A hierarchy of homogeneous two-fluid models and numerical methods for simulating various regimes of two-phase flows

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Part 1

Introduction

CONTEXT

Simulation of liquid fuel injection for design of new combustion chambers :

Credit : V. Le Chenadec

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1. D. Kah. *Prise en compte des aspects polydispersés pour la modélisation d'un jet de carburant dans les moteurs à combustion interne*. PhD thesis, Ecole Centrale Paris, 2010

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Modelling and simulation issues : a wide range of scales must be taken into account

- DNS would be unconceivable,
- two main regimes of flow : **separated phases** and **disperse phase**,
- two categories of Eulerian reduced-order models :
  - **two-fluid** models (and methods for locating gas-liquid interface),
  - **spray** models and kinetic theory basis. [1]

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Aim of our work

Design a unified approach using reduced-order models, with specific numerical strategies applicable on HPC resources.

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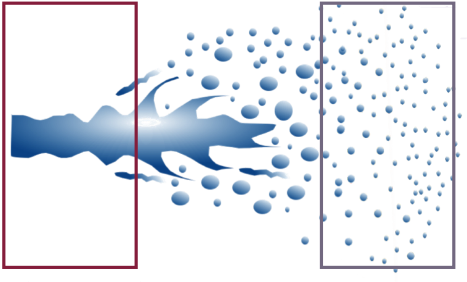
STRATEGY



Spray models for disperse phase.

Two-fluid models for interfacial flows.

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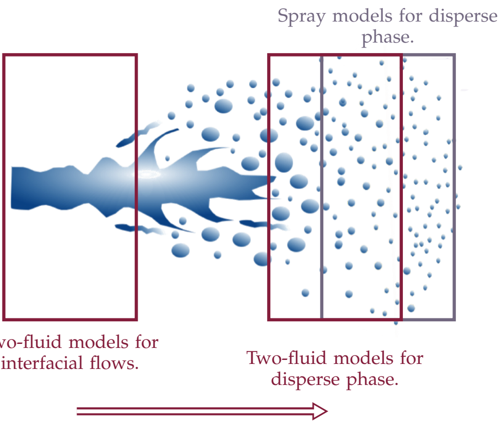
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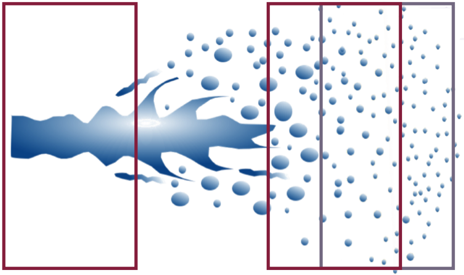

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$$\Longrightarrow$$

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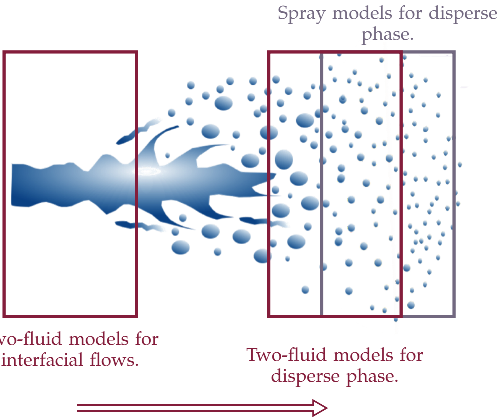

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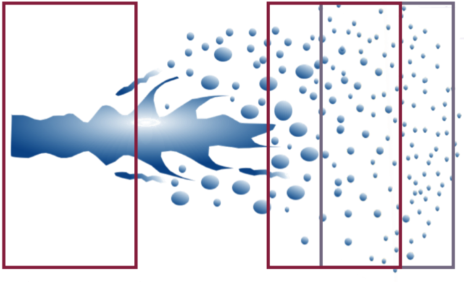

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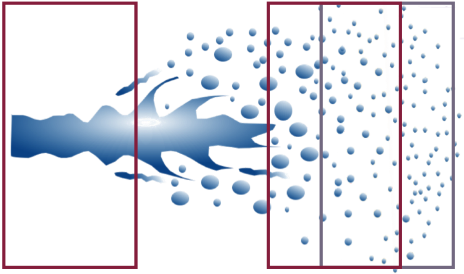
- Hierarchy of models as simple as possible,
- associated numerical schemes,
- adapted to highly parallel simulations.

STRATEGY

Outline of the presentation :

1. Modeling
   - derivation of two-fluid models,
   - identification of parameters.
2. Numerical schemes
   - AP schemes,
   - first results.
3. 2D / 3D simulations :
   - AMR framework,
   - results for simple interfacial flows.

Spray models for disperse phase.



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Part 2

Models

TWO-FLUID MODELS

Why choosing two-fluid models ?

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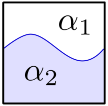
- widely used for separated phases :
  - incompressible for free surface flows / low-Mach
  - compressible for cases with pressure waves or shocks



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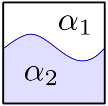

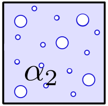

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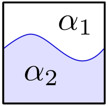

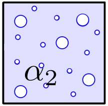

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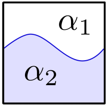

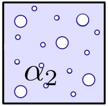

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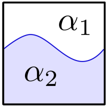

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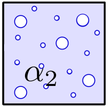

How to derive two-fluid models ?

Two approaches :

- Description of physics at micro-scale and averaging procedure.[2]

  $\Rightarrow$ **Issues of closures and well-posedness.**

$$\left\{\begin{array}{llll}
\partial_t\, m_1 & + & \nabla \cdot (m_1 \mathbf{u}_1) & = 0 \\
\partial_t\, m_2 & + & \nabla \cdot (m_2 \mathbf{u}_2) & = 0 \\
\partial_t\, (m_1 \mathbf{u}_1) & + & \nabla \cdot \left(m_1 \mathbf{u}_1 \otimes \mathbf{u}_1\right) + \alpha \nabla p_1 & = \mathbf{M} - \tau_1 \\
\partial_t\, (m_2 \mathbf{u}_2) & + & \nabla \cdot \left(m_2 \mathbf{u}_2 \otimes \mathbf{u}_2\right) + (1-\alpha) \nabla p_2 & = -\mathbf{M} - \tau_2 \\
\partial_t\, (m_1 h_1) & + & \nabla \cdot (m_1 h_1 \mathbf{u}_1) - \alpha \left(\partial_t p_1 + \mathbf{u}_1 \cdot \nabla p_1 \right) & = -\mathbf{u}_1 \tau_1 + \dfrac{q''_{1i}}{L_s} \\
\partial_t\, (m_2 h_2) & + & \nabla \cdot (m_2 h_2 \mathbf{u}_2) - (1-\alpha) \left(\partial_t p_2 + \mathbf{u}_2 \cdot \nabla p_2 \right) & = -2\tau_2 + \dfrac{q''_{2i}}{L_s}
\end{array}\right.$$

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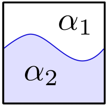

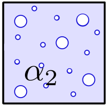

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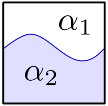

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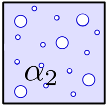

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Well-posed systems of equations ?

- hyperbolicity,
- entropic dissipation.

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- Choice of kinetic and potential energies,

Example

- $\frac{1}{2}\rho|\mathbf{u}|^2$, $\rho f(\rho, Y, \alpha)$, $\frac{1}{2}\mu(\alpha)|D_t\alpha|^2$

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- $\frac{1}{2}\rho|\mathbf{u}|^2$, $\rho f(\rho, Y, \alpha)$, $\frac{1}{2}\mu(\alpha)|D_t\alpha|^2$
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- Action of the Lagrangian :
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- definition of infinitesimal displacement in eulerian coordinates,
- postulation of mass cosnervation,

$\Rightarrow$ **conservative system of equations :**

$$\begin{array}{ccccc}
\partial_t \rho & + & \nabla \cdot (\rho \mathbf{u}) & = & 0 \\
\partial_t(\rho Y) & + & \nabla \cdot (\rho Y \mathbf{u}) & = & 0 \\
\partial_t\, (\rho \mathbf{u}) & + & \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \left(p + \frac{1}{2}(\rho Y w)^2\right) & = & 0 \\
\partial_t \alpha & + & \mathbf{u} \cdot \nabla \alpha & = & \dfrac{\rho Y w}{\sqrt{\mu}} \\
\partial_t w & + & \mathbf{u} \cdot \nabla w & = & \dfrac{p_g - p_l}{\rho Y \sqrt{\mu}}
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SECOND PRINCIPLE OF THERMODYNAMICS

Homogeneous barotropic two-fluid model (conservative) :

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- Entropy of the system[4]
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SECOND PRINCIPLE OF THERMODYNAMICS

Homogeneous barotropic two-fluid model (conservative) :

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Development of inequality and grouping of terms	$(\frac{1}{Y\sqrt{\mu}}\frac{\partial f}{\partial\alpha}+D_t w)\cdot(\frac{w}{\mu})\leq 0$
Introduction of dissipative parameters to ensure inequality	$D_t w=-\frac{\epsilon}{\mu}w+\frac{p_g-p_l}{\rho Y\sqrt{\mu}},\ \ \epsilon>0$

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Mathematical properties of the system :

- Hyperbolicity of the conservative part,
- characteristic sound velocity : $c^2 = Y c_g^2 + (1 - Y) c_l^2 + \rho (Y w)^2$,
- dissipative source terms.

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hyp : homogeneous, isothermal, micro-inertia, dissipative
→ **5-equation model**

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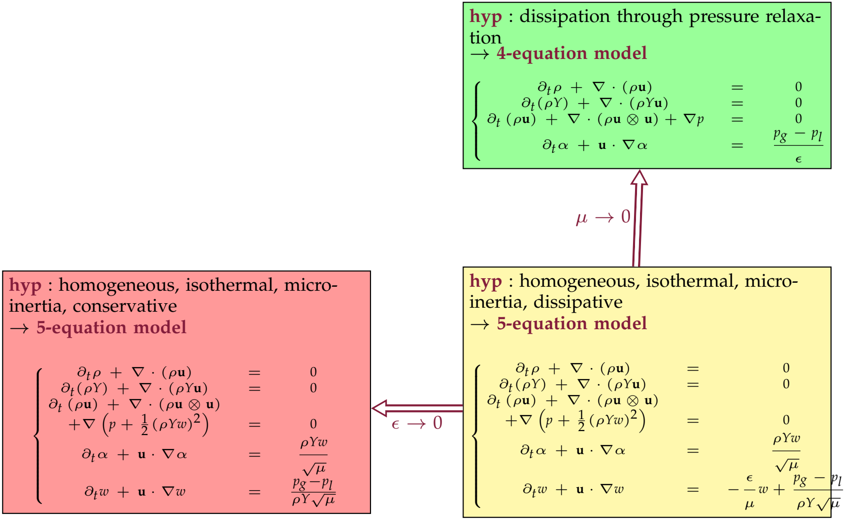

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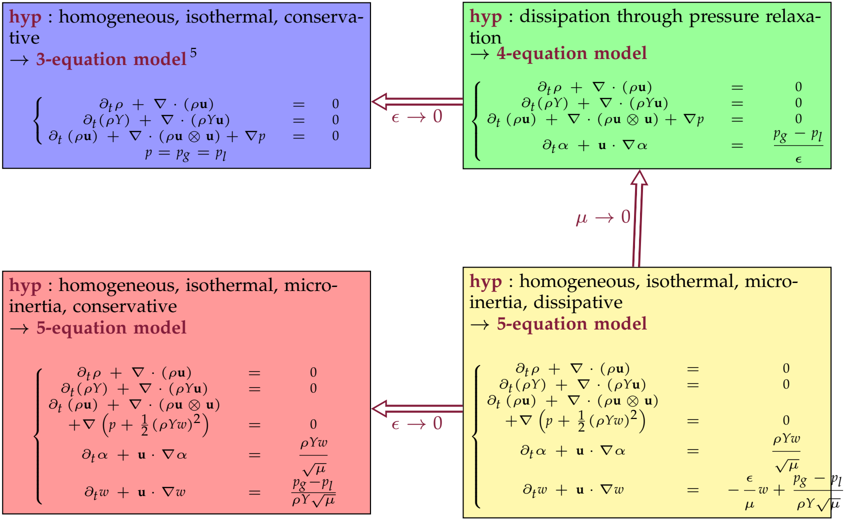

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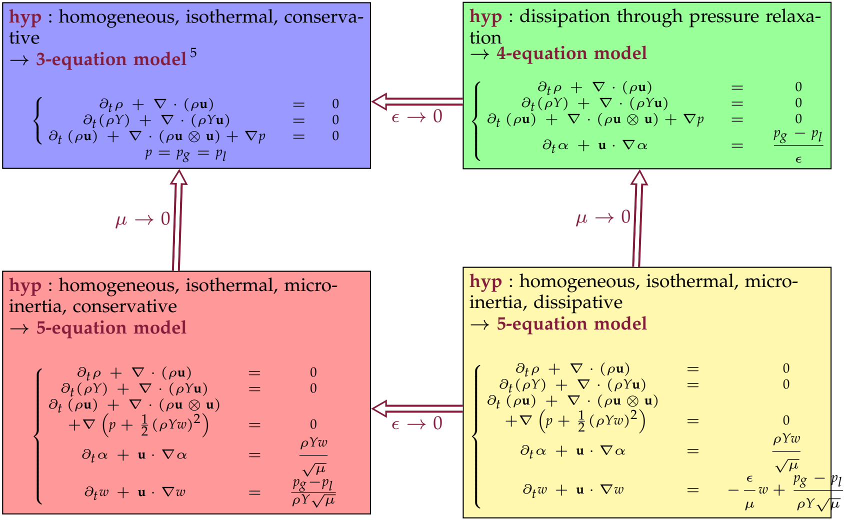

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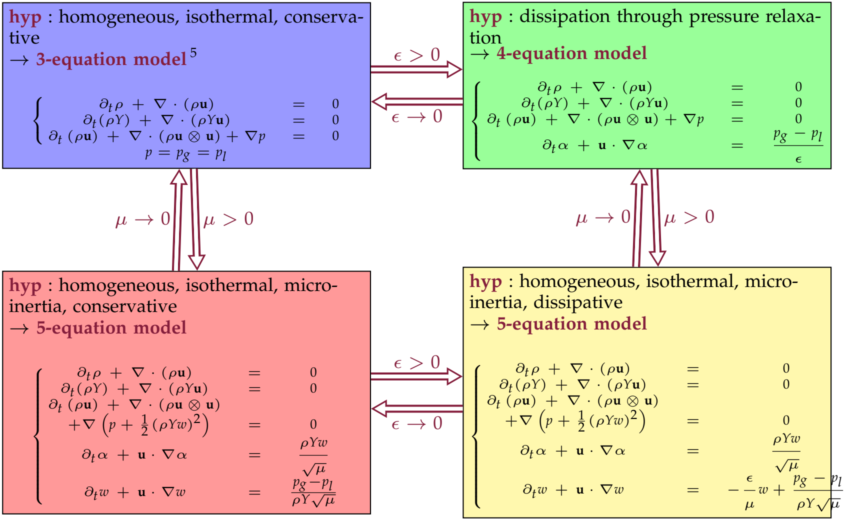

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⇒ we propose here physical values for the mathematical parameters !

COMPARISON WITH MEASURES AND REFERENCE MODEL

Measures of acoustic waves dispersion in bubbly media :

- Measure of phase velocity and spatial attenuation for different sizes of bubbles and different volume fractions of gas,
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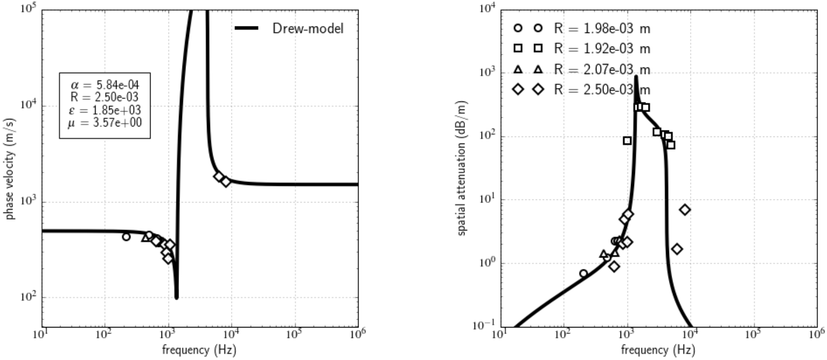

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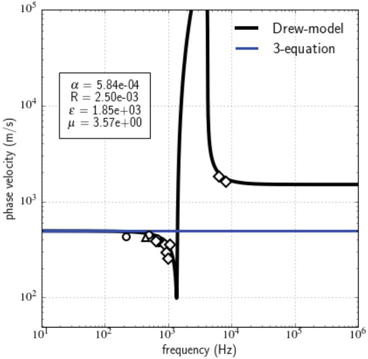

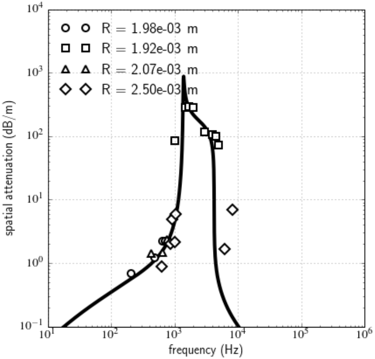

COMPARISON WITH MEASURES AND REFERENCE MODEL

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- Measure of phase velocity and spatial attenuation for different sizes of bubbles and different volume fractions of gas,
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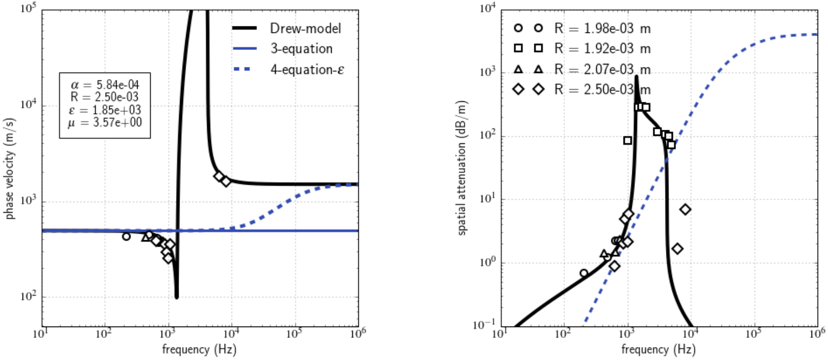

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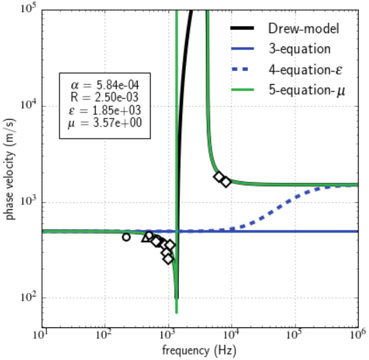

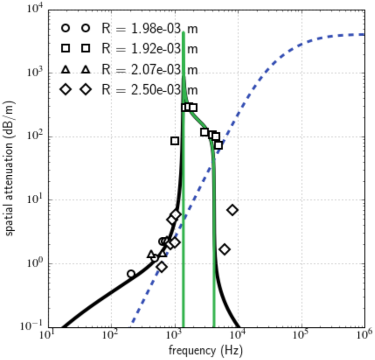

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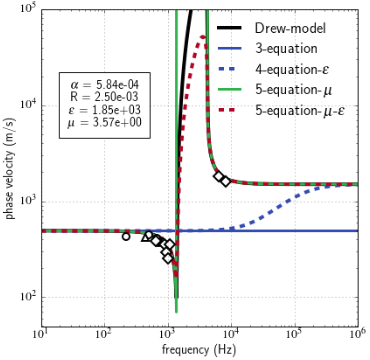

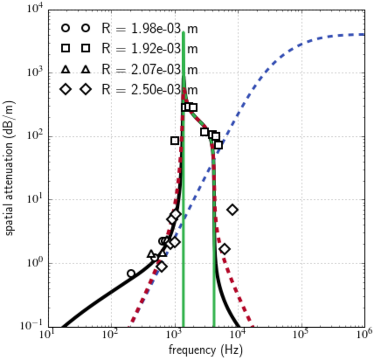

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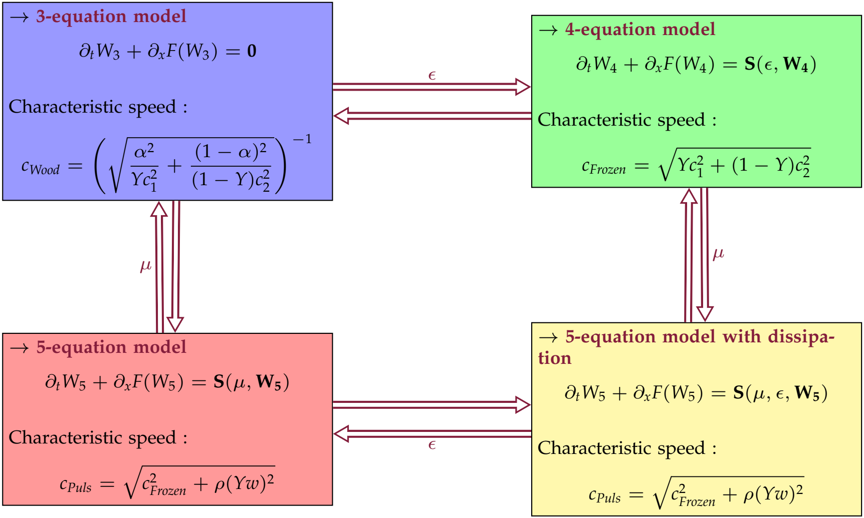
To go further

By defining relevant energies for the system, one can complete the hierarchy to comes closer to spray models.

A NUMERICAL SCHEME FOR THE WHOLE HIERARCHY ?



→ **3-equation model**

$$\partial_t W_3 + \partial_x F(W_3) = \mathbf{0}$$

Characteristic speed :

$$c_{Wood} = \left(\sqrt{\frac{\alpha^2}{Yc_1^2} + \frac{(1-\alpha)^2}{(1-Y)c_2^2}}\right)^{-1}$$

→ **4-equation model**

$$\partial_t W_4 + \partial_x F(W_4) = \mathbf{S}(\epsilon, \mathbf{W_4})$$

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→ **5-equation model**

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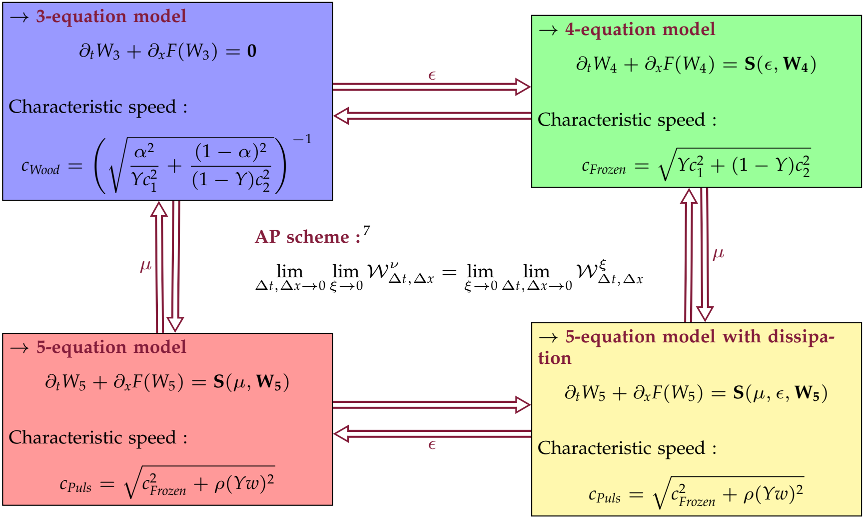

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Part 3

Numerical methods

ASYMPTOTIC PRESERVING SCHEMES : THEORY

Equations with stiff source term[8] : $\partial_t W + \partial_x F(W) = S(\xi, W)$

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Classical integration of source terms :

- Godunov splitting :

$$\begin{cases} W_t + F(W)_x = 0 \\ W_t = S(\xi, W) \end{cases}$$

- explicit integration of source terms may lead to strong CFL constraints (so as to ensure $\alpha \in [0, 1]$ for instance),
- not always accurate for large time steps when ξ is small,
- for our models, constraint on α : $\alpha \in [0, 1]$

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A more consistent way (issued from well-balanced schemes) :

- modification of Riemann solver to integrate source terms with fluxes,
- satisfying integral consistency [9] :

$$\int_x \int_t \left(\tilde{W}_t + F(\tilde{W})_x - S(\xi, \tilde{W}) \right) \, dt \, dx = 0$$

- use of generalized jump relations across the waves :

$$F(W_R) - F(W_L) - \Delta x \tilde{S} = \sum_k \lambda_k (W_{k+1} - W_k)$$

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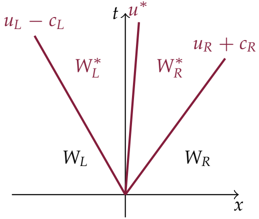
$$\begin{cases} \partial_t \rho & + & u\partial_x \rho & + & \rho\partial_x u & = & 0 \\ \partial_t Y & + & u\partial_x Y & & & = & 0 \\ \partial_t(\rho u) & + & u\partial_x(\rho u) & + & \rho u\partial_x u + \partial_x p & = & 0 \\ \partial_t \alpha & + & u\partial_x \alpha & & & = & \frac{p_g - p_l}{\epsilon} \end{cases}$$



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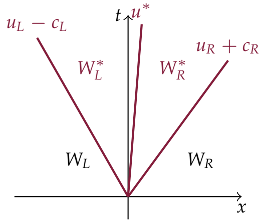
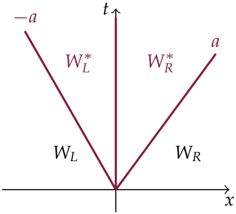


- Suliciu's relaxation scheme for the acoustic part :

$$\begin{cases} \partial_t \tau & - & \partial_m u & = & 0 \\ \partial_t Y & & & = & 0 \\ \partial_t u & + & \partial_m \Pi & = & 0 \\ \partial_t \alpha & & & = & \frac{p_g - p_l}{\epsilon} \\ \partial_t \Pi & + & a^2 \partial_m u & = & \lambda(p - \Pi) \end{cases}$$



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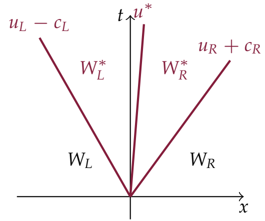

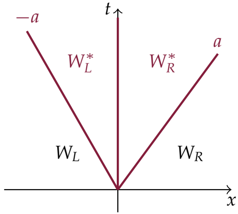

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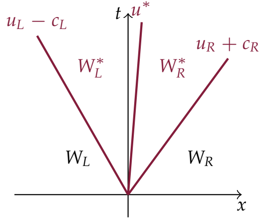

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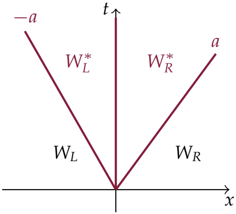

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Behavior of pressure waves for different wavelengths.

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Conclusions :

- Numerical dissipation is different between 4-eq and 3-eq models,
- 4-eq model tends to 3-eq model when $\epsilon \to 0$.
- 5-eq model tends to 4-eq model when $\mu \to 0$.

AP SCHEMES : VERIFICATION TESTS (2)

Behavior of pressure waves for different wavelengths.

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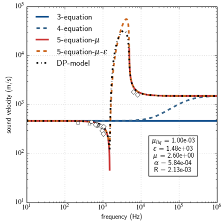
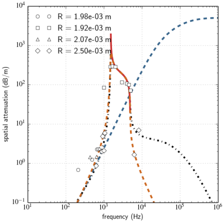
Behavior of pressure waves for different wavelengths.

- Wave propagating from liquid to bubbly medium.





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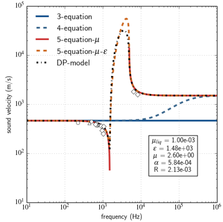

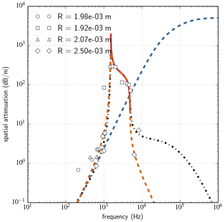

Pressure at low frequencies :

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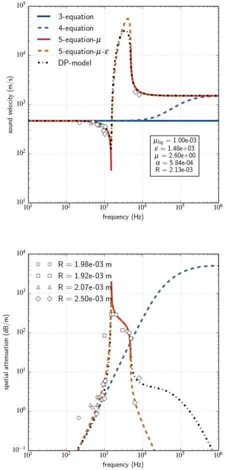

Pressure near resonance :

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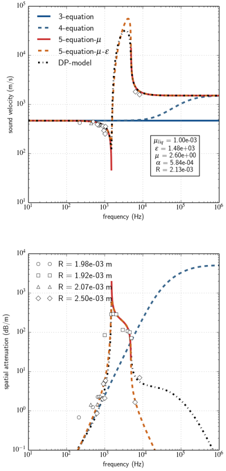

Pressure at high frequencies :

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Behavior of pressure waves for different wavelengths.

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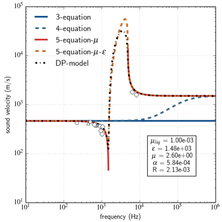
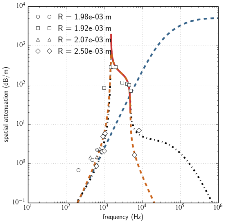




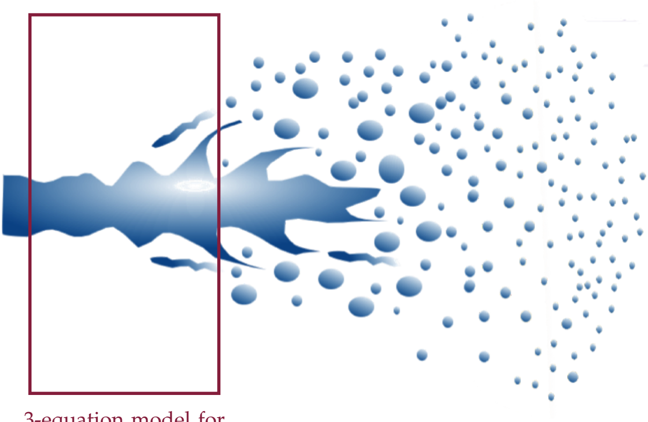
Observations :

- Different regimes according to frequency :
  - different models $\Rightarrow$ different velocities of propagation in bubbles,
  - different models $\Rightarrow$ different acoustic impedances.
- Numerical dissipation is equivalent in liquid part for all models.

Part 4

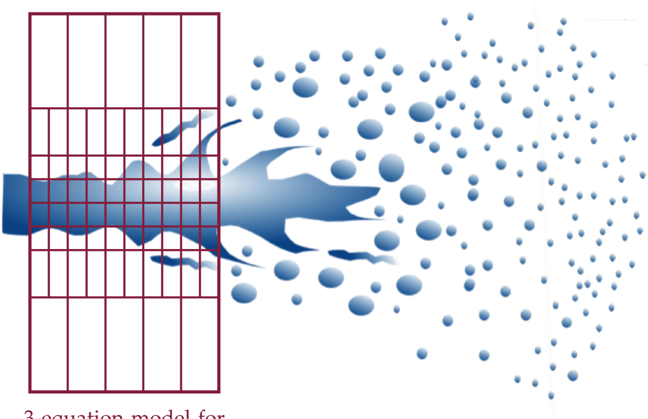
Numerical strategies for 2D and 3D simulations

NUMERICAL STRATEGIES FOR 2D AND 3D SIMULATIONS



3-equation model for interfacial flows.

NUMERICAL STRATEGIES FOR 2D AND 3D SIMULATIONS

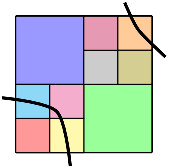


3-equation model for interfacial flows.

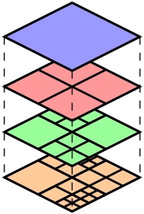
CELL-BASED AMR

Use of AMR to save computational costs.

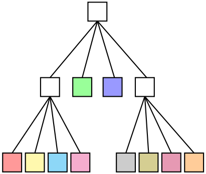
Mesh representation :



Cell refinement :



Tree structure equivalence :



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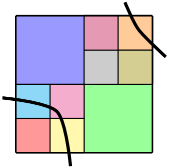

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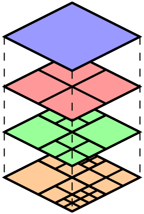

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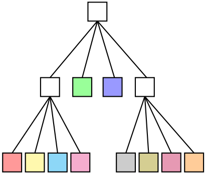

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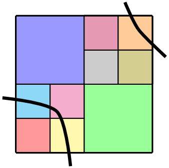

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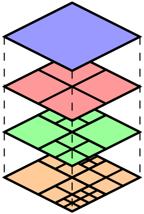

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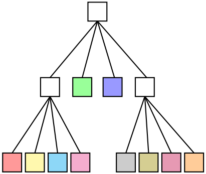

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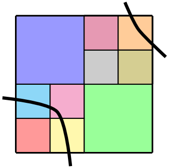

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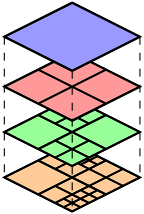

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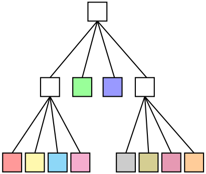

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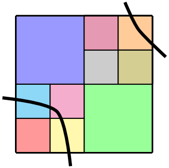

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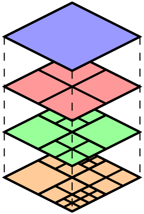

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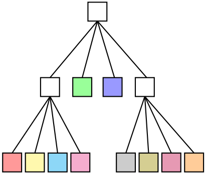

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- Other AMR techniques :
  - block-based AMR,
  - multi-resolution techniques (using wavelets).

FVS AND HLLC RIEMANN SOLVER

3-equation model :

$$\left\{\begin{array}{ccccc} \partial_t \rho & + & \nabla \cdot (\rho \mathbf{u}) & = & 0 \\ \partial_t (\rho Y) & + & \nabla \cdot (\rho Y \mathbf{u}) & = & 0 \\ \partial_t \left(\rho \mathbf{u}\right) & + & \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p & = & \rho \mathbf{g} \end{array}\right.$$

---

11. E. F. Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics - A Practical Introduction*. Springer, 3rd edition, 2009
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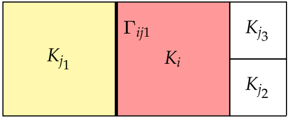

- First order Finite Volume Scheme,

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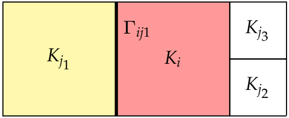

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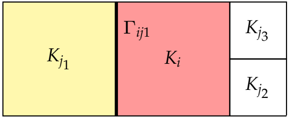

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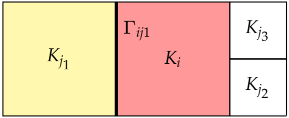

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- First order Finite Volume Scheme,
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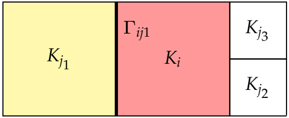
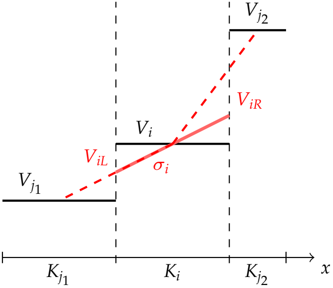
- One-direction approximate Riemann solver using HLLC, [11]
- Work on well-balanced aspects (for gravity source term),
- MUSCL-Hancock space and time second-order method :
  - `minmod` slope reconstruction at cell interfaces,
  - Hancock prediction step. [12]





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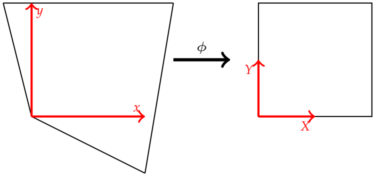
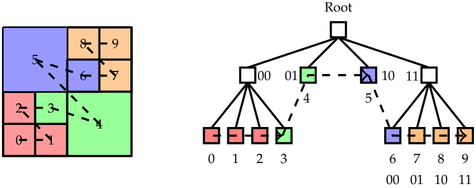
PARALLEL ALGORITHMS

p4est[13] library offers parallel algorithms to treat 2D and 3D meshes.

Principles :

- One-to-one transformation from physical space to unit cubes (trees),
- Morton space-filling curve inside each tree,
- storage of indexed cells into one array,
- subdivision of the array into MPI processes.





p4est algorithms are shown to scale on several thousands of MPI processes.

---

[13] C. Burstedde, L. C. Wilcox, and O. Ghattas. `p4est` : Scalable algorithms for parallel adaptive mesh refinement on forests of octrees. *SIAM Journal on Computing*, 33(3) :1103–1133, 2011

PRESENTATION OF CANOP

p4est library is used in CanoP.

Presentation :

- C/C++ code,
- FVS and approximate Riemann solvers (HLLC, Suliciu)
- 4 systems of equations :
  - scalar advection,
  - 3-equation two-fluid model,
  - MHD equations,
  - spray model.
- different refinement criteria (based on gradients),
- inputs :
  - specific connectivities and initial conditions,
  - use of p4est functions to read external connectivities (ABAQUS-type file) or initial conditions.
- outputs : HDF5 files, statistics.

Scaling and AMR advantages :[14]

---

[14] F. Drui, A. Fikl, P. Kestener, S. Kokh, A. Larat, V. Le Chenadec, and M. Massot. Experimenting with the p4est library for amr simulations of two-phase flows. to be published in ESAIM : Proceedings and Surveys, 2016

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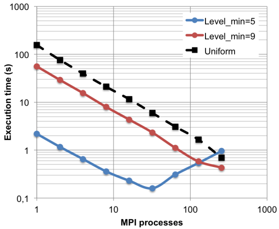

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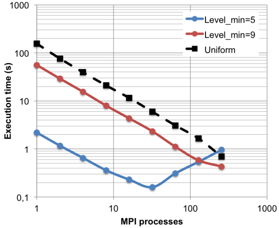
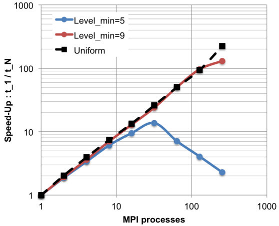


- Strong scaling :



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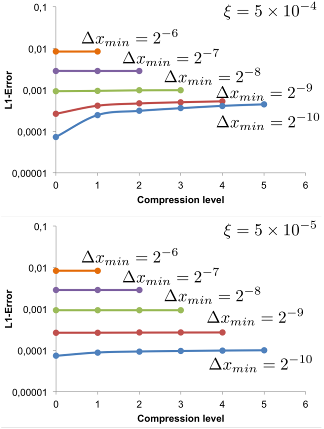
- Influence of refinement criterion :



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SIMULATION CONFIGURATIONS AND INTEREST

Simulation of interfacial flows : break of a dam.

- to test model and schemes,
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- possibility to compare with experimental measures.

Description :

Scheme :

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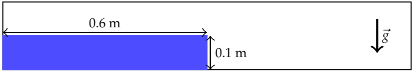

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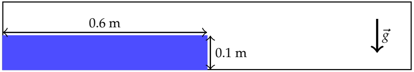

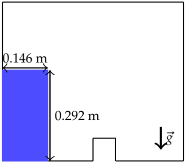

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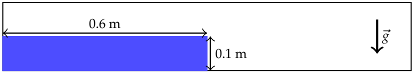

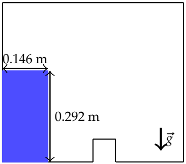

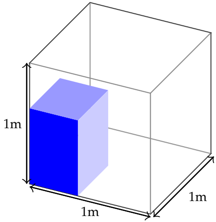

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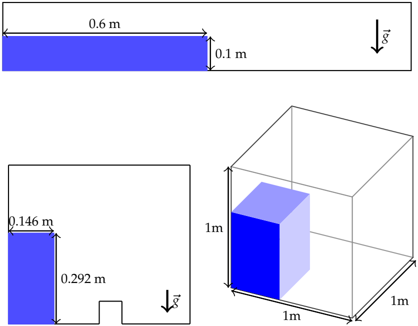

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- cartesian mesh,
- triangular mesh,
- all-regime schemes (low-Mach)

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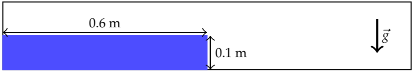

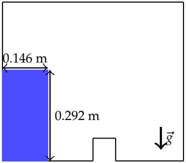

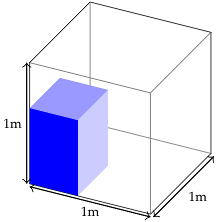

2D DAM BREAK

Reference simulation :[15]

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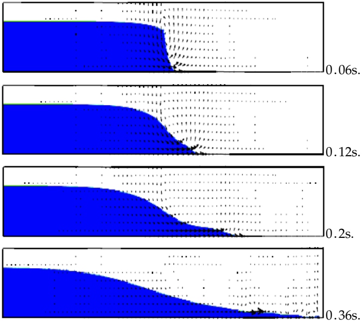

Credit S. Vincent

Results :

- Uniform mesh :
  - 3072×512 cells, 4.2×10^6 iterations,
  - 66 h on 120 MPI processes (Intel Xeon X5650)

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15. S. Vincent. *Modélisation d'écoulements incompressibles de fluides non-miscibles*. PhD thesis, Université de Bordeaux, 1999

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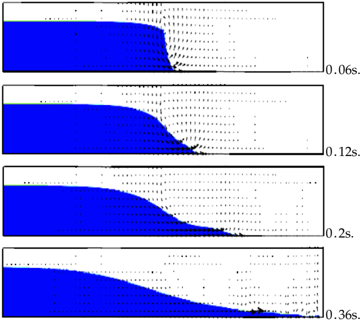
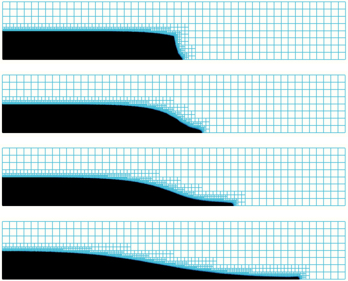


Credit S. Vincent

Results :

- Refinement in liquid phase :
  - $\sim 4.0 \times 10^5$ cells ($\sim$ 75% compression rate),
  - 22 h on 120 MPI processes (Intel Xeon X5650)



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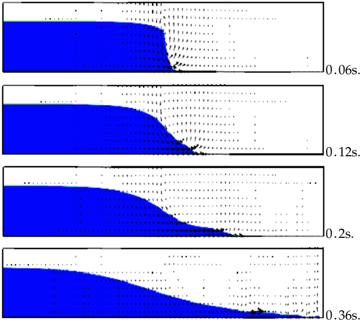
[15] S. Vincent. *Modélisation d'écoulements incompressibles de fluides non-miscibles*. PhD thesis, Université de Bordeaux, 1999

2D DAM BREAK

Reference simulation : [15]

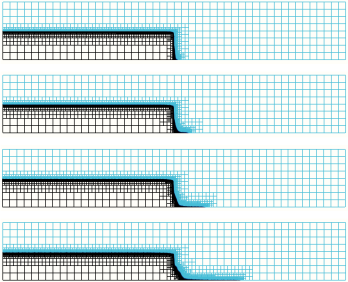
- Incompressible fluids,
- Augmented Lagrangian method.



Credit S. Vincent

Results :

- Refinement near interface ($\Delta\alpha$) :
  - from 1.1×10^4 to 7.8×10^4 cells ($>$ 95% compression rate),
  - 5 h on 120 MPI processes (Intel Xeon X5650)



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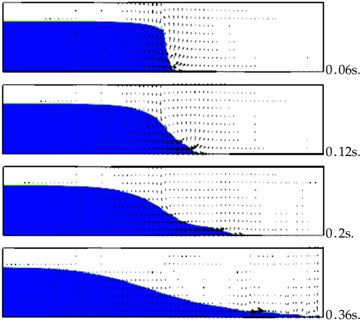

Credit S. Vincent

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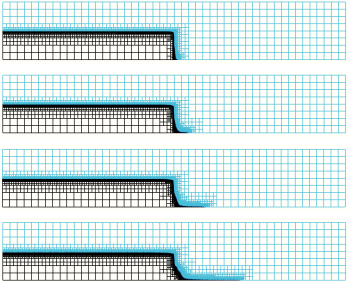


Observations :

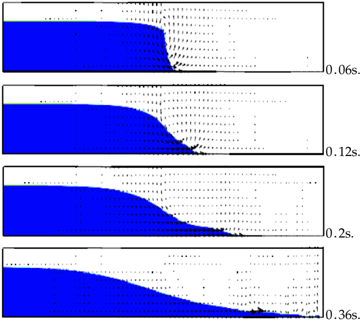
- the refined solution is far from the uniform solution,
- and far from the incompressible solution.
- We suspect a low-Mach problem in the coarsest cells !

$\Rightarrow$ test with a triangular mesh...

2D DAM BREAK

Reference simulation : [15]

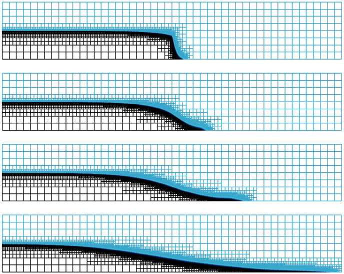
- Incompressible fluids,
- Augmented Lagrangian method.



Credit S. Vincent

Results :

- Triangular mesh and refinement near interface ($\Delta\alpha$) :



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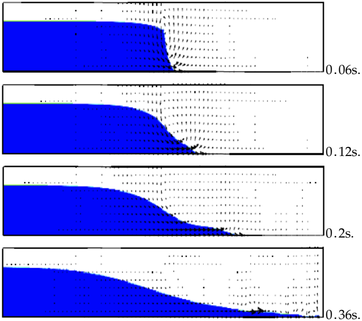
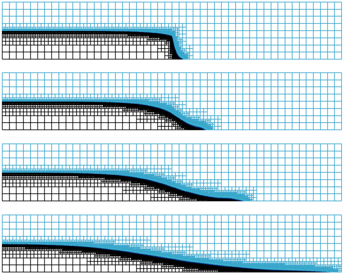


Credit S. Vincent

Results :

- Triangular mesh and refinement near interface ($\Delta\alpha$) :



Observations :

- the solution with the triangular mesh is much better !
- very probably low-Mach difficulties !

$\Rightarrow$ use the low-Mach regime strategy [16]

---

[16] S. Vincent. *Modélisation d'écoulements incompressibles de fluides non-miscibles*. PhD thesis, Université de Bordeaux, 1999

2D DAM BREAK

Reference simulation : [15]

- Incompressible fluids,
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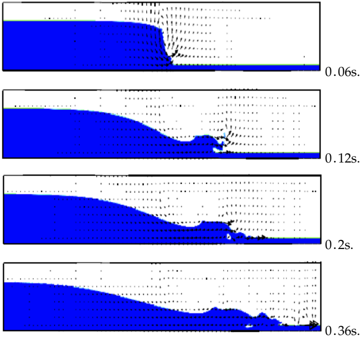
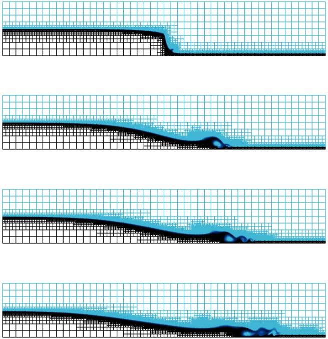


Credit S. Vincent

Results :

- Triangular mesh and refinement near interface ($\Delta\alpha$) :



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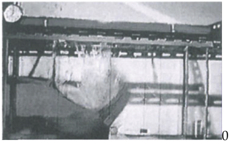
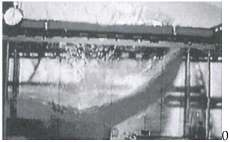
[15] S. Vincent. *Modélisation d'écoulements incompressibles de fluides non-miscibles*. PhD thesis, Université de Bordeaux, 1999

2D DAM BREAK WITH OBSTACLE

Experiment :[16]

Simulations :


0.2s


0.3s


0.4s

Credit F. Golay

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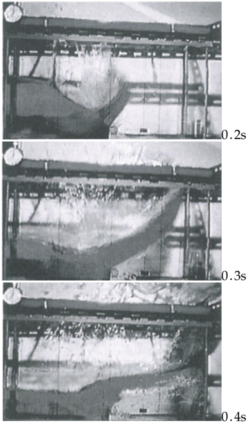
[16] S. Koshizuka, H. Tamako, and Y. Oka. A particle method for incompressible viscous flow with fluid fragmentations. *Computational Fluid Dynamics Journal*, 4(1) :29–46, 1995

2D DAM BREAK WITH OBSTACLE

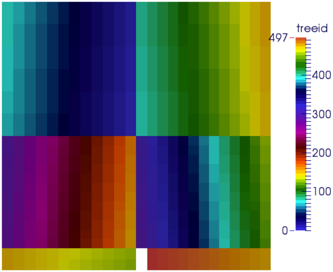
Experiment :[16]



Credit F. Golay

Simulations :

- Forest of 498 *quadtrees* :



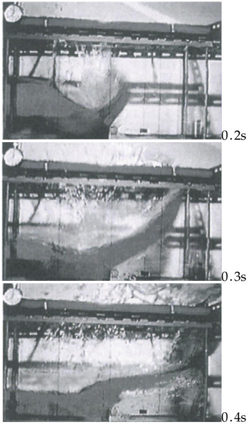
- Refinement on pressure gradient and near interface.
- Computation characteristics :
  - Min number of cells : 5.5×10^4
  - Max number of cells : 5.5×10^5
  - Number of iterations : 5.6×10^4
  - Machine : Igloo (ECP Mesocenter)
  - MPI processes : 120
  - Computation time : 35 min

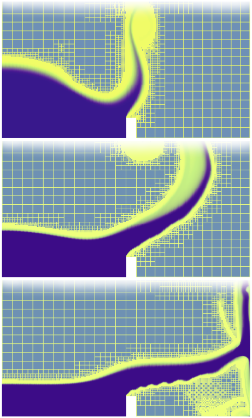
---

[16] S. Koshizuka, H. Tamako, and Y. Oka. A particle method for incompressible viscous flow with fluid fragmentations. *Computational Fluid Dynamics Journal*, 4(1) :29–46, 1995

2D DAM BREAK WITH OBSTACLE

Experiment :[16] **Simulations :**





Credit F. Golay

Conclusion :

- Cost of computation could be reduced using criterion on interface only,
- but numerical problems have to be solved before !

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[16] S. Koshizuka, H. Tamako, and Y. Oka. A particle method for incompressible viscous flow with fluid fragmentations. *Computational Fluid Dynamics Journal*, 4(1) :29–46, 1995

3D DAM BREAK

Description :

- Unit cube,
- artificially low sound velocities (in pressure laws : $\tilde{c}_k = c_k/100$),
- refinement on volume fraction gradient ($\nabla\alpha$),
- up to 8 levels of refinement (equivalent mesh is 256^3),
- 512 MPI processes, 4h of computation.

3D DAM BREAK

Description :

- Unit cube,
- artificially low sound velocities (in pressure laws : $\tilde{c}_k = c_k/100$),
- refinement on volume fraction gradient ($\nabla\alpha$),
- up to 8 levels of refinement (equivalent mesh is 256^3),
- 512 MPI processes, 4h of computation.

Simulation performed on Jade (former CINES supercomputer)

Part 5

Conclusions

CONCLUSION AND FUTURE WORK

In conclusion, we have developed :

- a general model taking into account subscale effects of interface dynamics,
- subsystems related to the general model by parameters,
- a model for monodisperse bubbles with simple topological assumption. ⇒ go further in modelling with the same derivation methods to get closer to spray models.
- a numerical strategy for managing multiple physical scales :
  - numerical scheme adapted to all models of the hierarchy,
  - 2D/3D tools using an AMR strategy.

⇒ solve for the last difficulties, ⇒ finish the implementation of the presented (and future) models, ⇒ perform a simulation in a real configuration.

Thank you for your attention !

Papers

F. Drui, A. Larat, V. Le Chenadec, S. Kokh, and M. Massot. A hierarchy of simple hyperbolic two-fluid models for bubbly flows. in the process of writing

F. Drui, A. Fikl, P. Kestener, S. Kokh, A. Larat, V. Le Chenadec, and M. Massot. Experimenting with the p4est library for amr simulations of two-phase flows. to be published in ESAIM : Proceedings and Surveys, 2016

Acknowledgements : Research funded by DGA (General Directorate for Armament), CEA and EM2C, CNRS, CentraleSupelec. Simulations performed on Mesocentre de l'ECP.