in \{-, 0, +\}}$.

$$\begin{cases} g_+ = \frac{\sqrt{\rho}}{2}\left(m_u + m_u^2 + \frac{p}{\rho s^2}\right)\\ g_0 = \sqrt{\rho}\left(1 - m_u^2 - \frac{p}{\rho s^2}\right)\\ g_- = \frac{\sqrt{\rho}}{2}\left(-m_u + m_u^2 + \frac{p}{\rho s^2}\right) \end{cases}$$



h_j are the same as g_i but with $m_v = \frac{v}{s}$ instead of $m_u = \frac{u}{s}$.

We tested our model on the dynamic of a compressed disc with periodic boundary conditions. We can see the evolution of the disc at different times. This case allows us to check the symmetry and rotational invariance as well as the stability during the propagation of the shock and the interactions between the waves. Results are encouraging but still with some robustness issues to understand.

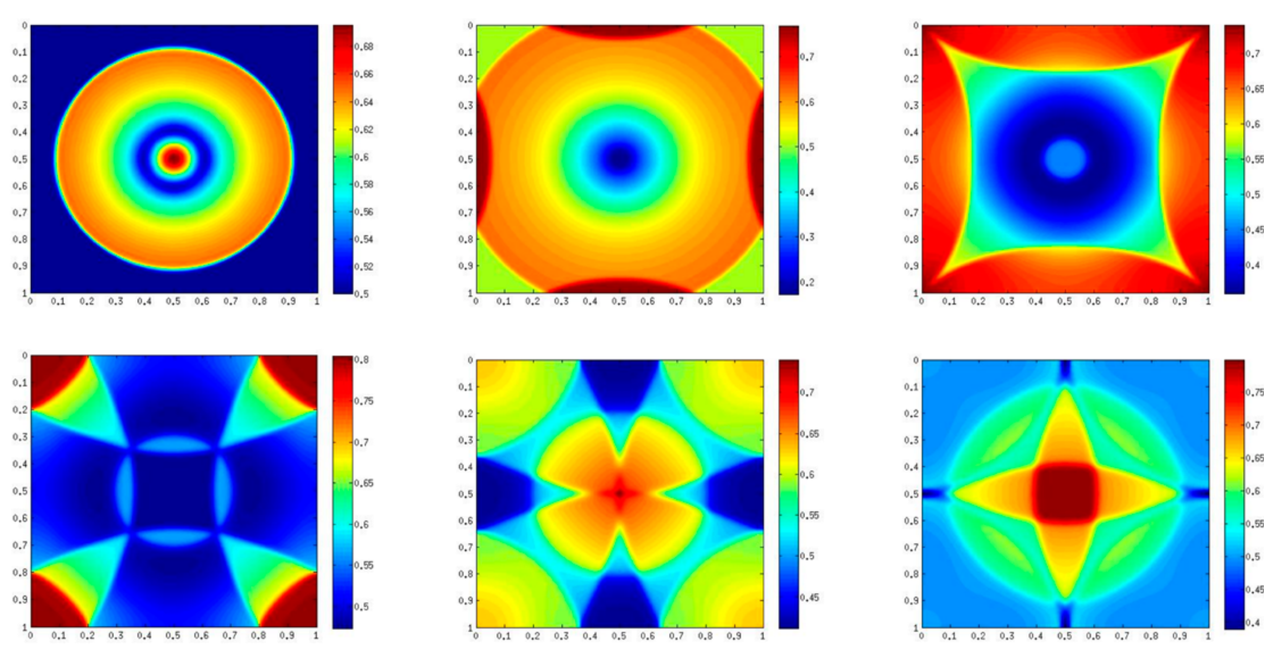


Figure 1: Example of shock propagation into the compressible medium captured by the Lattice Boltzmann solver.

For now, we only have a LBM for compressible fluids with EOS $p = p(\rho)$ in two dimensions. To extend this to air-liquid flows, we use method (A) of Larrouturou's work (Ref. [3]) for dealing with mass fractions. It works fine in 1D and we already made a successful 2D test on a Kelvin-Helmholtz instability test case and got accurate results.

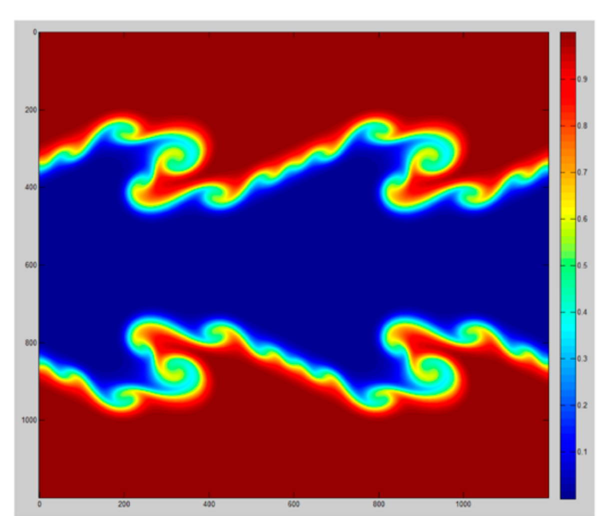


Figure 2: Kelvin-Helmholtz instabilities developing at the interface of contrary flow

Lagrange-remap (or remapped Lagrange) scheme

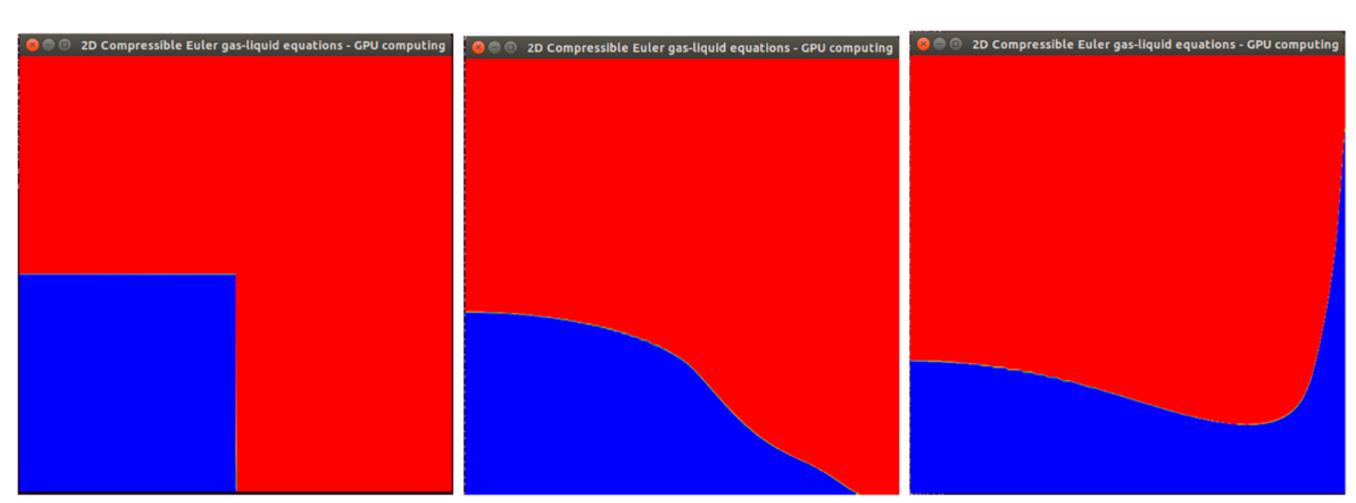
This method solves the Euler system in its Lagrangian formulation (Reynolds' transport theorem). Then we need to project the values from the moving referential on the fixed Eulerian grid.

Code	Time (s)		SpeedUp
Matlab		371.465	1
CUDA AoS	125.760	122.950	3.03
CUDA SoA	12.740	17.710	20.97

Table 1: Execution time (in single and double precision) and speed ups for the codes

With

- Results obtained on a Quadro K2100M,
- Final time of the simulation $T_{\text{final}} = 0.8$s
- Squared grid of size 128^2



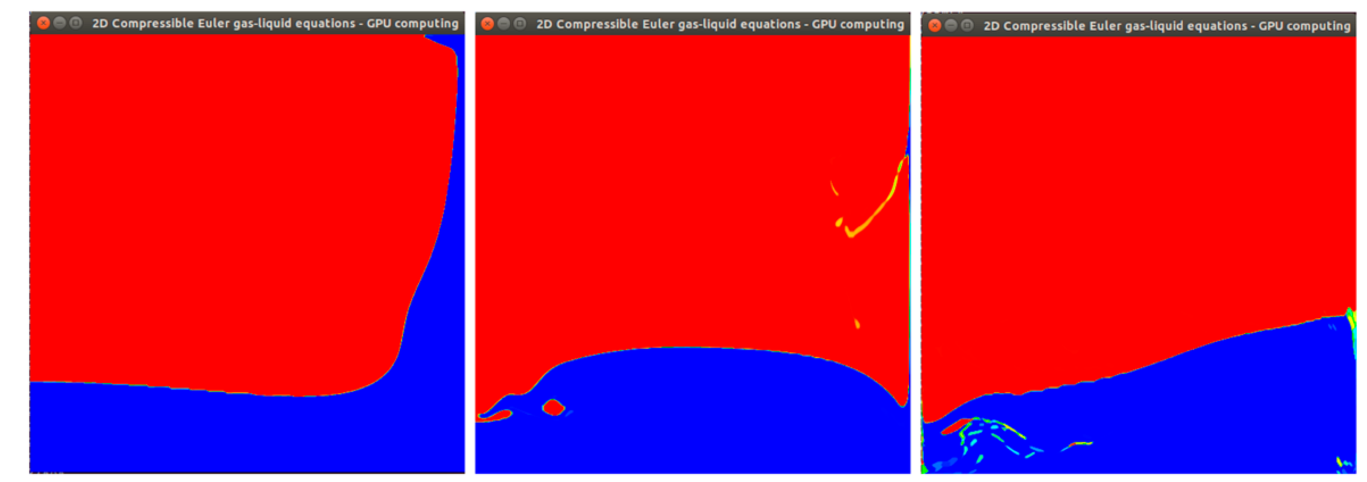


Figure 3: Evolution of the dambreak over time with Lagrange Remap scheme

Size	Time (s)
128×128	12.740
512×512	591.037 $\sim$ 10min

Table 2: CUDA SoA single precision, $T_{\text{final}} = 0.8$s

During this simulation time, we observe the collapse of the initial water column, then the collision with the rightward wall, the bounce-back and a wave breaking with formation of a compressible air pocket. Secondary waves then appear. The numerical solver use here is from (ref. [1]).

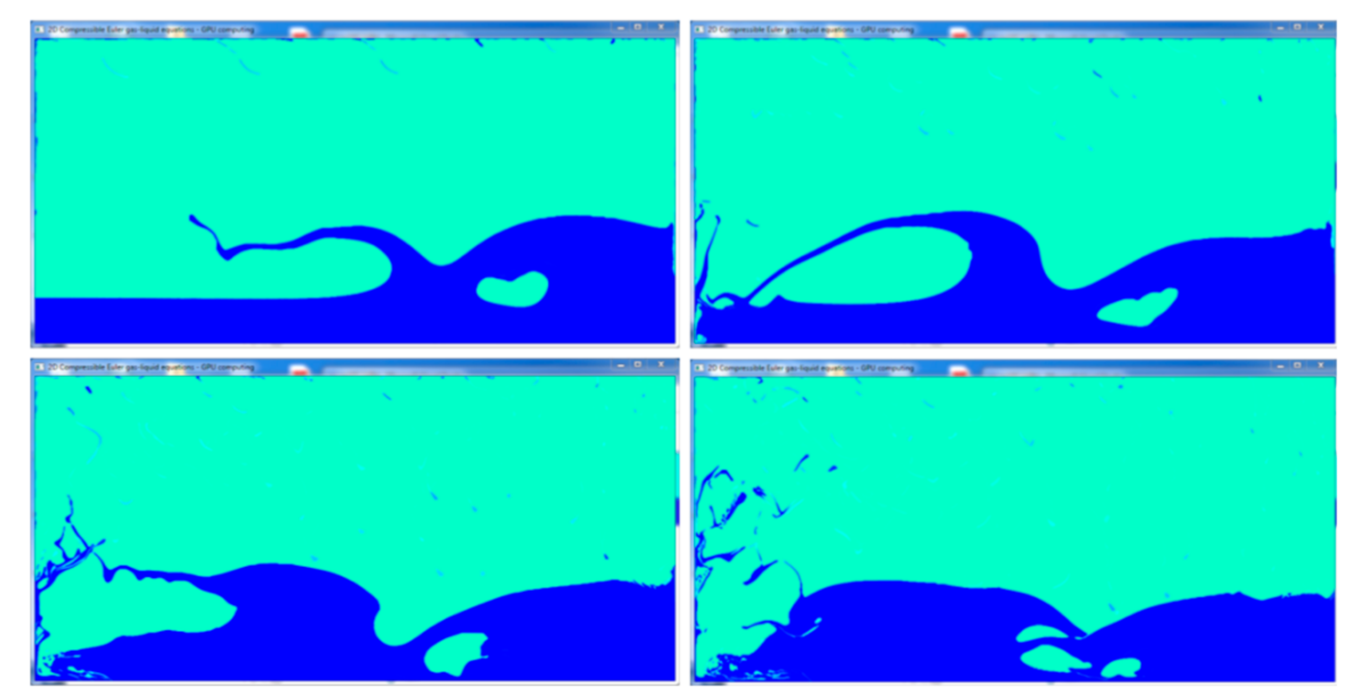


Figure 4: Yet another dam break case with different geometry and initial conditions.

Conclusion and forthcoming research

We have developed a model which is effective and accurate but we chose a pressure equation of state for the liquid that gives a gas fraction α written in closed form, allowing for high-efficiency GPU parallelism. Others EOS may be more physical but they imply the need of an iterative solver for α. We also notice some numerical instabilites occuring at phase interfaces for high density ratios by the multiphase Lattice Boltzmann model.

But we have ideas and plan to derive a hybrid mixed approach that combines both Lagrange-remap scheme and Lattice-Boltzmann solver, taking advantage of each of the methods. We are currently working on that and preliminary results are quite promising. We will make some performances comparison with Tesla K20 and K40 soon.

References

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Acknowledgements

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