Simulation of Multi-Material Compressible Flows with Interfaces

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Congrès SMAI – Guidel
May 26, 2011

Outline

Collaborations

The present work is the result of several collaborations

- M. Billaud-Friess
- B. Boutin
- F. Caetano
- F. Faccanoni
- F. Lagoutière
- L. Navoret
- CCRT Support Team
- A. Geay
- V. Michel
- V. Faucher
- P. Salvatore
- O. Grégoire

Outline

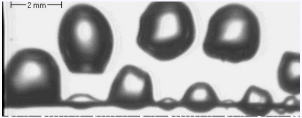
1. Framework and Interface Capture Methods
   - Industrial Application Problem Examples
   - Simulation Framework
   - Model Main Properties

A Target (Open) Problem for Nuclear Safety Simulation

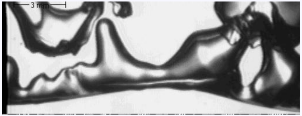
Phenomenon

- Liquid phase heated by a wall (pool boiling) at a given temperature T_{wall}.
- As T_{wall} increases there is a transition from the Nucleate Boiling Regime to the Film Boiling Regime. This transition is still not understood.

Nucleate Boiling



Critical Flux



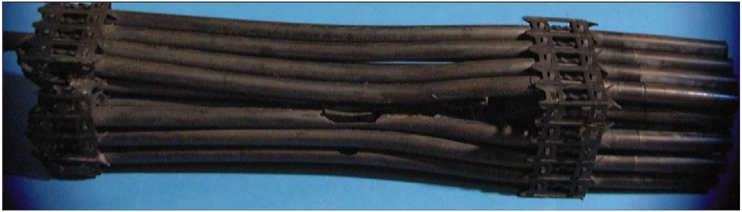
Film Boiling

source : `http://www.spaceflight.esa.int/users/fluids/TT_boiling.htm`

A difficult problem

- Determining the most significant physical scale is still an open issue
- Performing experiments is difficult.

Damage after “insulation” by a vapor film



(Omega Experiment, CEA)

More Application Examples

Nuclear Safety

- Boiling Crisis
- Vapor Explosion
- Fluid-Structure Interaction
- Security Study Involving Free Surface Dynamics

Comubstion Engines

Fuel Injection(subsonic and supersonic jets)

And More...

Fluid Flow in Food Processing

- mixing
- paste injection
- ...

Laser ICF

Study of N-Components Flow (M. Billaud-Friess)

Simulation Framework

Physical Framework

- Simulation of two-component flows with interfaces
- Each fluid $k = 0, 1$ is compressible, EOS_k: $(\rho_k, P_k) \mapsto \varepsilon_k$
- Single velocity kinematics and the interface is passively advected at the local velocity

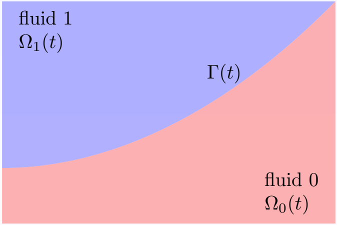
Numerical Method "Guidelines"

- Focus on scalable methods
- No interface reconstruction

A First Model Problem: Free Boundary Coupling Problem

Coupling Problem with a Free Boundary

The problem can be expressed as a simple Euler×Euler coupling problem across a moving boundary $\Gamma(t)$ where both pressure and velocity are continuous.



$$e = \varepsilon + u^2/2$$

Coupled Euler Systems

$$\frac{\partial}{\partial_t}\begin{bmatrix}\rho\\ \rho u\\ \rho e\end{bmatrix} + \frac{\partial}{\partial_x}\begin{bmatrix}\rho u\\ \rho u^2 + P_0\\ (\rho e + P_0)u\end{bmatrix} = 0, x \in \Omega_0(t)$$

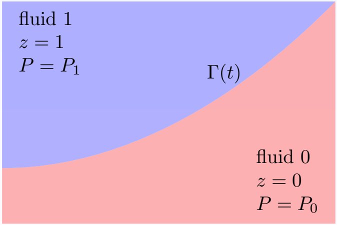
$$\frac{\partial}{\partial_t}\begin{bmatrix}\rho\\ \rho u\\ \rho e\end{bmatrix} + \frac{\partial}{\partial_x}\begin{bmatrix}\rho u\\ \rho u^2 + P_1\\ (\rho e + P_1)u\end{bmatrix} = 0, x \in \Omega_1(t)$$

P and u continuous across $\Gamma(t)$

A Second Model Problem: Global Formulation

"Equivalent" Problem: Coupling via an Augmented System

The boundary = the discontinuity locus of an additional variable z called a "color function" which is passively advected at local velocity.



Extended Euler System

$$\frac{\partial}{\partial_t}\begin{bmatrix}\rho\\ \rho u\\ \rho e\\ \rho z\end{bmatrix}+\frac{\partial}{\partial_x}\begin{bmatrix}\rho u\\ \rho u^2+P\\ (\rho e+P)u\\ \rho u z\end{bmatrix}=0, \quad x\in\Omega$$

$z(t=0,x)\in\{0,1\}$

P such that $P(z,\rho,\varepsilon)=\begin{cases}P_0(\rho,\varepsilon), & \text{if } z=0\\ P_1(\rho,\varepsilon), & \text{if } z=1\end{cases}$

Modelling Issues

Values $z \in \{0, 1\}$, $t = 0$

Classical approx. strategies for

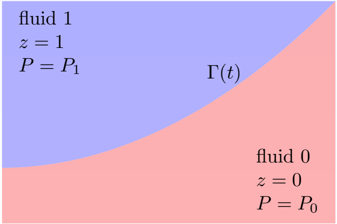
$$\partial_t \rho z + \mathrm{div}(\rho \mathbf{u} z) = 0$$

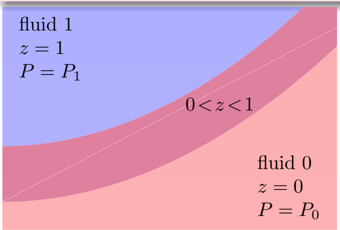
or

$$\partial_t z + \mathbf{u} \cdot \nabla z = 0$$

Values $0 < z < 1$, $t > 0$

$$\mathrm{EOS} = \begin{cases} \mathrm{EOS}_0 & \text{if } z = 0 \\ ? & \text{if } 0 < z < 1 \\ \mathrm{EOS}_1 & \text{if } z = 1 \end{cases}$$





Modelling Issues

Values $z \in \{0, 1\}$, $t = 0$

Classical approx. strategies for

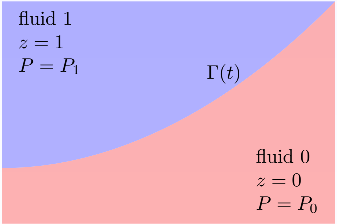
$$\partial_t \rho z + \mathrm{div}(\rho \mathbf{u} z) = 0$$

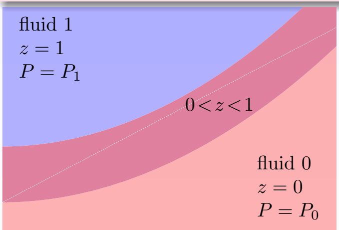
or

$$\partial_t z + \mathbf{u} \cdot \nabla z = 0$$

Values $0 < z < 1$, $t > 0$

$$\mathrm{EOS} = \begin{cases} \mathrm{EOS}_0 & \text{if } z = 0 \\ \text{Numerical Mixture Model} & \text{if } 0 < z < 1 \\ \mathrm{EOS}_1 & \text{if } z = 1 \end{cases}$$





(Numerical?) Mixture Model: Abgrall, Allaire, Clerc, Coquel, Dellacherie, Després, Hérard, Karni, Kokh, Lagoutière, Larrouturou, Massoni, Saurel, Seguin, Shyue, Kapila, Menikoff, Miller, Puckett...

Five-Equation Model (with isobaric closure)

Conservative Form

$$
\begin{cases}
\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\
\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P\mathrm{Id}) = 0 \\
\partial_t(\rho e) + \operatorname{div}[(\rho e + P)\mathbf{u}] = 0 \\
\\
\partial_t(\rho y) + \operatorname{div}(\rho y \mathbf{u}) = 0 \quad \text{(partial mass conservation)} \\
\partial_t(\rho z) + \operatorname{div}(\rho z \mathbf{u}) = 0, \quad \text{(color function transport)}
\end{cases}
$$

(Allaire, Clerc, Kokh)

$$
\rho = z\rho_1 + (1-z)\rho_0, \quad e = \varepsilon + |u|^2/2, \quad y = z\rho_1/\rho,
$$

$$
\rho\varepsilon = z\rho_1\varepsilon_1(\rho_1, P) + (1-z)\rho_0\varepsilon_0(\rho_0, P) \quad \text{(Isobaric closure)}
$$

Five-Equation Model (with isobaric closure)

Quasi-Conservative Form (used for discretization)

$$
\begin{cases}
\partial_t \rho + \mathrm{div}(\rho \mathbf{u}) = 0 \\
\partial_t (\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u} + P \mathrm{Id}) = 0 \\
\partial_t (\rho e) + \mathrm{div}[(\rho e + P)\mathbf{u}] = 0 \\
\\
\partial_t (\rho y) + \mathrm{div}(\rho y \mathbf{u}) = 0 \quad \text{(partial mass conservation)} \\
\partial_t z + \mathbf{u} \cdot \nabla z = 0, \quad \text{(color function transport)}
\end{cases}
$$

(Allaire, Clerc, Kokh)

$$
\rho = z\rho_1 + (1-z)\rho_0, \quad e = \varepsilon + |u|^2/2, \quad y = z\rho_1/\rho,
$$

$$
\rho\varepsilon = z\rho_1\varepsilon_1(\rho_1, P) + (1-z)\rho_0\varepsilon_0(\rho_0, P) \quad \text{(Isobaric closure)}
$$

Rankine-Hugoniot Relations: Weak solutions are well defined. No ambiguity with the non-conservative product $\mathbf{u} \cdot \nabla z$

Model Main Properties

- The system can be expressed in an equivalent full conservative form
- The solution of the Riemann problem is available.
- Hyperbolicity (real characteristics) is ensured when $\xi_k = (\partial \rho_k \varepsilon_k / \partial P_k)_{\rho_k} > 0$ (reads $\gamma_k > 1$ for perfect gases)
- Eigenstructure of the system: $\{u - c, u, u, u, u + c\}$
- $u \pm c$: GNL field (acoustic waves), u: LD field (material waves)
- Sound velocity c given by

$$\xi c^2 = y \xi_1 c_1^2 + (1 - y) \xi_0 c_0^2,$$

$$\xi = z \xi_1 + (1 - z) \xi_0, \quad c_k = \text{pure fluid } k \text{ sound velocity}$$

- No entropy so far for the general case...

A Few Remarks about Mixture Models

Holy Cow! This Void Fraction Equation is Wrong!!

Numerous other models use: $\partial_t z + \mathbf{u} \cdot \nabla z = \beta \mathrm{div} \mathbf{u}$

Where is β? (Murrone, Kapila, Guillard, Massoni, Saurel, Puckett, Miller, Koren...)

Sacrebleu! The Mixture Model is Wrong!!

$P_1 = P_0$ is wrong in a physical mixture (strong shock impacting a mixture)

Similar Equations but Very Different Physics

- Numerical Mixture $\neq$ Physical Mixture:
  Parent averaged scale model $\Rightarrow$ Reduced averaged scale model.
- Our model cannot produce mixture zone in the exact solution for initial values such that.

$$\forall x, \quad z(x, t = 0) \in \{0, 1\} \Rightarrow \forall x, \quad z(x, t > 0) \in \{0, 1\}$$

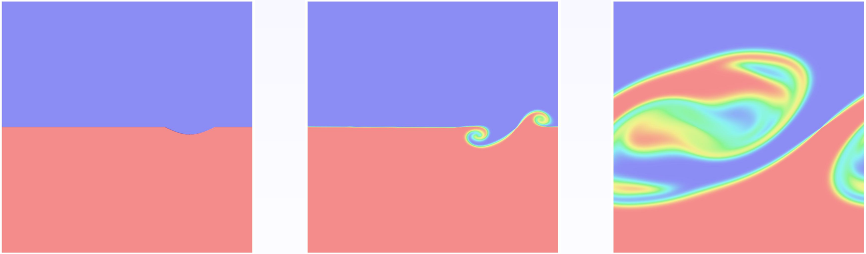
z is governed by a LD Field $=$ z values are advected.

Numerical Issues (1)

Drawback

Most schemes tend to smear (sooner or later) the interface until it cannot be properly located.

Kelvin-Helmholtz Instability.



Possible cure without interface reconstruction?

Outline

"Target" Discretization Strategy

We aim at deriving a time-explicit quasi-conservative Finite-Volume type discretization of the system.

$$\rho\mathbf{W} = (\rho y, \rho, \rho u, \rho e)^T$$

$$\rho_j^{n+1}\mathbf{W}_j^{n+1} - \rho_j^n\mathbf{W}_j^n + \lambda(\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}) = 0$$

$$z_j^{n+1} - z_j^n + \lambda(u_{j+1/2}\widetilde{z}_{j+1/2} - u_{j-1/2}\widetilde{z}_{j-1/2}) - \lambda z_j^n(u_{j+1/2} - u_{j-1/2}) = 0$$

Finite-Volume via a Lagrange-Remap Approach

Lagrange-Remap

The discretization of the convection operator is splitted into two step

- Lagrange Step:
  - the convection via a Lagrangian description
  - transport is frozen (while the mesh is distorted in the original Eulerian mesh)
- Remap (or Projection) Step:
  - resample the solution over the original Eulerian mesh
  - equivalent to account for the fluid transport

Lagrangian Coordinates

$$\frac{\partial \mathscr{X}}{\partial t}(x,t) = u(\mathscr{X}(x,t),t), \quad \mathscr{X}(x,t=0) = x$$

$$D_t a = (\partial \tilde{a}/\partial t)_{\mathscr{X}}, \quad (\partial a/\partial x)_t = (\widetilde{\rho}_{|t=0}/\widetilde{\rho})(\partial \tilde{a}/\partial \mathscr{X})_t$$

The system reads (for regular solutions)

$$\begin{cases} \mathrm{D}_t z = 0, \quad \mathrm{D}_t y = 0 \\ \rho \mathrm{D}_t \begin{bmatrix} 1/\rho \\ u \\ e \end{bmatrix} + \begin{bmatrix} -u \\ P \\ Pu \end{bmatrix}_x = 0 \end{cases}$$

$$\mathrm{D}_t \cdot = \partial_t \cdot + u \partial_x \cdot$$

Euler Coord. $a(x,t) \longleftrightarrow$ Lagrange Coord. $\widetilde{a}(\mathscr{X},t)$

$$(\mathrm{L}) \begin{cases} \widetilde{z}_t = 0, \quad \widetilde{y}_t = 0 \\ \widetilde{\rho}_{t=0} \begin{bmatrix} 1/\widetilde{\rho} \\ \widetilde{u} \\ \widetilde{e} \end{bmatrix}_t + \begin{bmatrix} -\widetilde{u} \\ \widetilde{P} \\ \widetilde{P}\widetilde{u} \end{bmatrix}_{\mathscr{X}} = 0 \end{cases}$$

Lagrange-Remap Process

We only consider a single timestep: $t^n \to t^{n+1}$.

Map the Euler variable onto the Lagrange variable.

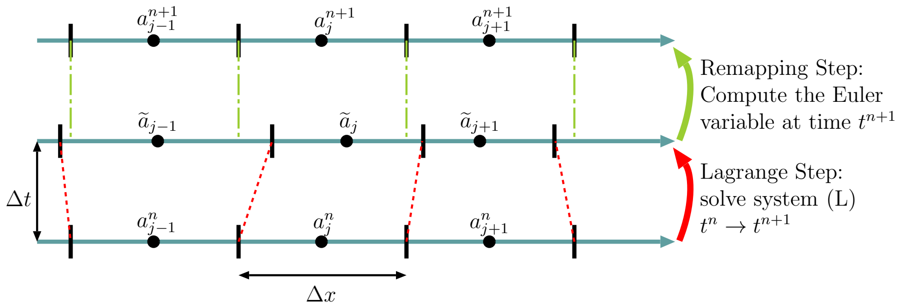
$a_j^n = \widetilde{a}_j^n$

Update the Lagrange Variable

$\widetilde{a}_j^{n+1} \sim \widetilde{a}_j$

Final Euler Variable: Resample the solution over the original mesh

a_j^{n+1}



Outline

3. The Numerical Scheme
   - Lagrange Step
   - Remapping Step: General Structure
   - Remapping Step: Optimizing the Numerical Diffusion

Scheme for the Lagrange Step

Acoustic Scheme (Després) / Suliciu-Type Relaxation Scheme

$$\left\{\begin{array}{c}\begin{pmatrix}1/\widetilde{\rho}_j - 1/\rho_j^n \\ \widetilde{u}_j - u_j^n \\ \widetilde{e}_j - e_j^n\end{pmatrix} + \dfrac{\lambda}{\rho_j^n}\begin{pmatrix}-u_{j+1/2} + u_{j-1/2} \\ P_{j+1/2} - P_{j-1/2} \\ P_{j+1/2}u_{j+1/2} - P_{j-1/2}u_{j-1/2}\end{pmatrix} = 0 \\ \widetilde{z}_j = z_j^n, \quad \widetilde{y}_j = y_j^n, \quad \lambda = \Delta t/\Delta x\end{array}\right.$$

Flux Formulas

$$(\rho c)^*_{j+1/2} = \sqrt{\max[\rho_j^n(c_j^n)^2, \rho_{j+1}^n(c_{j+1}^n)^2]\min(\rho_j^n, \rho_{j+1}^n)}$$

$$P_{j+1/2} = \frac{1}{2}(P_j^n + P_{j+1}^n) - \frac{1}{2}(\rho c)^*_{j+1/2}(u_{j+1}^n - u_j^n)$$

$$u_{j+1/2} = \frac{1}{2}(u_j^n + u_{j+1}^n) - \frac{1}{2}\frac{1}{(\rho c)^*_{j+1/2}}(P_{j+1}^n - P_j^n)$$

This step preserves (P, u)-constant profiles.

CFL Condition

In the sequel we shall suppose that $\lambda = \Delta t/\Delta x$ verifies

$$\lambda \times \max_{j\in\mathbb{Z}} \Big(|u_{j+1/2}|, (\rho c)^*_{j+1/2} / \min(\rho^n_j, \rho^n_{j+1}) \Big) \leq C \qquad (\bigstar)$$

where usually $C \simeq 0.8$.
(numerical of the present talks performed with $C = 0.999$)

Scheme for the Remapping Step

General Form

$$\rho \mathbf{W} = (\rho y, \rho, \rho u, \rho e)^T$$

$$\rho_j^{n+1}\mathbf{W}_j^{n+1} - \widetilde{\rho_j \mathbf{W}}_j + \lambda\Big(u_{j+1/2}\widetilde{(\rho\mathbf{W})}_{j+1/2} - u_{j-1/2}\widetilde{(\rho\mathbf{W})}_{j-1/2}\Big)$$
$$-\lambda\widetilde{(\rho\mathbf{W})}_j(u_{j+1/2} - u_{j-1/2}) = 0$$

$$(z_j^{n+1} - z_j^n) + \lambda(u_{j+1/2}\widetilde{z}_{j+1/2} - u_{j-1/2}\widetilde{z}_{j-1/2}) - \lambda z_j^n(u_{j+1/2} - u_{j-1/2}) = 0$$

Building the scheme boils down to specify the following terms

$$\widetilde{y}_{j+1/2}, \quad \widetilde{\rho}_{j+1/2}, \quad \widetilde{u}_{j+1/2}, \quad \widetilde{\varepsilon}_{j+1/2}, \quad \widetilde{z}_{j+1/2}$$

Defining the Fluxes

$$\widetilde{z}_{j+1/2} = ?$$

$$\widetilde{u}_{j+1/2} = ?$$

$$\widetilde{y}_{j+1/2} = ?$$

$$\widetilde{\rho}_{j+1/2} = ?$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = ?$$

Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

Upwind choice $(j + 1/2 = \mathrm{upw})$ according to the sign of $u_{j+1/2}$ for phasic quantities ρ_0, ρ_1 and $\rho_0\varepsilon_0$, $\rho_1\varepsilon_1$.

Upwind choice too for u

Defining the Fluxes

$$\widetilde{z}_{j+1/2} = ?$$

$$\widetilde{u}_{j+1/2} = ?$$

$$\widetilde{y}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{j+1/2}/\widetilde{\rho}_{j+1/2}$$

$$\widetilde{\rho}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{j+1/2} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0)}_{j+1/2}$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1\varepsilon_1)}_{j+1/2} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0\varepsilon_0)}_{j+1/2}$$

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Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

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Defining the Fluxes

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$$\widetilde{\rho}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{\text{upw}} + (1 - \widetilde{z}_{j+1/2})\widetilde{(\rho_0)}_{\text{upw}}$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1\varepsilon_1)}_{\text{upw}} + (1 - \widetilde{z}_{j+1/2})\widetilde{(\rho_0\varepsilon_0)}_{\text{upw}}$$

Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

Upwind choice ($j + 1/2 = \text{upw}$) according to the sign of $u_{j+1/2}$ for phasic quantities ρ_0, ρ_1 and $\rho_0\varepsilon_0$, $\rho_1\varepsilon_1$.

Upwind choice too for u

Defining the Fluxes

$$\widetilde{z}_{j+1/2} = ?$$

$$\widetilde{u}_{j+1/2} = \widetilde{u}_{\mathrm{upw}}$$

$$\widetilde{y}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{\mathrm{upw}}/\widetilde{\rho}_{j+1/2}$$

$$\widetilde{\rho}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1)}_{\mathrm{upw}} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0)}_{\mathrm{upw}}$$

$$\widetilde{(\rho\varepsilon)}_{j+1/2} = \widetilde{z}_{j+1/2}\widetilde{(\rho_1\varepsilon_1)}_{\mathrm{upw}} + (1-\widetilde{z}_{j+1/2})\widetilde{(\rho_0\varepsilon_0)}_{\mathrm{upw}}$$

Enforce consistency for $\widetilde{y}_{j+1/2}$, $\widetilde{\rho}_{j+1/2}$, $\widetilde{\varepsilon}_{j+1/2}$.

Upwind choice ($j+1/2=\mathrm{upw}$) according to the sign of $u_{j+1/2}$ for phasic quantities ρ_0, ρ_1 and $\rho_0\varepsilon_0$, $\rho_1\varepsilon_1$.

Upwind choice too for u

Constraints for the flux $\widetilde{z}_{j+1/2}$

Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Under CFL condition ($\bigstar$), we have a "trust interval" for $\widetilde{z}_{j+1/2}$ that ensures stability for both y and z, and consistency for both fluxes $\widetilde{z}_{j+1/2}$ and $\widetilde{y}_{j+1/2}$.

stability for z_j^{n+1}

stability for y_j^{n+1}

consistency for $\widetilde{z}_{j+1/2}$

consistency for $\widetilde{y}_{j+1/2}$

$$\widetilde{z}_{j+1/2} \in \left[m_{j-1/2}, M_{j-1/2}\right] \bigcap \left[a_j, A_j\right] \bigcap \left[b_j, B_j\right] \bigcap \left[d_{j+1/2}, D_{j+1/2}\right]$$

Constraints for the flux $\widetilde{z}_{j+1/2}$

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$$\widetilde{z}_{j+1/2} \in \underbrace{\overbrace{\left[m_{j-1/2}, M_{j-1/2}\right]}^{\text{consistency for } \widetilde{z}_{j+1/2}} \bigcap \overbrace{\left[a_j, A_j\right]}^{\text{stability for } z_j^{n+1}} \bigcap \overbrace{\left[b_j, B_j\right]}^{\text{stability for } y_j^{n+1}} \bigcap \overbrace{\left[d_{j+1/2}, D_{j+1/2}\right]}^{\text{consistency for } \widetilde{y}_{j+1/2}}}_{\substack{\Cup \\ z_j^n}} \neq \emptyset$$

Constraints for the flux $\widetilde{z}_{j+1/2}$

Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Under CFL condition ($\bigstar$), we have a "trust interval" for $\widetilde{z}_{j+1/2}$ that ensures stability for both y and z, and consistency for both fluxes $\widetilde{z}_{j+1/2}$ and $\widetilde{y}_{j+1/2}$.

stability for z_j^{n+1} stability for y_j^{n+1}

consistency for $\widetilde{z}_{j+1/2}$ consistency for $\widetilde{y}_{j+1/2}$

$$\widetilde{z}_{j+1/2} \in \underbrace{\left[m_{j-1/2}, M_{j-1/2}\right] \bigcap \left[a_j, A_j\right] \bigcap \left[b_j, B_j\right] \bigcap \left[d_{j+1/2}, D_{j+1/2}\right]}_{\substack{\Cup \\ z_j^n}} \neq \emptyset$$

How should we choose $\widetilde{z}_{j+1/2}$?

Choosing the z-flux $\widetilde{z}_{j+1/2}$ (1)

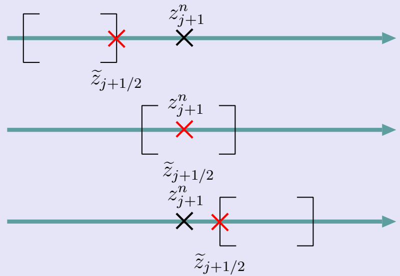
Suppose $u_{j-1/2} > 0$ and $u_{j+1/2} > 0$.

Després-Lagoutière Strategy: Limited Downwind Strategy

We choose the most downwinded possible value for $\widetilde{z}_{j+1/2}$ such that

$$\widetilde{z}_{j+1/2} \in \left[m_{j-1/2}, M_{j-1/2}\right] \bigcap \left[a_j, A_j\right] \bigcap \left[b_j, B_j\right] \bigcap \left[d_{j+1/2}, D_{j+1/2}\right]$$

$\widetilde{z}_{j+1/2}$ values axis



Choosing the $\widetilde{z}_{j+1/2}$ value is an explicit step: no CPU cost is needed, nor any recursive procedure.

Choosing the flux $\widetilde{z}_{j+1/2}$ (2)

What if $u_{j-1/2} < 0$ and $u_{j+1/2} > 0$?

For sake of "security" we opt for the upwind choice, i.e.

$$\widetilde{z}_{j+1/2} = z_j^n$$

Other cases

The cases $u_{j-1/2} > 0$, $u_{j+1/2} < 0$ and $u_{j-1/2} < 0$, $u_{j+1/2} < 0$ can be examined following the same lines and provide similar formulas for the flux $\widetilde{z}_{j+1/2}$.

Outline

4. Numerical Results
   - 1D Interface Advection
   - Sod-Type Shock Tube
   - 2D Air-R22 Shock-Interface Interaction
   - Kelvin-Helmholtz Instability

1D Interface Advection(1)

Test Description

Advection of a 1D "bubble" (pulse) involving two fluids

Inner bubble state

Analytical EOS

$\rho = 10^3, \quad P = 10^5, \quad u = 10^3$

Outter bubble State

Tabulated EOS

$\rho = 50, \quad P = 10^5, \quad u = 10^3$

- $1\,\mathrm{m}$ long domain discretized over a 100-cell mesh
- Periodic boundary conditions
- $t = 3.0\,\mathrm{s}$ (1 524 000 time steps)

1D Interface Advection(2)

EOS for the Inner Bubble Fluid (Stiffened Gas Equation)

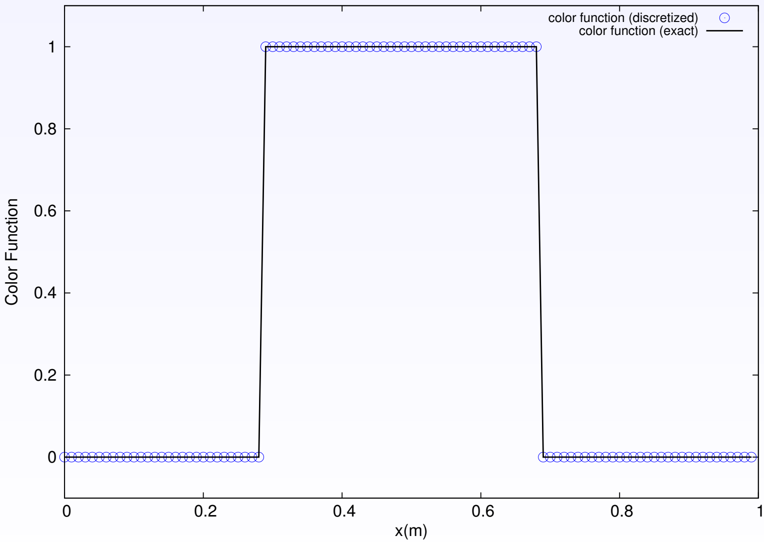
$$P = (\gamma_1 - 1)\rho\varepsilon - \gamma_1\pi_1, \quad \gamma_1 = 4.4, \quad \pi_1 = 6 \times 10^8\,\mathrm{Pa}$$

EOS for the Outter Bubble Fluid (Tabulated van der Waals Fluid)

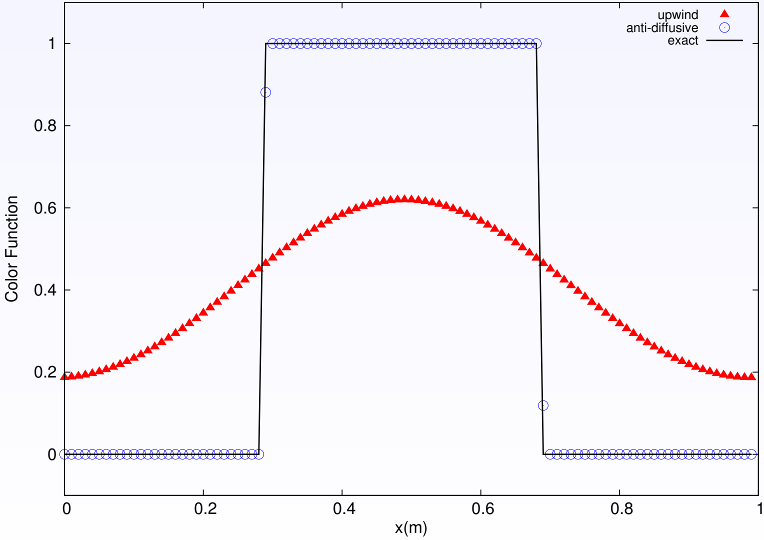
$$P = \left(\frac{\gamma_0 - 1}{1 - b_0\rho}\right)(\rho\varepsilon + a_0\rho^2) - a_0\rho^2, \quad \gamma_0 = 1.4, b_0 = 10^{-3}, a_0 = 5.$$

- Discretization of the $(\rho, P) \in [0, 990] \times [10^4, 10^9]$ over a uniform $10^3 \times 10^3$ grid.
- $(\rho, P) \mapsto \rho\varepsilon$ is provided thanks to a Q_1 interpolation
- $(\rho, \varepsilon) \mapsto P$ computed with a Newton method
- $P_1 = P_0$ resolved with a Dichotomy Algorithm

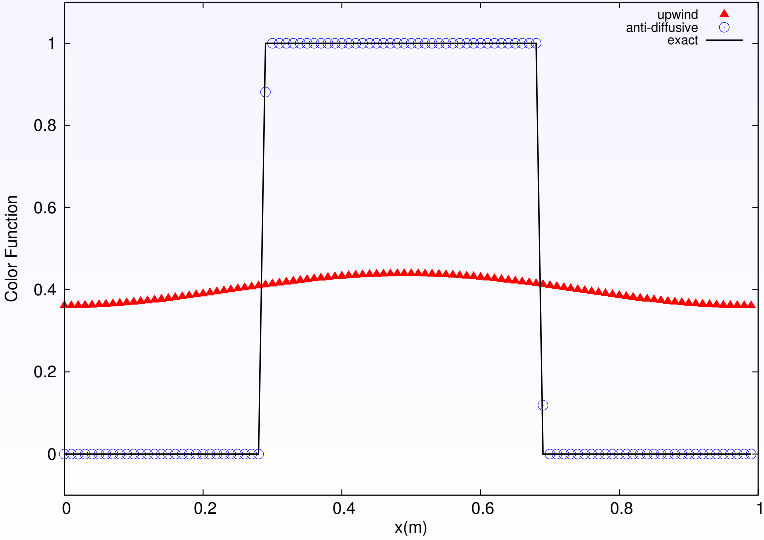
1D Interface Advection(3): Initial State



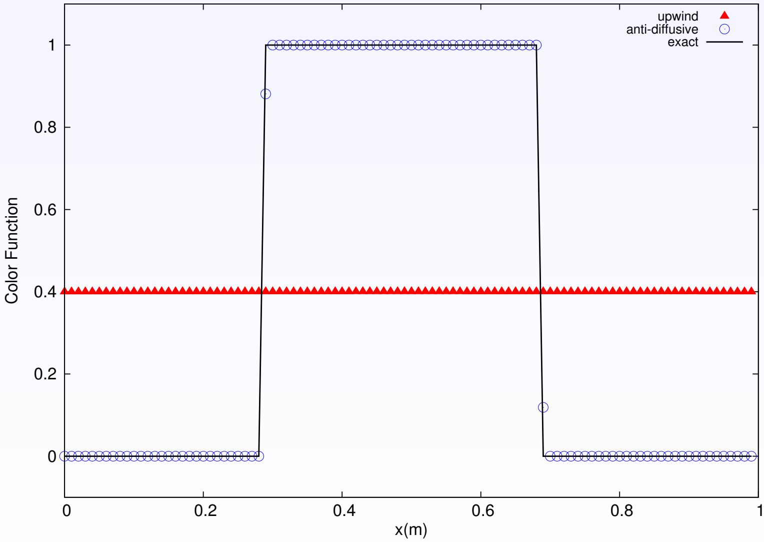
Interface Advection (4): Color Function at $t = 0.01$ s (step 5080)



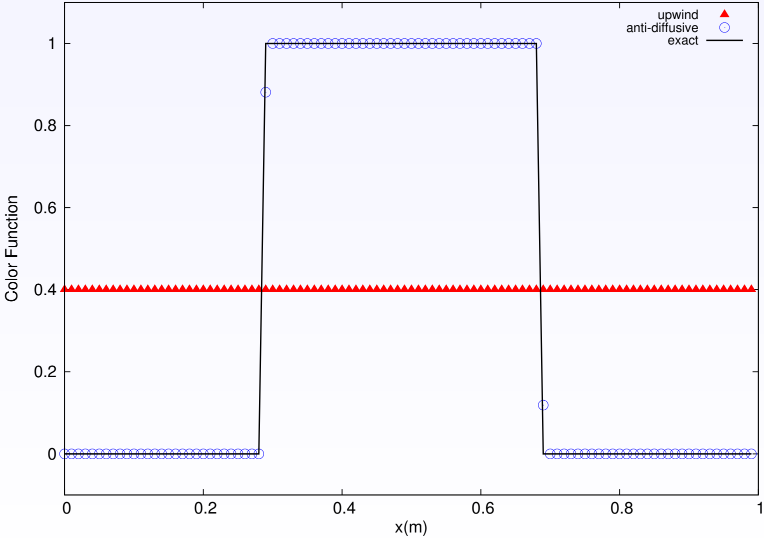
Interface Advection (5): Color Function at $t = 0.03$ s (step 15240)



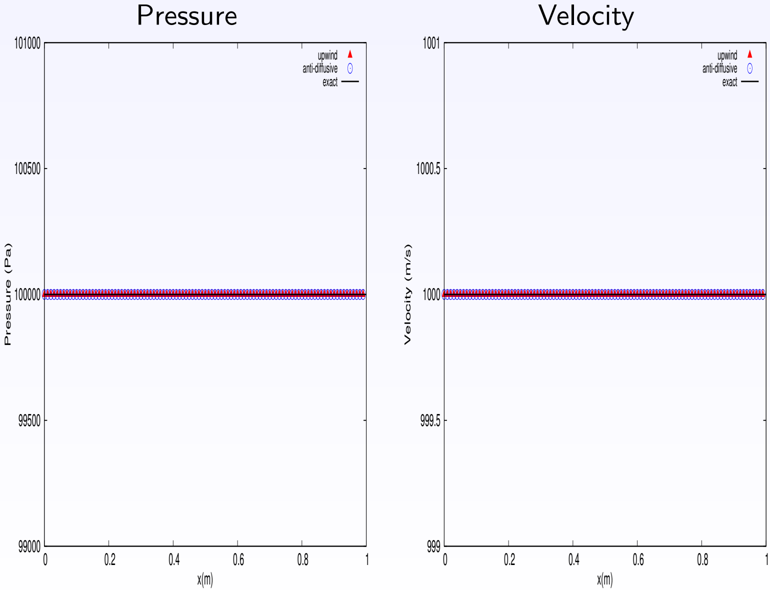
Interface Advection (6): Color Function at $t = 0.1$ s (step 50800)



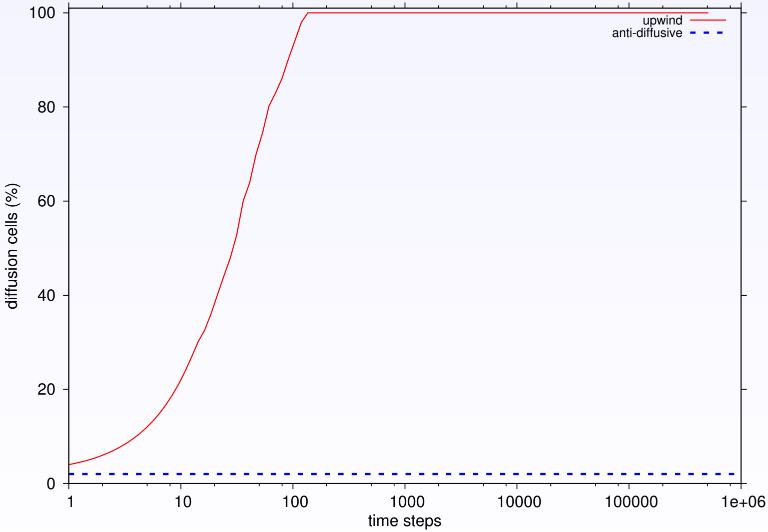
Interface Advection (7): Color Function at $t = 3.0\ \mathrm{s}$ (step 1524000)



Interface Advection (8): Pressure & Velocity at $t = 3.0$ s



Interface Advection (9): Numerical Diffusion



Shock Tube 1 (1)

Test Description

Riemann Problem with two perfect gases, adapted from the Sod Shock Tube Test

Left State

$\gamma = 1.4$

$\rho = 1.0$

$P = 1.0$

$u = 0.0$

Right State

$\gamma = 2.4$

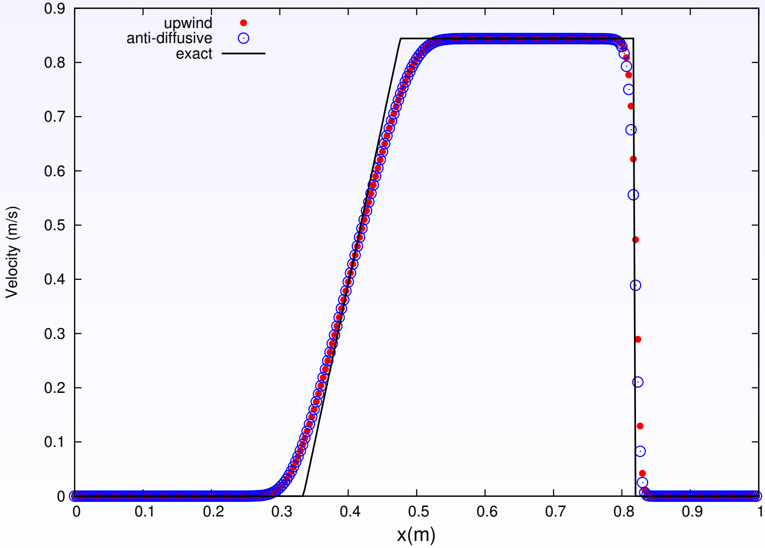
$\rho = 0.125$

$P = 0.1$

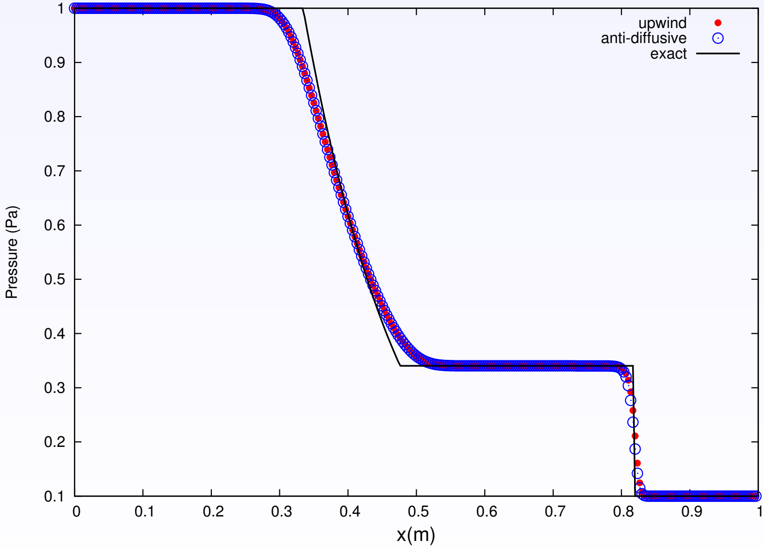
$u = 0.0$

- The domain is discretized over a 300-cell mesh.
- $t = 0.14s$

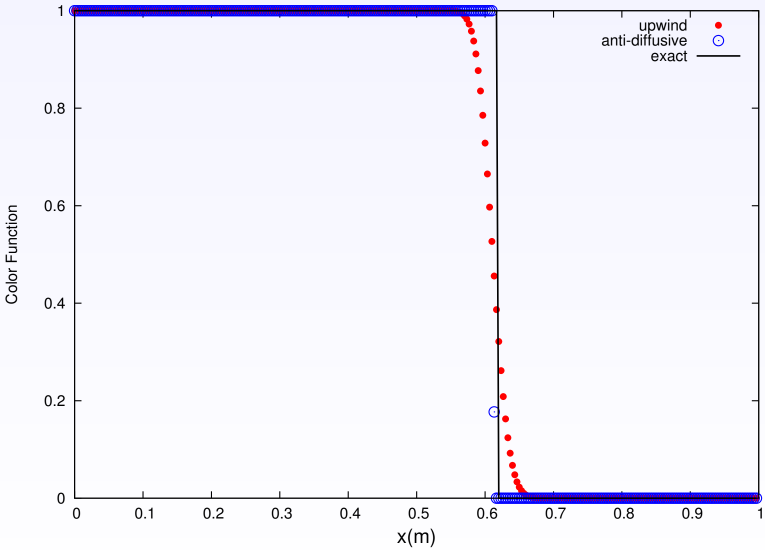
Shock Tube 1 (2): Velocity



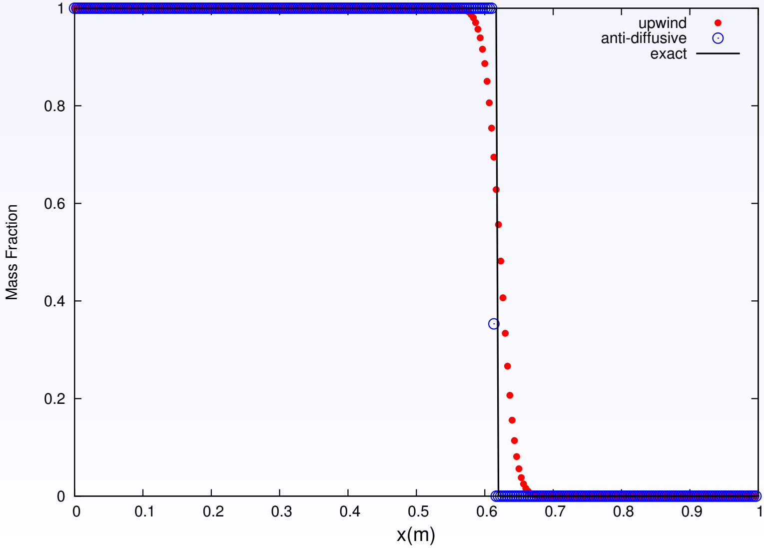
Shock Tube 1 (3): Pressure



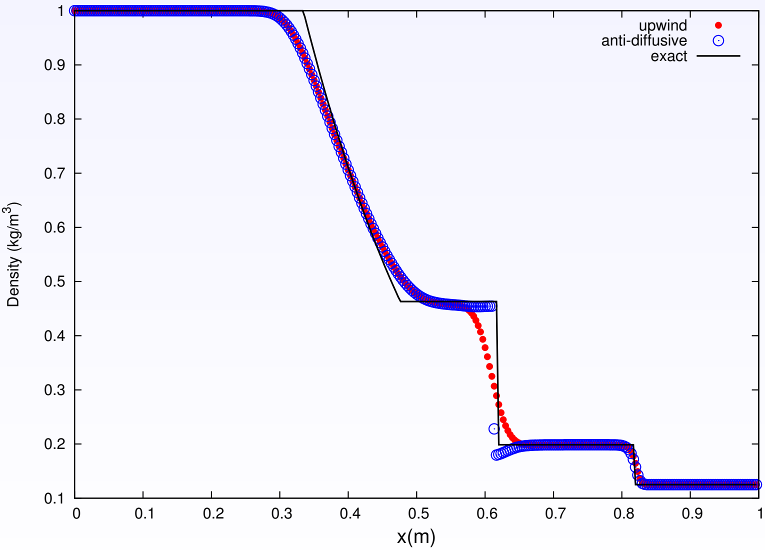
Shock Tube 1 (4): Color Function



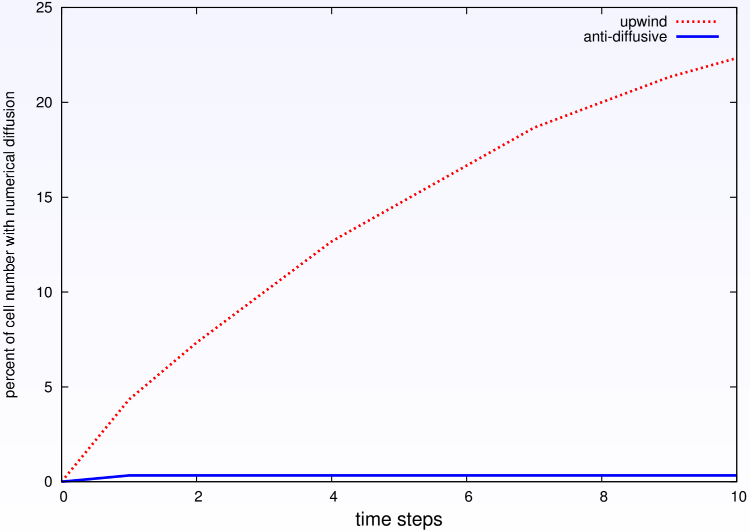
Shock Tube 1 (5): Mass Fraction



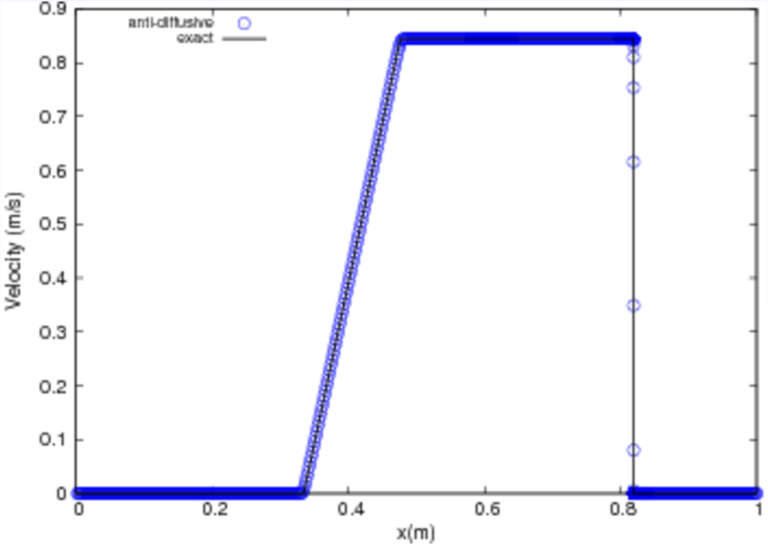
Shock Tube 1 (6): Density



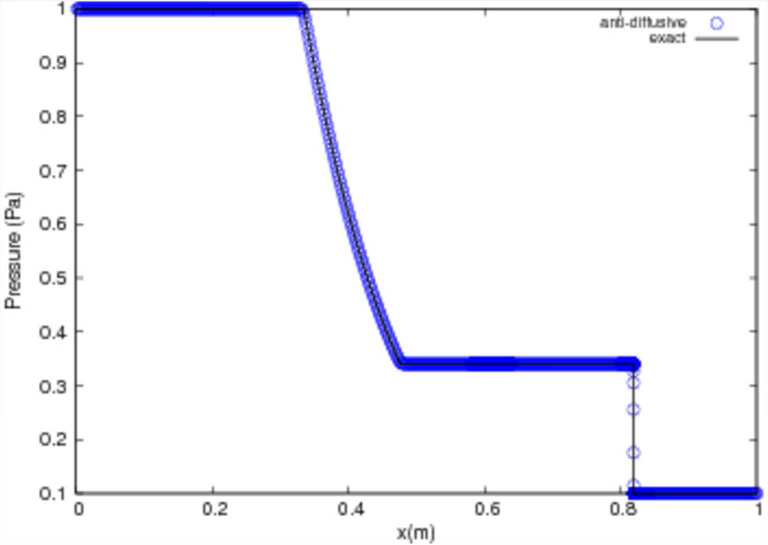
Shock Tube 1 (7): Numerical Diffusion of The Color Function



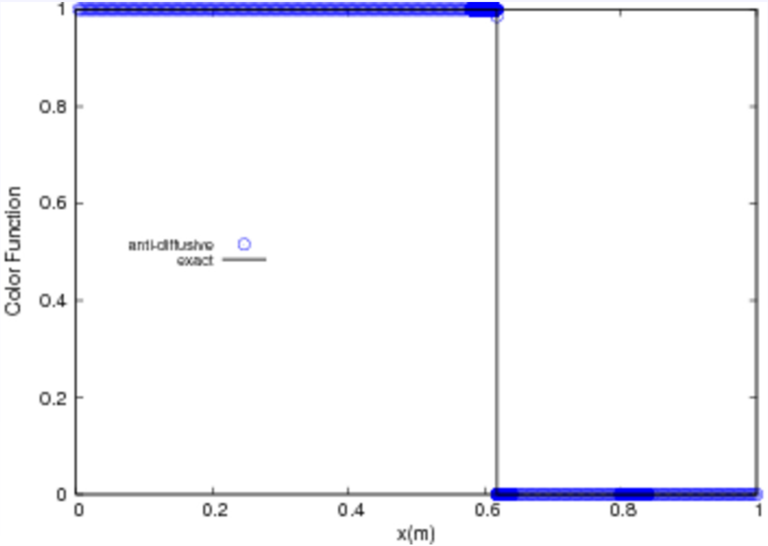
Shock Tube 1 (8): Velocity (50 000 cells)



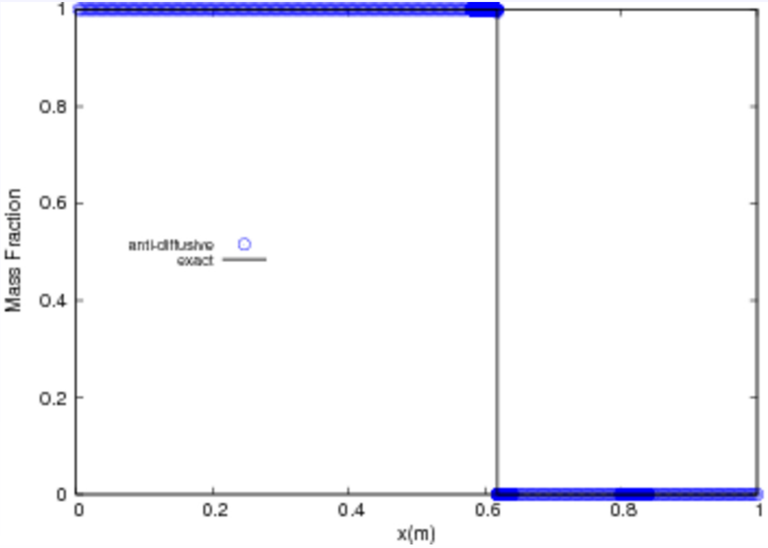
Shock Tube 1 (9): Pressure (50 000 cells)



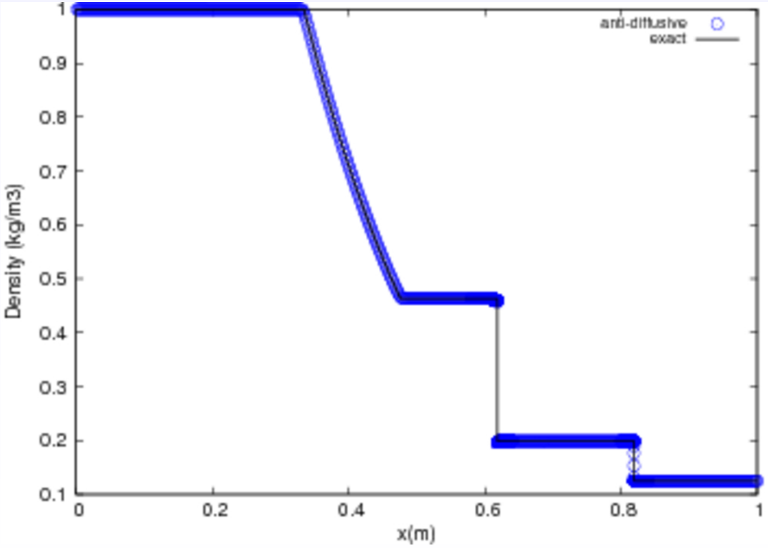
Shock Tube 1 (10): Color Function (50 000 cells)



Shock Tube 1 (11): Mass Fraction (50 000 cells)



Shock Tube 1 (12): Density (50 000 cells)

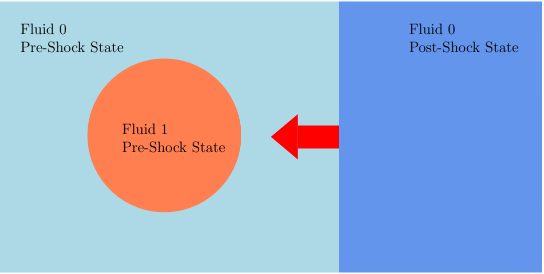


2D Air-R22 Shock-Interface Interaction (1)

Test Description

A planar shock hits a bubble initially at rest.

- Domain discretized over a 5000×1000 mesh
- Two perfect gases



Ref : Haas&Sturtevant(Experiment), Quirk&Karni, Shyue, . . .

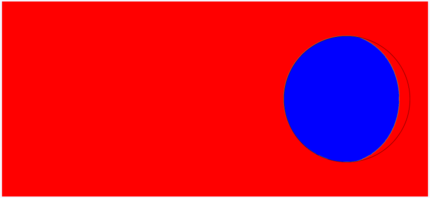
2D Air-R22 Shock-Interface Interaction (2)

EOS Parameters & Initial Values

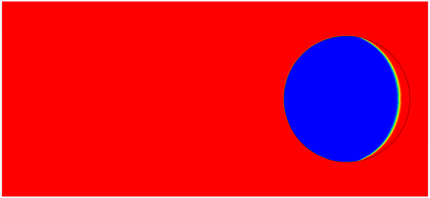
location	density $(\mathrm{kg.m^{-3}})$	pressure (Pa)	u_1 $(\mathrm{m.s^{-1}})$	u_2 $(\mathrm{m.s^{-1}})$	γ
air (post-shock)	1.686	1.59×10^5	-113.5	0	1.4
air (pre-shock)	1.225	1.01325×10^5	0	0	1.4
R22	3.863	1.01325×10^5	0	0	1.249

2D Air-R22 Shock-Interface Interaction (3)

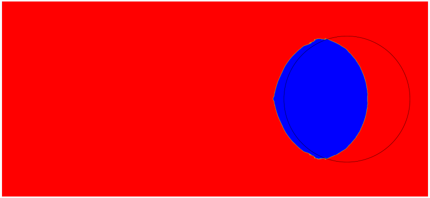
Color Function



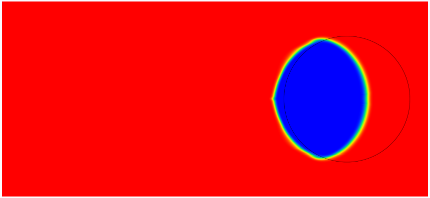
$t = 50, \mu\mathrm{s}$ (anti-diffusive)



$t = 50\ \mu\mathrm{s}$ (upwind)



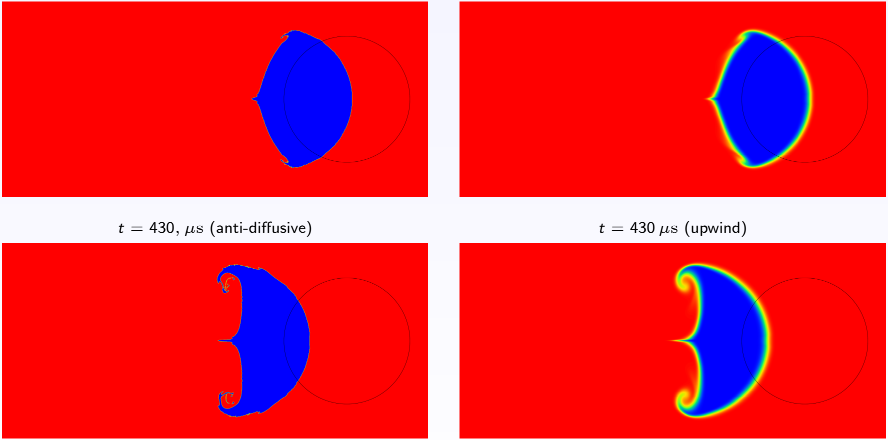
$t = 239\ \mu\mathrm{s}$ (anti-diffusive)



$t = 239\ \mu\mathrm{s}$ (upwind)

2D Air-R22 Shock-Interface Interaction (4)

Color Function



t = 430, μs (anti-diffusive)

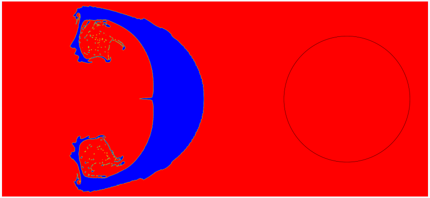
t = 430 μs (upwind)

t = 540 μs (anti-diffusive)

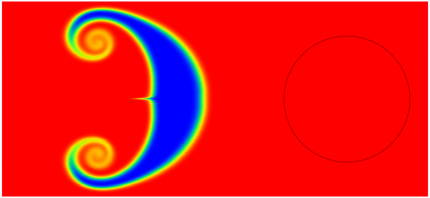
t = 540 μs (upwind)

2D Air-R22 Shock-Interface Interaction (5)

Color Function



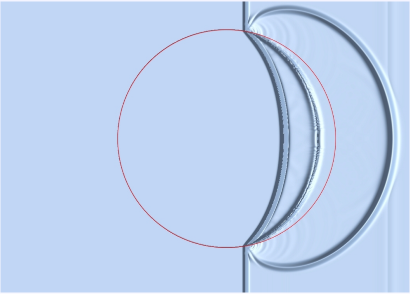
$t = 1020$, $\mu\mathrm{s}$ (anti-diffusive)

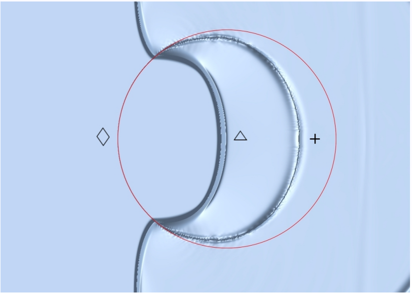


$t = 1020\,\mu\mathrm{s}$ (upwind)

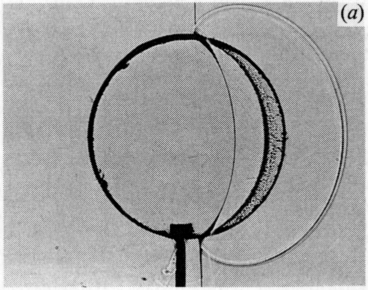
2D Air-R22 Shock-Interface Interaction (6)

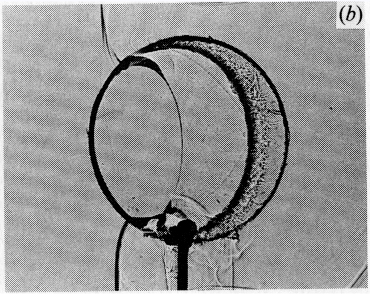
Anti-Diffusive Solver





Experiment

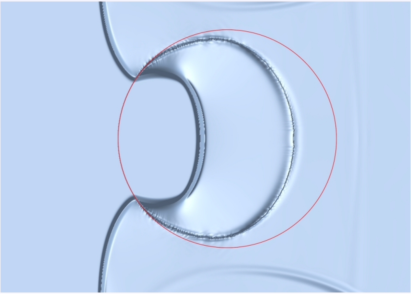


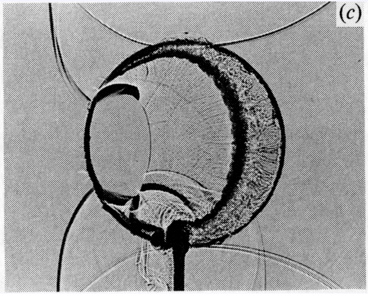


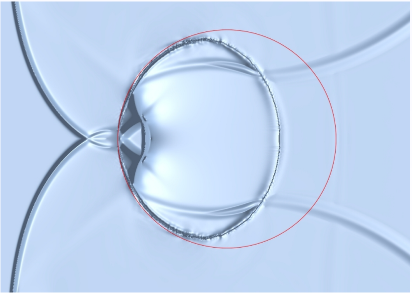
2D Air-R22 Shock-Interface Interaction (7)

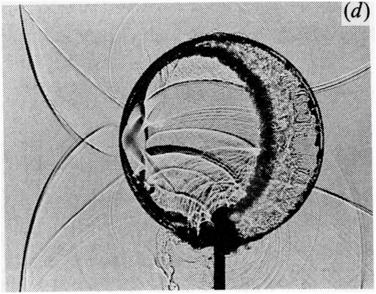
Anti-Diffusive Solver

Experiment



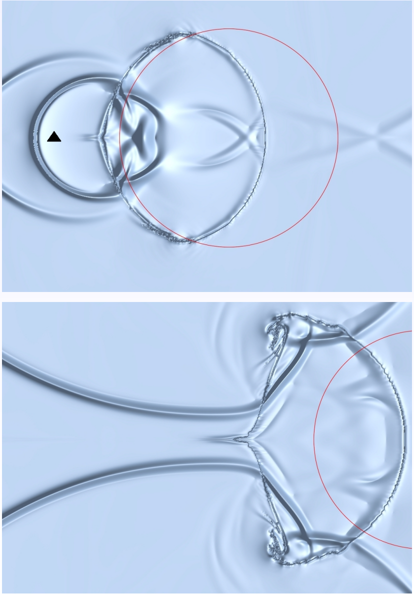




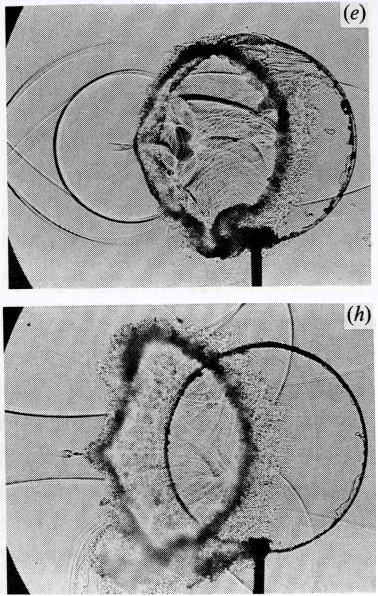


2D Air-R22 Shock-Interface Interaction (8)

Anti-Diffusive Solver

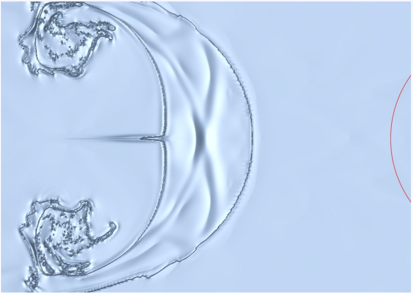


Experiment

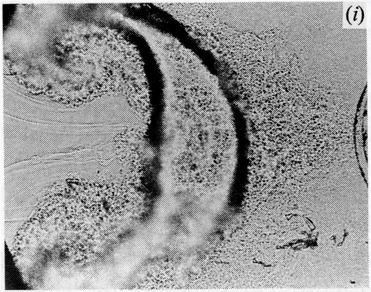


2D Air-R22 Shock-Interface Interaction (9)

Anti-Diffusive Solver

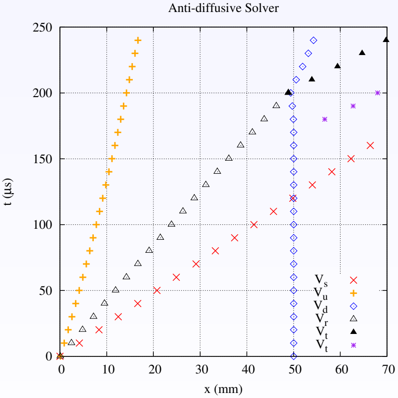


Experiment

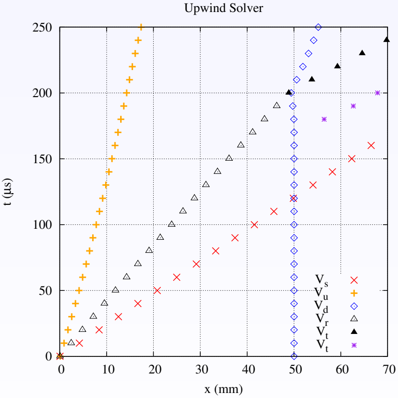


2D Air-R22 Shock-Interface Interaction (10)

Anti-Diffusive Solver



Upwind Solver

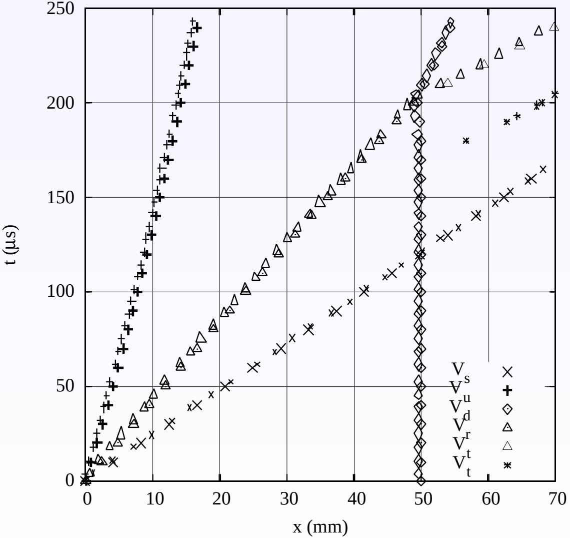


2D Air-R22 Shock-Interface Interaction (11)

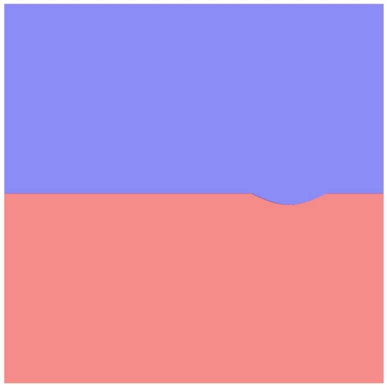
Velocity (m/s)	V_s	V_R	V_T	V_{ui}	V_{uf}	V_{di}	V_{df}
Haas & Sturtevant (Exp.)	415	240	540	73	90	78	78
Quirk & Karni	420	254	560	74	90	116	82
Shyue (tracking)	411	243	538	64	87	82	60
Shyue (capturing)	411	244	534	65	86	98	76
Upwind Solver	411	243	524	66	86	83	62
Anti-Diffusive Solver	411	243	525	65	86	85	64

2D Air-R22 Shock-Interface Interaction (12)

Anti-Diffusive Solver vs Results of obtained by Shyue.



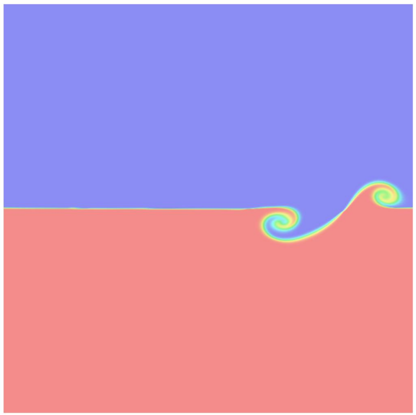
Kelvin-Helmholtz Instability (1)



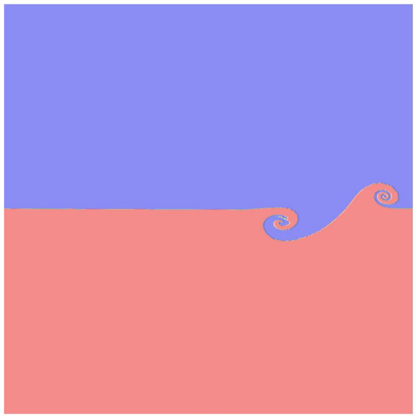
The domain is discretized over a 1000×1000 mesh

Kelvin-Helmholtz Instability (2)

upwind

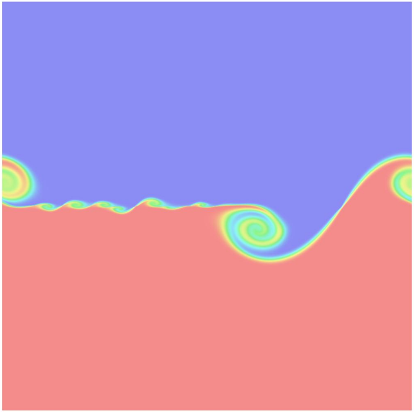


anti-diffusive

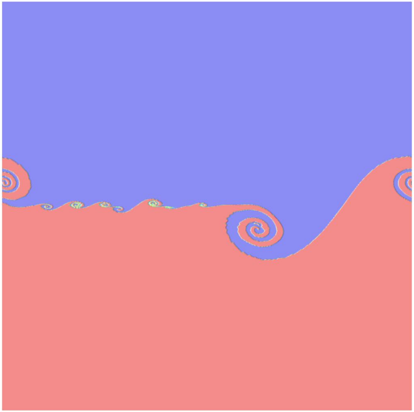


Kelvin-Helmholtz Instability (3)

upwind



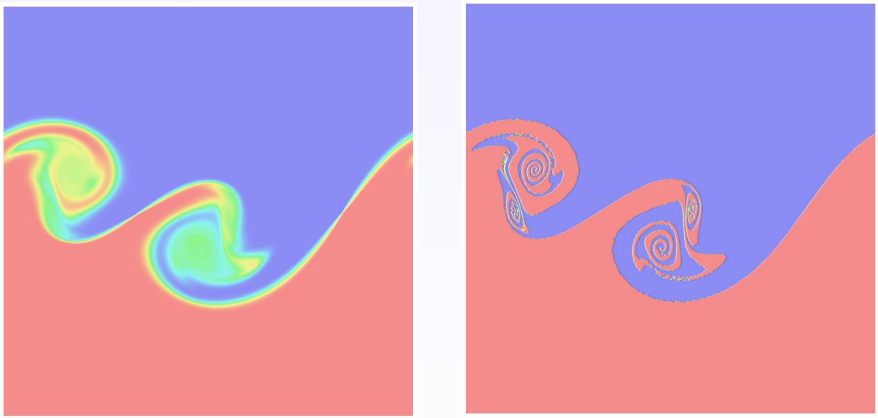
anti-diffusive



Kelvin-Helmholtz Instability (4)

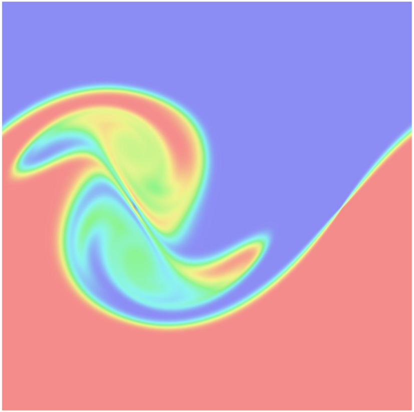
upwind

anti-diffusive

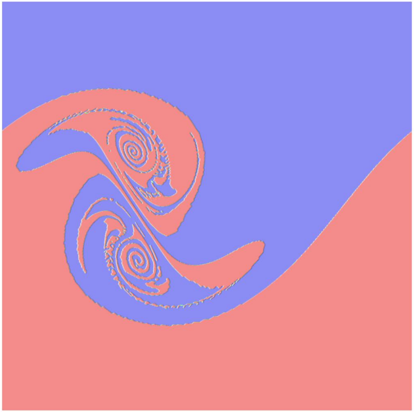


Kelvin-Helmholtz Instability (5)

upwind

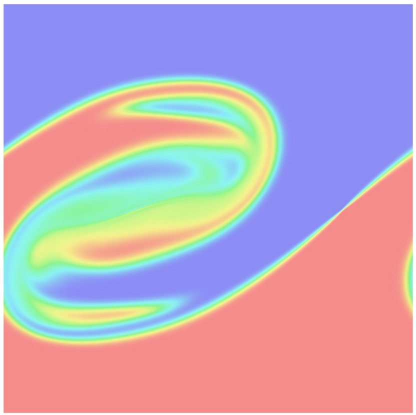


anti-diffusive

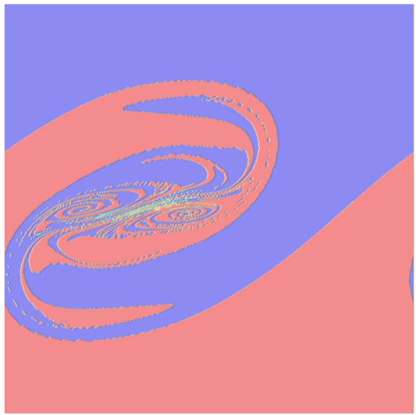


Kelvin-Helmholtz Instability (6)

upwind

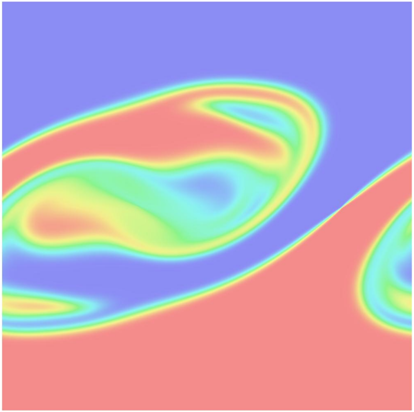


anti-diffusive

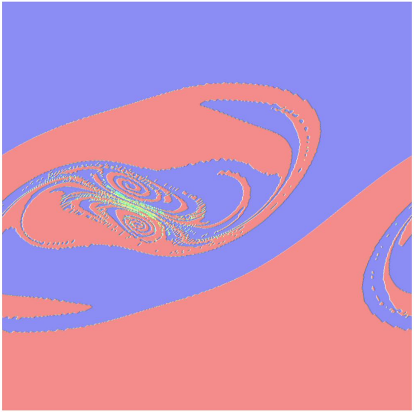


Kelvin-Helmholtz Instability (7)

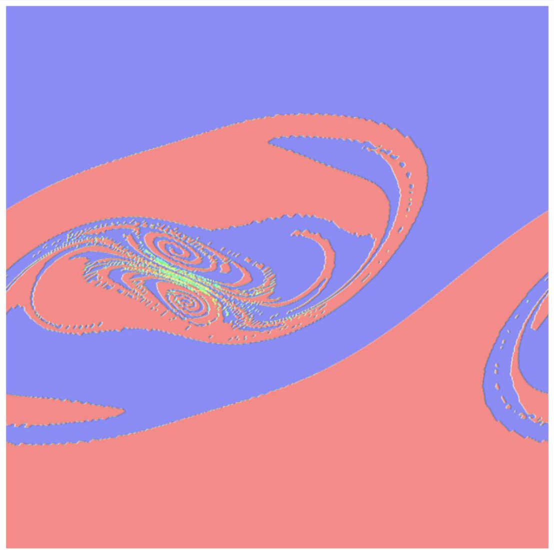
upwind



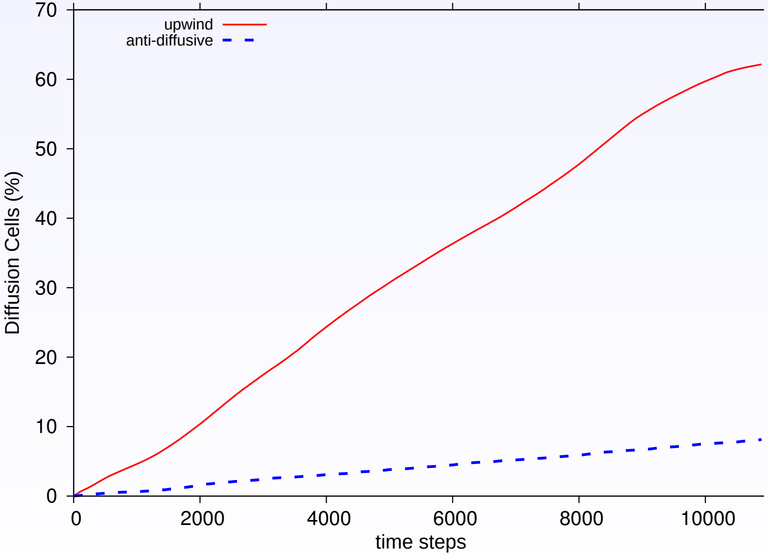
anti-diffusive



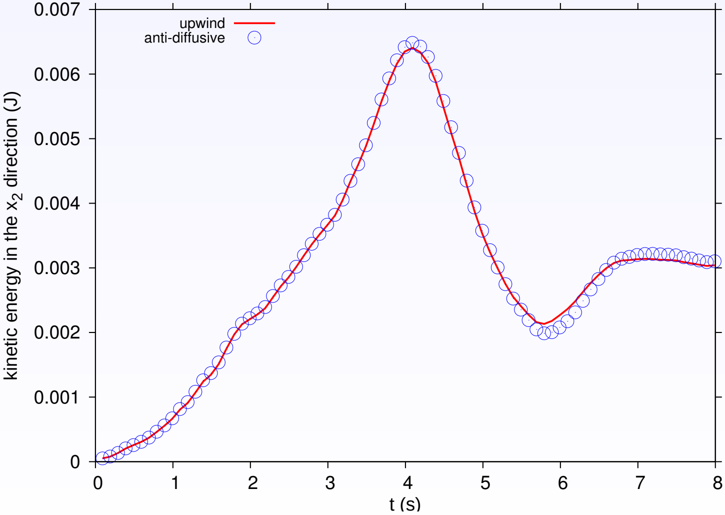
Kelvin-Helmholtz Instability (8)



Kelvin-Helmholtz Instability (9): Numerical Diffusion



Kelvin-Helmholtz Instability (10): Evolution of the Kinetic Energy in the x_2-Direction $t \mapsto \iint \frac{1}{2}\rho u_2^2 \mathrm{d}x_1 \mathrm{d}x_2$



Outline

Parallel Implementation: about Goals & Methods

Numerical Tools for Physical Modelization in an Ideal World

Taking advantage of the increasing CPU power and mature distributed computing techniques

Series of "fine scale" simulations ➡ Data Processing ➡ "average scale" Models

Methodology / Guidelines

Large meshes / Scalability

"Reasonably Simple" Choices

The above features condition our choices regarding numerical methods but also regarding physical models. **We hope that simplicity will provide us computational power through scalability.**

Parallel Algorithm

TRITON Code

TRITON: 3D parallel code developped at CEA Saclay (DM2S/SFME/LETR) dedicated to compressible with interface

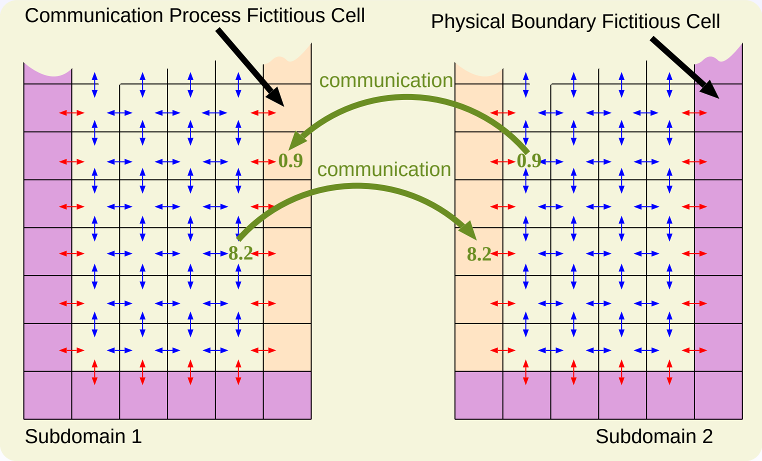
Code History

- A first 3D "Toy Code" developped in collaboration with R. Tuy
- Parallel version 0 by Ph. Fillion (CEA) and R. Tuy
- The present algorithm based on the work of Ph. Huynh and M. Flores (CS software support team of the CCRT)

"Natural Choice"

- Domain Decomposition
- Distributed memory

Managing the Communications



1: Communication

Inter-subdomain non-blocking communications

2: Computation

Compute the inner fluxes in the subdomains

3: Communication

Wait until step 1 is over.

4: Computation

Compute the fluxes at the subdomains boundaries

Speed Up Results

Preliminary Tests Only!!

These results must be confirmed and refined.

Tests performed with the cluster PLATINE at CCRT.

Number of CPUs	**1**	**2**	**50**	**100**	**200**
Averaged Elapsed Time (s)	405.45	201.7	9.78	4.9	2.06
Speed-Up	1	2.01	41.46	82.74	196.82
Speed-Up (%)	100	100.51	82.91	82.74	98.41

Outline

Example of 3D Simulation Performed with TRITON

Context of The Test

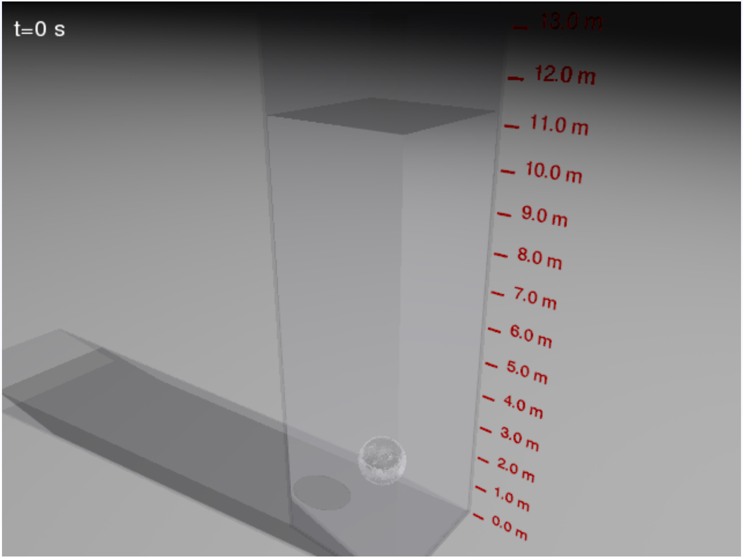
- Safety Study: Acid Test (Engineer Study)
- Blind Test: no parameter tuning was allowed.

3D Gas Bulk Rising Towards a Free Surface

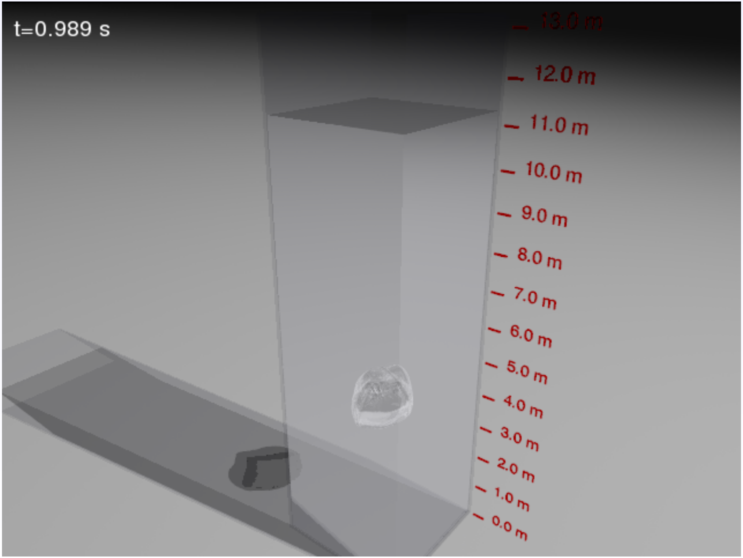
- Domain restricted to a quarter of space (due to time constraints)
- $54 \times 54 \times 400 = 1\,166\,400$ cells mesh
- Test performed on a 1024 nodes cluster (PLATINE) at CCRT
- "Wall clock" time: about 60 h

(Joint work with CEA coworkers: O. Grégoire & P. Salvatore)

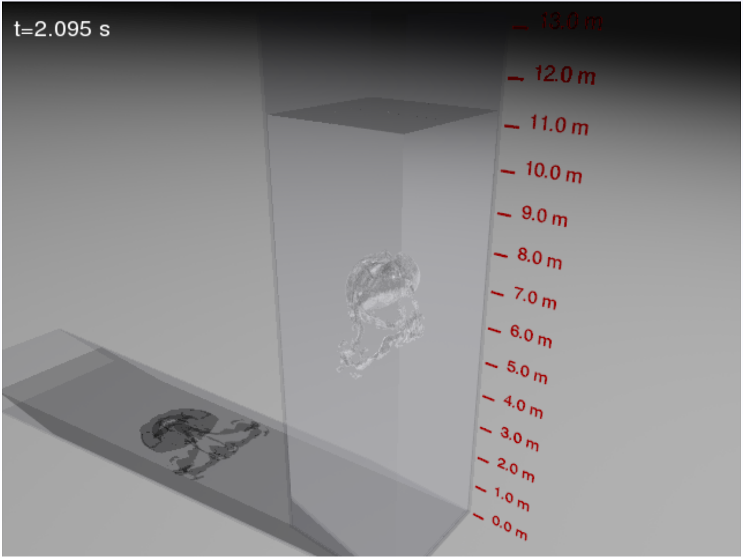
3D Gas Bulk Rising (1)



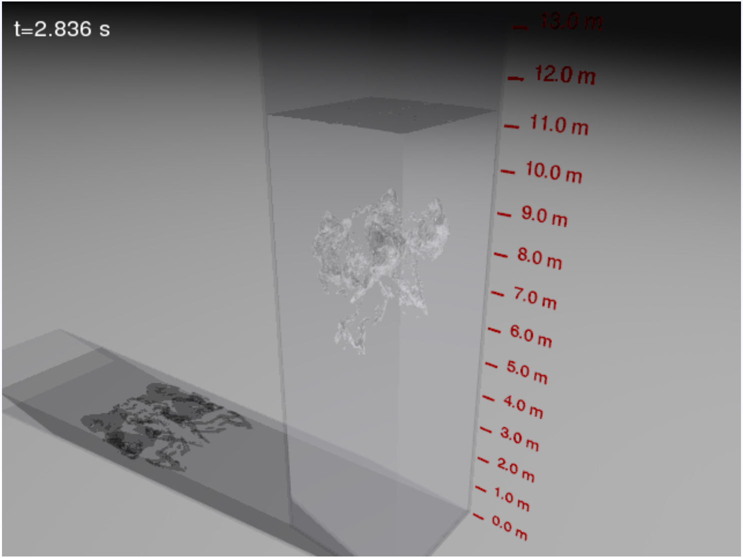
3D Gas Bulk Rising (2)



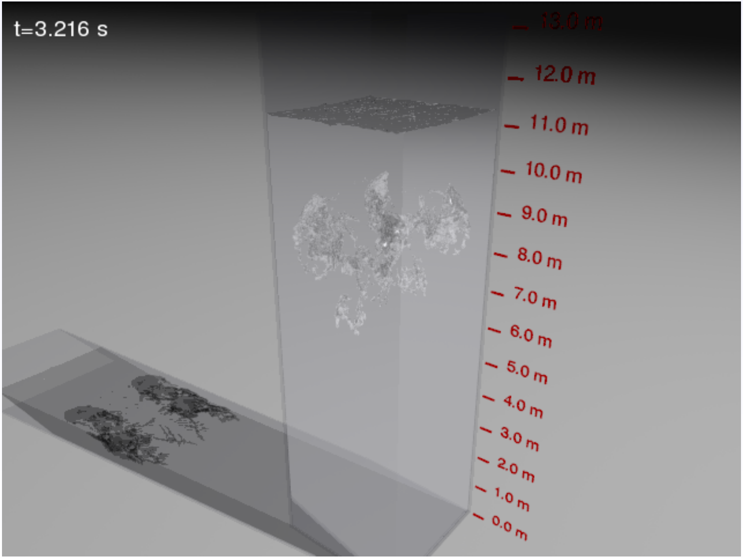
3D Gas Bulk Rising (3)



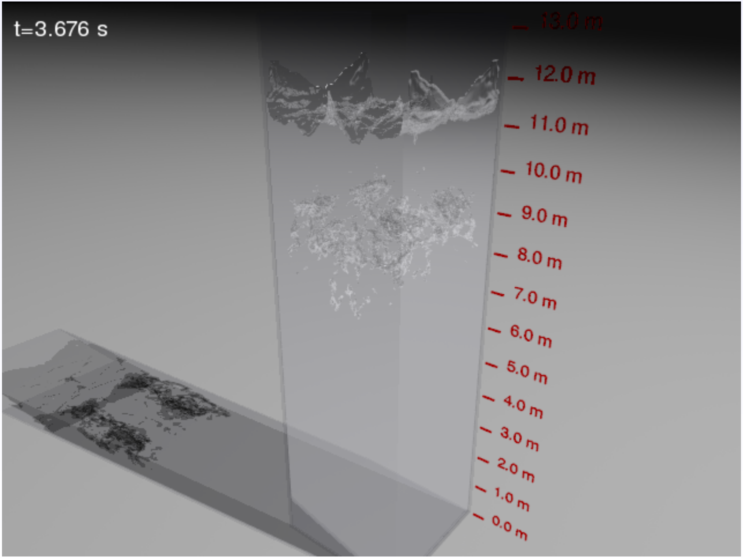
3D Gas Bulk Rising (4)



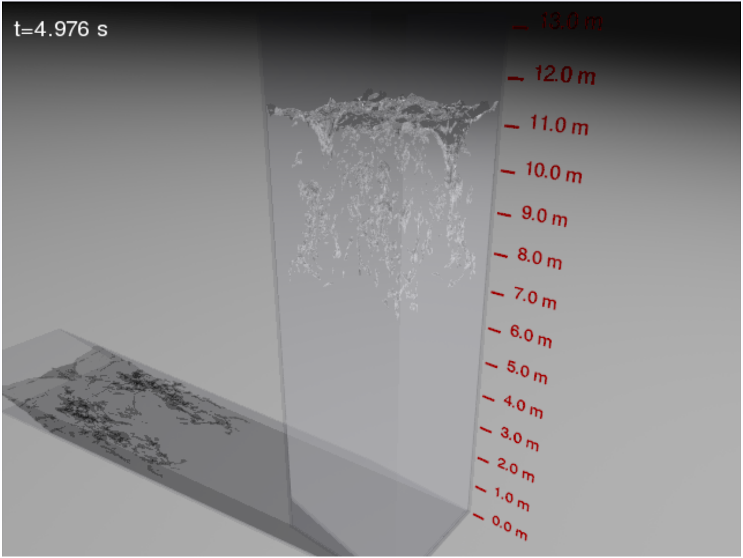
3D Gas Bulk Rising (5)



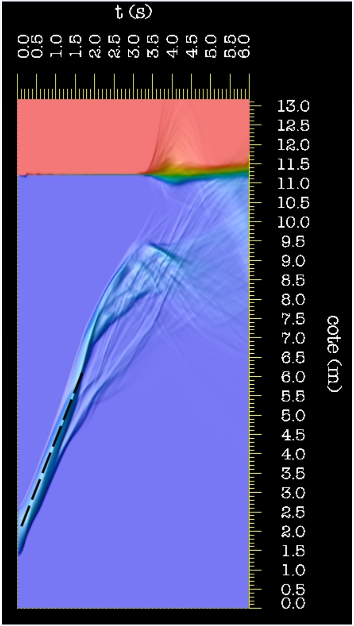
3D Gas Bulk Rising (6)



3D Gas Bulk Rising (7)



3D Gas Bulk Rising (8)



Averaged Volume Fraction Estimate

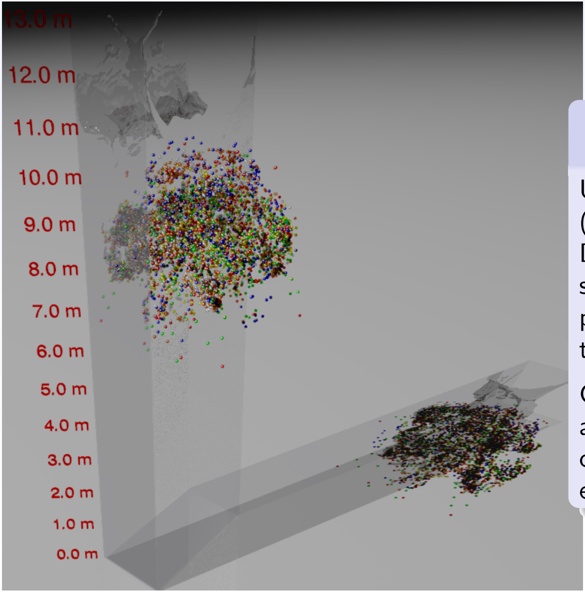
$$<z>(x_3,t) = \iint z(x_1,x_2,x_3,t)\,\mathrm{d}x_1\mathrm{d}x_2$$

Comparison with Theoretical Estimates

The gas bulk reaches its asymptotic velocity quasi-instantaneously

The rising velocity measured on the 3D results provides a match with the theoretical results with a 2.6×10^{-2} relative error.

3D Gas Bulk Rising (9)



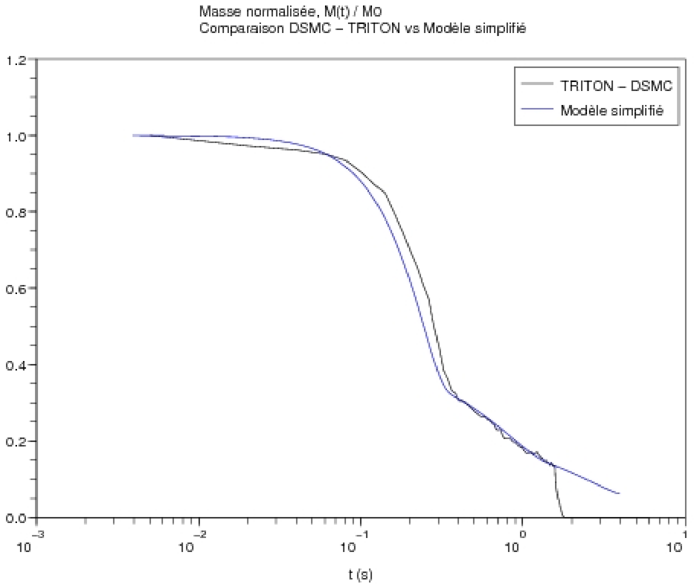
Particle Dynamics within the Flow

Use of the DSMC code (Lagrangian Particle Dynamics) for simulating the motion of particles within the two-phase flow.

Chaining both codes allowed to precisely corroborate engineers estimates.

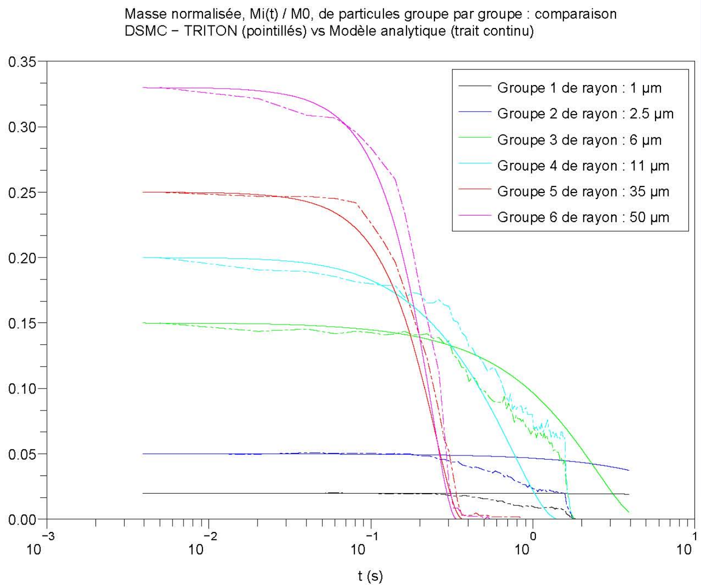
3D Gas Bulk Rising (10)

Estimate of the global residual mass of particle within the gas bulk



3D Gas Bulk Rising (11)

Estimate of the residual mass of particle within the gas bulk group by group



Outline

7. High-Order Strategy

Extension to High-Order Methods

CEMRACS 2010 — SimCapIAD project

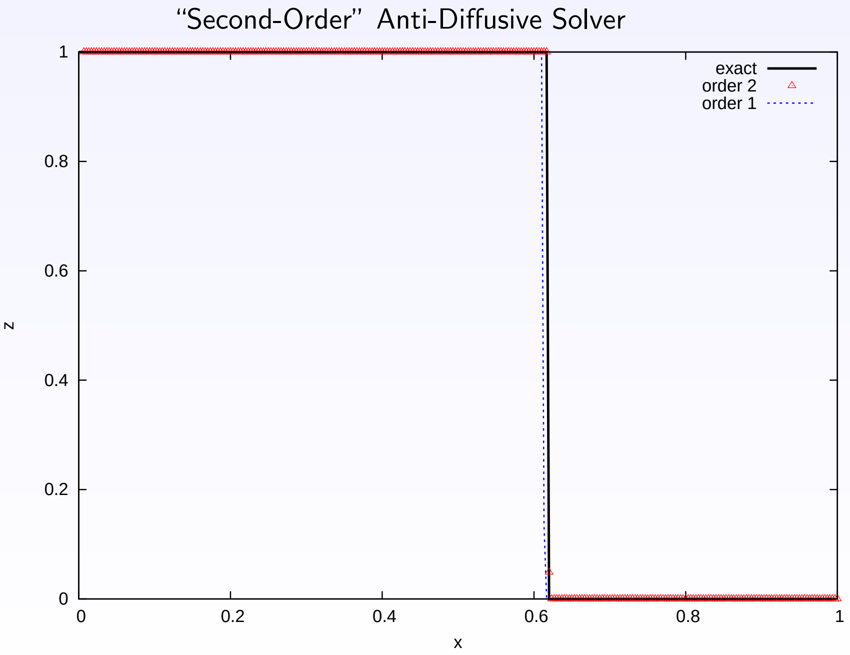
M. Billaud, B. Boutin, F. Caetano, G. Faccanoni,
S. Kokh, F. Lagoutière, L. Navoret.

funding: Univ. Paris-Sud 11

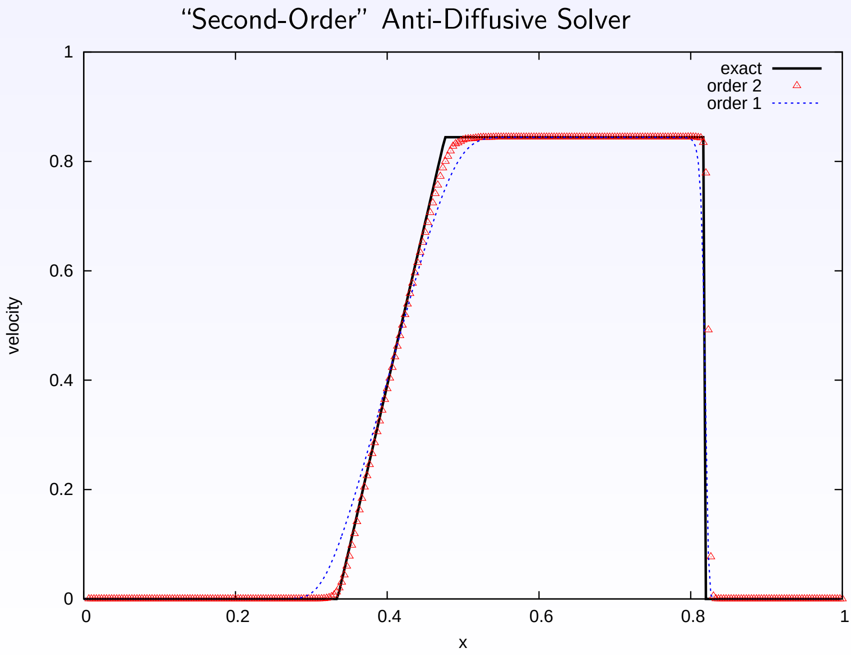
Design of several anti-diffusive schemes based on second order numerical methods (with respect to space and/or time).


"Second-Order" Anti-Diffusive Solver
exact
order 2
order 1
pressure
x
0
0.2
0.4
0.6
0.8
1
0
0.2
0.4
0.6
0.8
1

“Second-Order” Anti-Diffusive Solver
exact
order 2
order 1
density
x
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1



“Second-Order” Anti-Diffusive Solver
exact
order 2
order 1
z
x
0
0.2
0.4
0.6
0.8
1



“Second-Order” Anti-Diffusive Solver
exact
order 2
order 1
velocity
x
0
0.2
0.4
0.6
0.8
1

Convergence Rate (for the Sod test-case)

	ρ	u	p
Order 1 upwind	0.63	0.82	0.77
Order 1 anti-diff	0.75	0.82	0.78
Lagrange order 2 anti-diff	0.86	0.88	0.85
Lagrange-projection order 2 upwind	0.83	1.03	1.08
Lagrange-projection order 2 anti-diff	1.08	1.04	1.10

- upwind $\rightarrow$ anti-diffusive : improve the order for ρ
- with the order 2 method, orders are improved

  but numerical order $\lesssim 1$ (discontinuous solutions)
- Lagrange order 2 + projection of order 2

  better than Lagrange order 2

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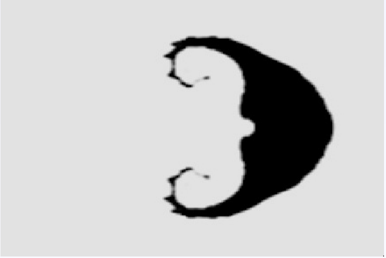
first order



second order

For the 2D shock/interface test: comparable accuracy between first and "second order" with a 25 times smaller grid.

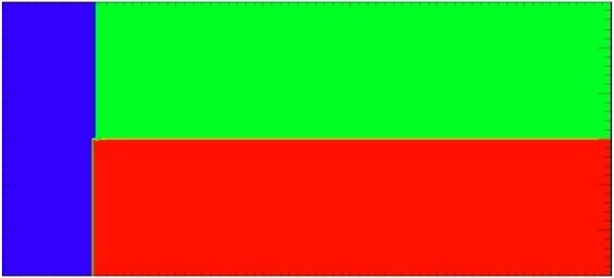
Outline

Extensions to Interface Flow Between N Compononents

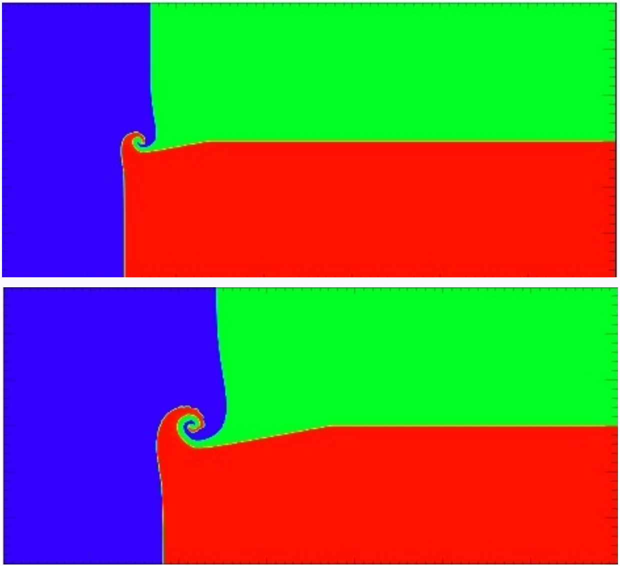
Joint work with M. Billaud-Friess (CEA/CELIA).

- Generalization of the two-component Five-Equation Model to a general model that can handle an arbitrary number of component
- Generalization of the Anti-Diffusive Lagrange-Remap Algorithm based on the transport algorithm proposed by Jaouen and Lagoutière

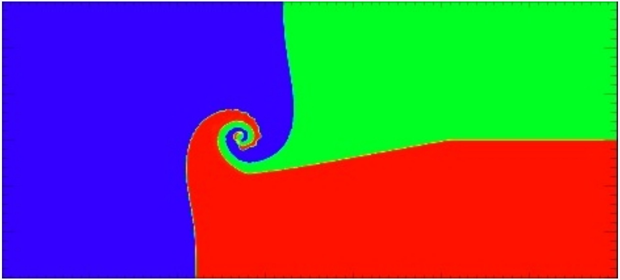
Simulation of a 3-component Kelvin-Helmholtz Instability

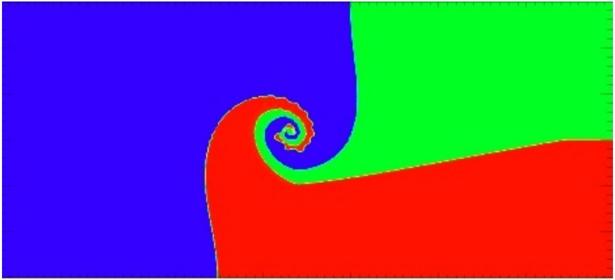


3-Component Kelvin-Helmholtz Instability

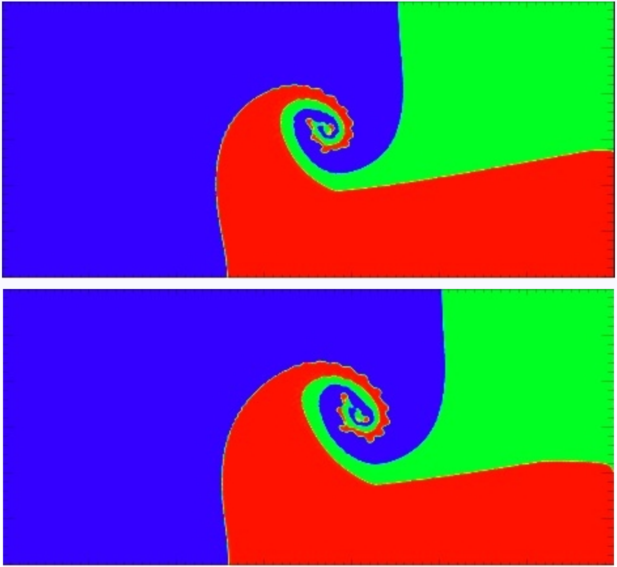


3-Component Kelvin-Helmholtz Instability

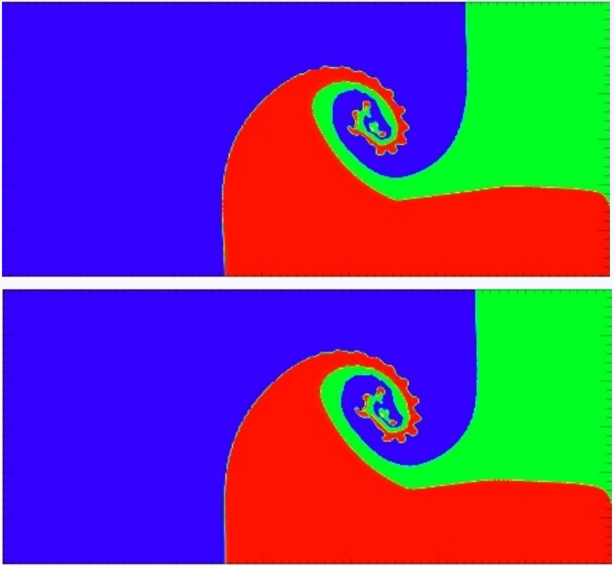




3-Component Kelvin-Helmholtz Instability



3-Component Kelvin-Helmholtz Instability



GPU Implementation (1)

GPU Port of the TRITON code

- CUDA
- achieved by the F. Dahm (CS CCRT Support Team)
- very constrained task: preserving the overall code structure
- Tesla S1070 : up to 3.4 faster than a single CPU test

GPU Implementation (2)

GPU Code Written From Scratch

- CUDA & OpenCL
- achieved by V. Michel (internship ENSIMAG) & A. Geay (CEA – SFME/LGLS)
- dedicated data structure architecture
- upwind version only
- GPU & multi-GPU implementation

CUDA: Results Overview

- shock/bubble interaction test over a $100 \times 50 \times 50$ grid
- Tesla C1050: up to 67.0 times faster than a single CPU test
- Fermi: untested but much better results are expected

Preliminary test run over a 10^9-cell mesh : 100 time steps in 91 seconds!

Outline

Conclusion & Perspectives(1)

- Design of a Lagrange-Remap scheme for the Five-Equation system with isobaric closure
- The scheme is conservative for ρy, ρ, ρu, ρe
- Good treatment of the Riemann Invariants across the material interface
- The scheme works "out of the box": no specific "numerical tuning" is required to optimize the scheme performance
- Anti-diffusive interface advection for both mass fraction y & color function z
- "Positivity" for both y & z variables
- no extra CPU cost
- The Després-Lagoutière approach is not restricted to its originating framework
- Good scalability

Conclusion & Perspectives (2)

...Conclusion

- SimCapiad (Cemarcs 2010): "Second Order" Extension
- Extension of the model and the scheme for N-component flows (joint work with M. Billaud-Friess)

Perspectives

- Similar strategy for unstructured meshes (Després & Lagoutière, V. Faucher)
- Fictitious boundaries (joint work with M. Belliard)
- Stable scheme for large time steps (Tran, Postel, Coquel)
- Capillarity
- Boundary Conditions (contact line, etc.)