FVCA5, Aussois, June 09-13, 2008

A Finite-Volume Approach to Fluids with Phase Transitions

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Plan of the Talk

1) Compressible Fluids with Phase Change

2) The Sharp-Interface Approach I

3) The Diffuse-Interface Approach

4) The Sharp-Interface Approach II

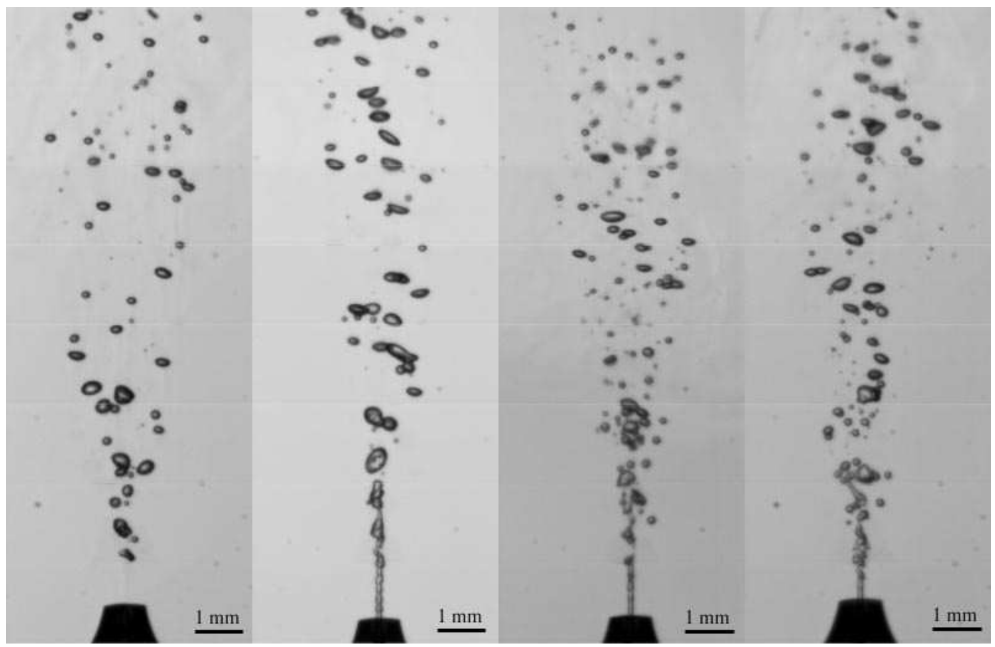
5) Outlook

DFG-CNRS Research Group: *Micro-Macro Modelling of Liquid-Vapor Flow*

1) Compressible Fluids with Phase Change

Compressible Effects in Liquid-Vapour Flow

Bubble rise after evaporation
of the liquid at different pressures

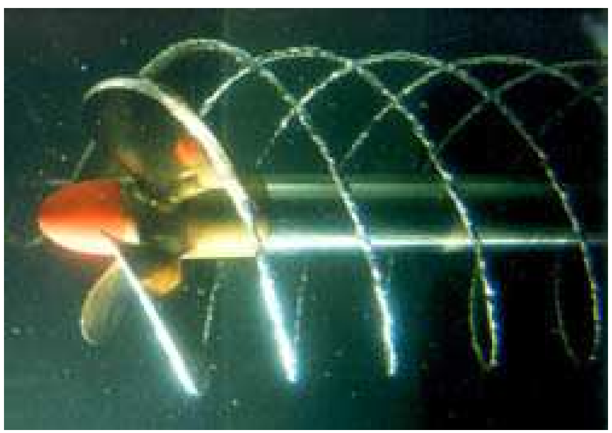


Pr = 0.836 0.892 0.900 0.929

(Source: F. D'Annibale, ENEA C.R. Casaccia, Institute of Thermal Fluid Dynamics,)

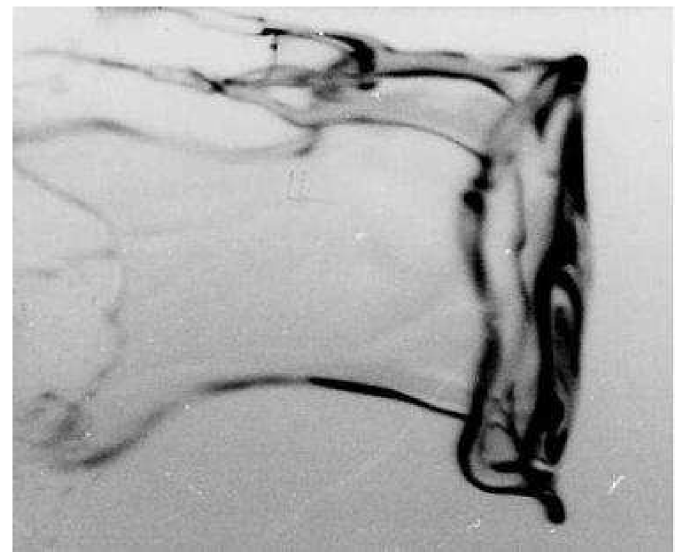
More Compressible Effects in Liquid-Vapour Flow

Cavitating bubbles



(Source: Tom Fink Cavitation Tunnel)

Deformation of drop by shock wave



(Source: Multiphase Flow and Spray Systems Laboratory, University of Toronto)

Requirements for the Mathematical Model

- Modelling on a macroscopic/continuum-mechanical level
- Correct description of phase transitions **and** fluid flow
- Consistency with laws of thermodynamics
- Compressibility in both phases
- Flexible numerical treatment possible

2) The Sharp-Interface Approach I:

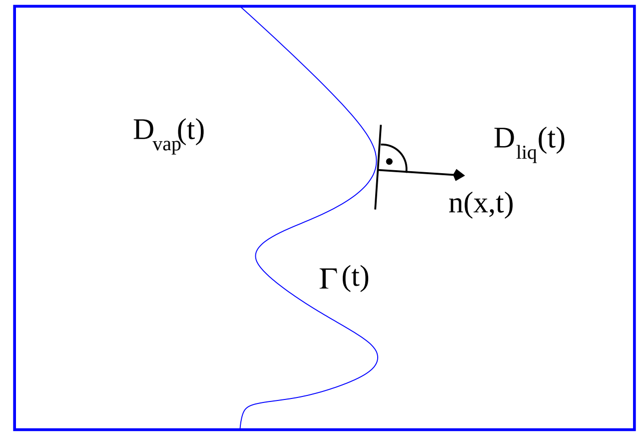
.....doesn't seem to be a good idea...

Sharp-Interface I

A Sharp-Interface Model: Isothermal Euler Equations

$$\left.\begin{array}{rcl} \rho_t + & \mathrm{div}(\rho\mathbf{v}) & = 0 \\ (\rho\mathbf{v})_t + & \mathrm{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) & = 0 \end{array}\right. \quad \text{in } D_{\text{vap/liq}}(t)$$

and trace conditions at free phase boundary $\Gamma(t)$



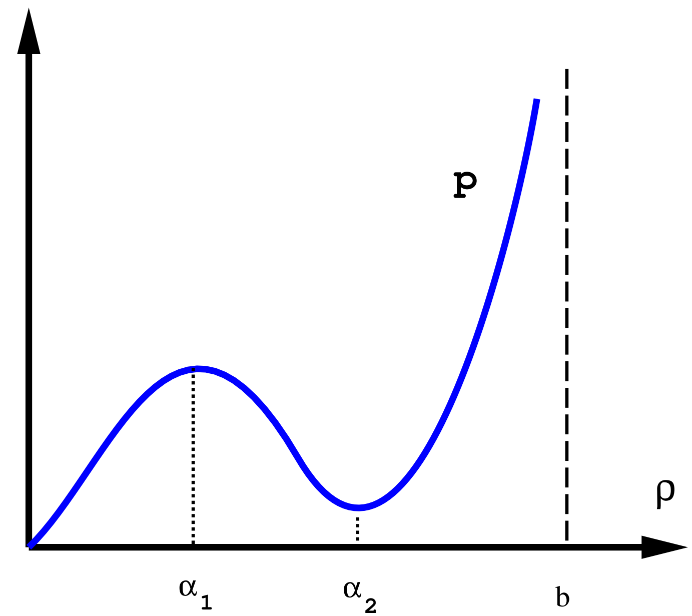
$$\mathbf{u} := (\rho, \rho\mathbf{v}), \qquad \begin{array}{ll} \rho = \rho(\mathbf{x},t) > 0 & : \text{Density} \\ \mathbf{v} = \mathbf{v}(\mathbf{x},t) \in \mathbb{R}^d & : \text{Velocity} \end{array}$$

Definition: The families $\{\Gamma(t)\}_{t\in[0,T]}$ and $\{\mathbf{u}_{\text{vap/liq}}(.,t) \in L^\infty(D_{\text{vap/liq}}(t)\}_{t\in[0,T]}$ are called an **admissible solution of the SI-model** iff

- $\mathbf{u}_{\text{vap/liq}}$ is an entropy solution in $\{(D_{\text{vap/liq}}(t), t) \,|\, t \in [0,T]\}$,
- $\rho_{\text{vap/liq}}$ is in the vapour/liquid phase,
- and the trace conditions are satisfied for $t \in [0,T]$.

Van-der-Waals Pressure Isotherm:

$$p = p(\rho, T_*) = \frac{RT_*\rho}{1 - d\rho} - a\rho^2$$



Pressure $p = p(\rho, T_*)$

Definition: (phases)

A density state ρ is in the **vapour** (**liquid**) phase iff we have

$$\rho \in (0, \alpha_1) \qquad \big(\rho \in (\alpha_2, b)\big).$$

It is called **elliptic** for $\rho \in (\alpha_1, \alpha_2)$.

SI-Model as a Conservation Law:

$$\mathbf{u}_t + \sum_{i=1}^{d} [\mathbf{f}^i(\mathbf{u})]_{x_i} \;=\; 0,$$
$$A(\mathbf{u}, \boldsymbol{\mu}) \;:=\; \sum_{i=1}^{d} \mu_i D\mathbf{f}^i(\mathbf{u}), \;\; |\boldsymbol{\mu}| = 1$$

$$\begin{aligned}
\lambda_1(\mathbf{u}, \boldsymbol{\mu}) &= \mathbf{v}\cdot\boldsymbol{\mu} - \sqrt{p'(\rho)},\\
\lambda_2(\mathbf{u}, \boldsymbol{\mu}) &= \mathbf{v}\cdot\boldsymbol{\mu},\\
&\vdots\\
\lambda_d(\mathbf{v}, \boldsymbol{\mu}) &= \mathbf{v}\cdot\boldsymbol{\mu},\\
\lambda_{d+1}(\mathbf{u}, \boldsymbol{\mu}) &= \mathbf{v}\cdot\boldsymbol{\mu} + \sqrt{p'(\rho)},
\end{aligned}$$

Difficulties of the SI-Model:

Modelling/Analysis:

- Choice of interface conditions not obvious
- Breakdown of notion of solution in case of topological changes of phases

Numerics:

- Numerical averaging might lead to elliptic density values
- Pointwise trace conditions but volume-oriented schemes

3) A Phase-Field Model
or Diffuse-Interface Model

A Diffuse-Interface Model: Navier-Stokes-Korteweg Equations

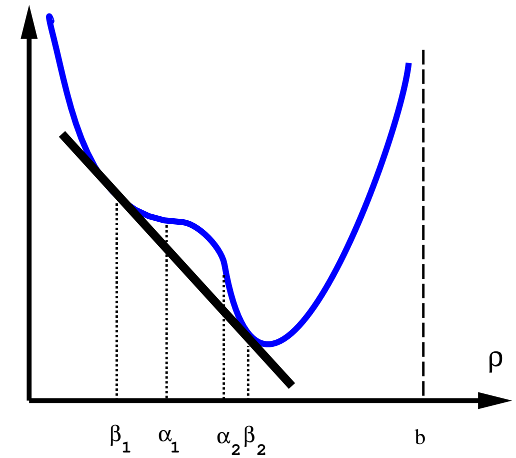
$$
\begin{aligned}
\rho_t \; + & \quad \text{div}(\rho \mathbf{v}) &= \; 0 \\
(\rho \mathbf{v})_t \; + & \; \text{div}(\rho \mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &= \; \text{div}(\mathbf{T}^\varepsilon) + \varepsilon^2 \rho \nabla \Delta \rho
\end{aligned}
$$

$$
\begin{aligned}
\rho = \rho(x,t) > 0 & \quad : \text{Density} \\
\mathbf{v} = \mathbf{v}(\mathbf{x},t) \in \mathbb{R}^d & \quad : \text{Velocity}
\end{aligned}
$$

$$
\mathbf{T}^\varepsilon = (T_{ij}^\varepsilon), \qquad T_{ij}^\varepsilon := \varepsilon \lambda \text{div}(\mathbf{v})\delta_{ij} + \varepsilon \mu (v_{j,x_i} + v_{i,x_j}).
$$

A Diffuse-Interface Model: Navier-Stokes-Korteweg Equations

$$
\begin{aligned}
\rho_t &+ \operatorname{div}(\rho\mathbf{v}) &&= 0\\
(\rho\mathbf{v})_t &+ \operatorname{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &&= \operatorname{div}(\mathbf{T}^\varepsilon) + \varepsilon^2\rho\nabla\Delta\rho
\end{aligned}
$$



$\rho = \rho(x,t) > 0$: Density

$\mathbf{v} = \mathbf{v}(\mathbf{x},t) \in \mathbb{R}^d$: Velocity

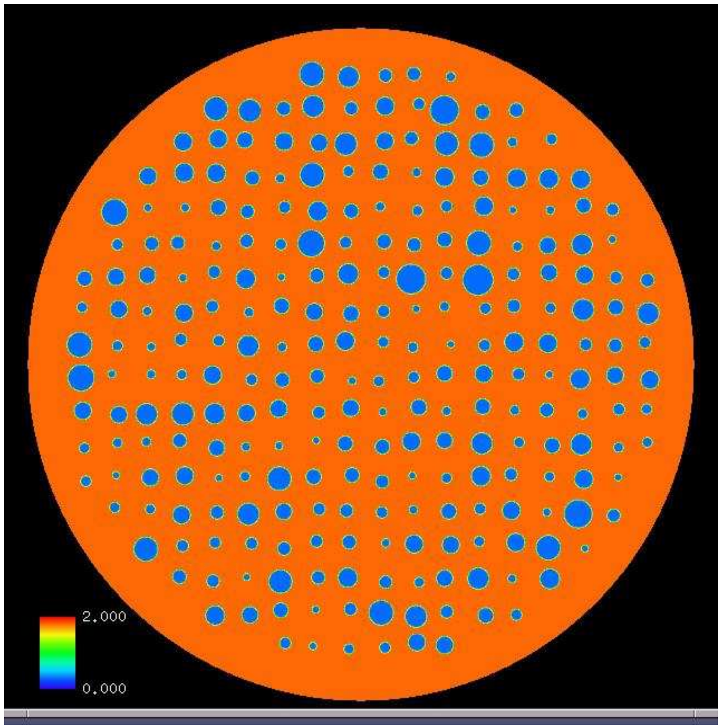
$$\mathbf{T}^\varepsilon = (T_{ij}^\varepsilon), \qquad T_{ij}^\varepsilon := \varepsilon\lambda\operatorname{div}(\mathbf{v})\delta_{ij} + \varepsilon\mu(v_{j,x_i} + v_{i,x_j}).$$

Energy: $p'(\rho) = \rho W''(\rho)$.

Energy inequality for the DI-model:

$$\frac{d}{dt}\Big(\int_{\mathbb{R}^d} \frac{1}{2}\rho(\mathbf{x},t)|\mathbf{v}(\mathbf{x},t)|^2 + W(\rho(\mathbf{x},t)) + \frac{\varepsilon^2}{2}|\nabla\rho(\mathbf{x},t)|^2\,d\mathbf{x}\Big) \le 0$$

A Simulation Example: (Phase separation)



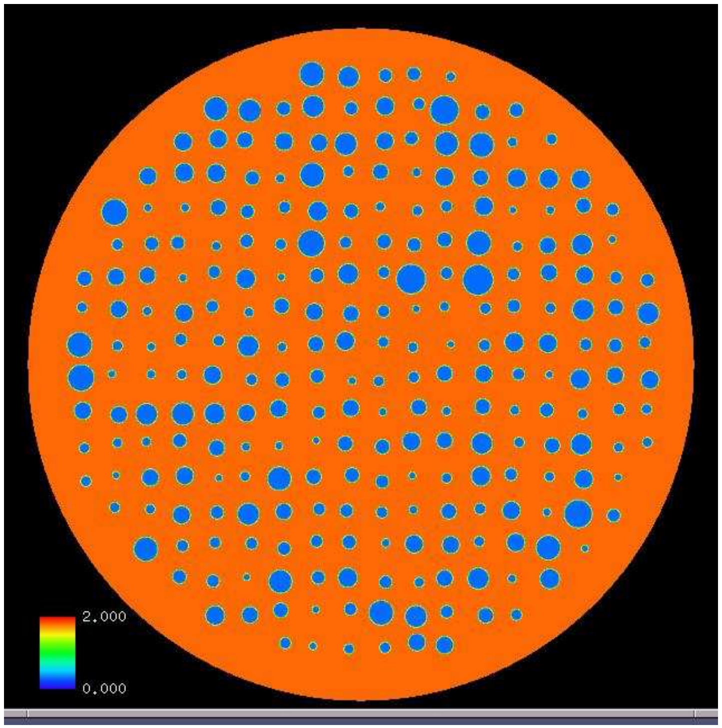
Initial density field with random bubble distribution.

Computations:

Local Discontinuous-Galerkin Code

(PhD-thesis, D. Diehl ’07).

A Simulation Example: (Phase separation)



Initial density field with random bubble distribution.

Computations:

Local Discontinuous-Galerkin Code

(PhD-thesis, D. Diehl '07).

Major Problems:

Interfacial width not realistic

Density variation not realistic

4) The Sharp-Interface Approach II:

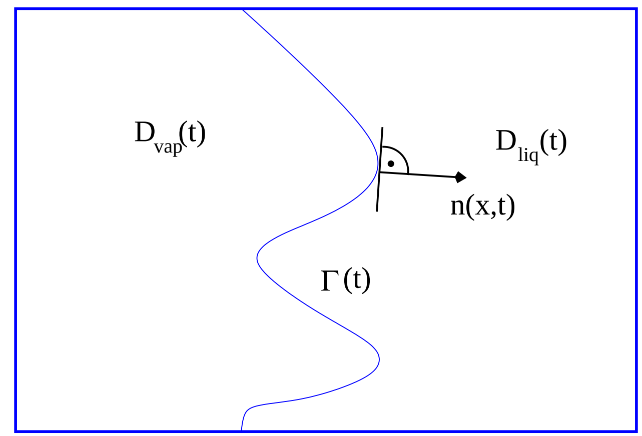
...not such a bad idea...

Isothermal Euler Equations:

$$\begin{aligned} \rho_t \ + \ \mathrm{div}(\rho\mathbf{v}) &= 0 \\ (\rho\mathbf{v})_t \ + \ \mathrm{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &= 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

$$\begin{aligned} [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)]\!] &= 0 \\ [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)\mathbf{v} + p\mathbf{n}]\!] &= (d-1)\sigma\kappa\mathbf{n} \quad \text{in } \Gamma(t) \end{aligned}$$

+ additional trace condition



$\rho = \rho(\mathbf{x}, t) > 0$: Density

$\mathbf{v} = \mathbf{v}(\mathbf{x}, t) \in \mathbb{R}^d$: Velocity

Here $\sigma > 0$ is the constant surface tension and

$s = s(\mathbf{x}, t)$ normal propagation speed of phase boundary $\Gamma(t)$

$\kappa = \kappa(\mathbf{x}, t)$ mean curvature of phase boundary $\Gamma(t)$

Kinetic Relation as Trace Condition:

Let $G : \mathbb{R} \to \mathbb{R}$ with $aG(a) \leq 0$, $a \in \mathbb{R}$, be given.
A phase boundary is called G**-admissible** iff we have

$$\underbrace{-s \left[\!\left[W(\rho) + \frac{1}{2}\rho|\mathbf{v}|^2 \right]\!\right] + \left[\!\left[\big(W(\rho) + \frac{1}{2}\rho v^2 + p(\rho)\big)\mathbf{v}\cdot\mathbf{n} \right]\!\right]}_{\text{entropy dissipation}} = jG(j),\ j = \rho_\pm(\mathbf{v}_\pm\cdot\mathbf{n} - s)$$

Examples:

(a) $G(a) = -a \quad \Rightarrow$ Phase boundary satisfies Clausius-Duhem inequality

(b) $G(a) = 0 \quad \Rightarrow$ Phase boundary satisfies Clausius-Duhem inequality (dissipation free)

Theorem (Benzoni-Gavage&Freistühler 04)
For $G \equiv 0$ there exists a local-in-time classical solution of the initial value problem for the SI-model.

Sharp-Interface Model for Planar Waves/Riemann Problem:

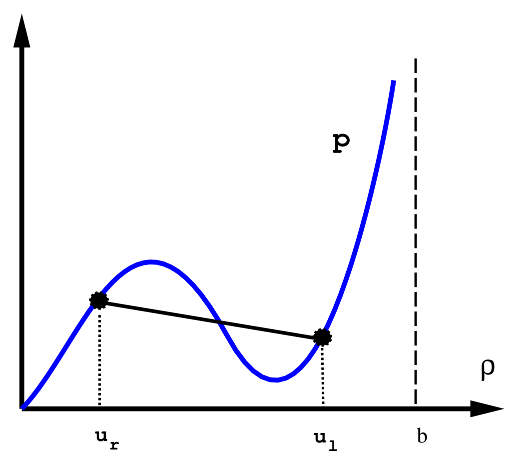
$$\begin{array}{ccccc} \rho_t & + & \rho v_x & = & 0 \\ (\rho v)_t & + & \left(\rho v^2 + p(\rho)\right)_x & = & 0 \end{array} \quad \text{in } \mathbb{R} \times (0,\infty)$$

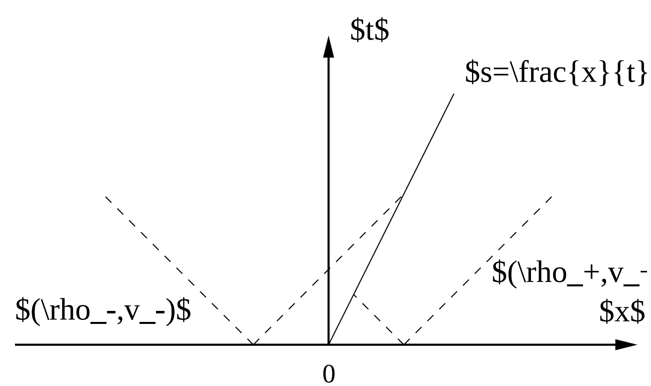
$$u := (\rho, \rho v)$$

$\rho = \rho(x,t) > 0$: Density

$v = v(x,t) \in \mathbb{R}$: Velocity

Subsonic Phase Boundary:





Sharp-Interface Model for Planar Waves/Riemann Problem:

$$\begin{array}{rcccl} \rho_t & + & \rho v_x & = & 0 \\ (\rho v)_t & + & \left(\rho v^2 + p(\rho)\right)_x & = & 0 \end{array} \text{ in } \mathbb{R} \times (0,\infty), \qquad u(x,0) = \begin{cases} u_l : x < 0 \\ u_r : x > 0 \end{cases}$$

$$u := (\rho, \rho v) \qquad \begin{array}{ll} \rho = \rho(x,t) > 0 & : \text{Density} \\ v = v(x,t) \in \mathbb{R} & : \text{Velocity} \end{array}$$

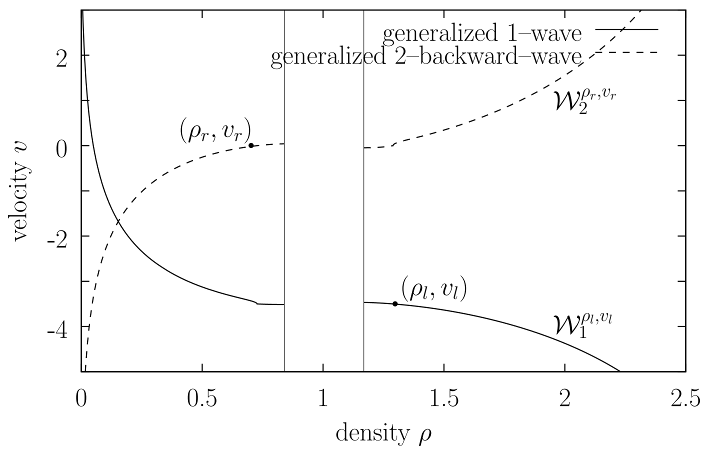
Theorem: (Merkle&R., M2AN 07)
For $G : \mathbb{R} \longrightarrow \mathbb{R}$, $aG(a) \leq 0$, we have

(i) The Riemann problem admits a weak solution $u : \mathbb{R} \times [0,\infty) \longrightarrow \mathcal{U}$ in the class of self-similar functions consisting of Laxian shock waves, G-admissible phase transitions, attached and rarefaction waves.

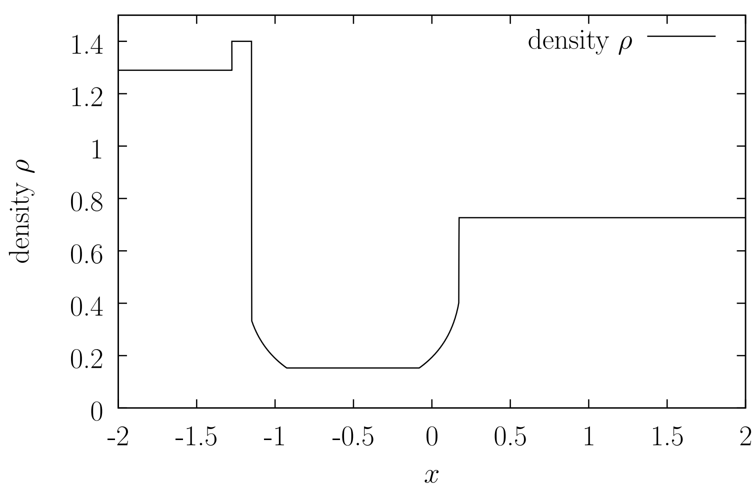
(ii) It is unique in this class if it satisfies the following properties.

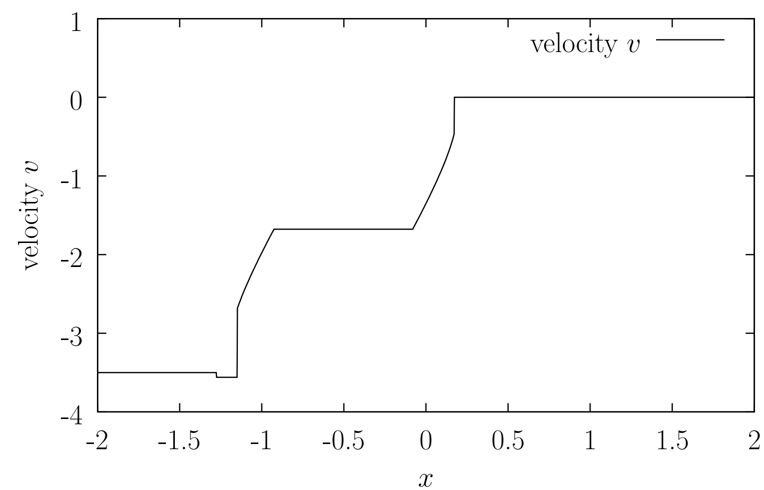
1. phase boundaries connecting states with the same pressure connect Maxwell–states,
2. a one-phase solution is used whenever it exists.

Analysis: Wave Curves and Solution for a Two-Phase Case



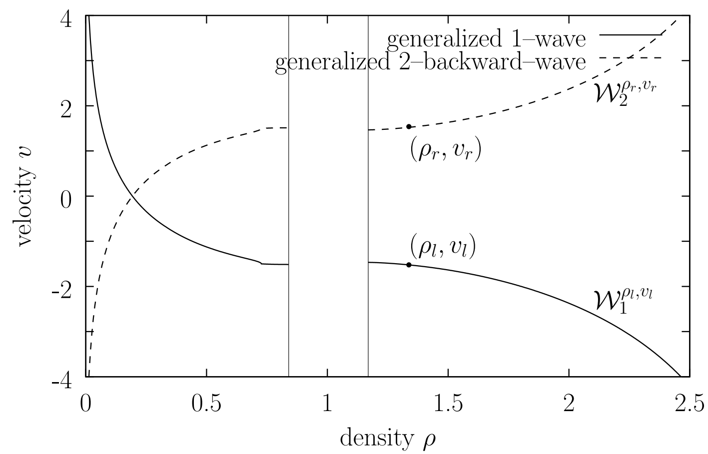
Generalized one-forward and two-backward curves



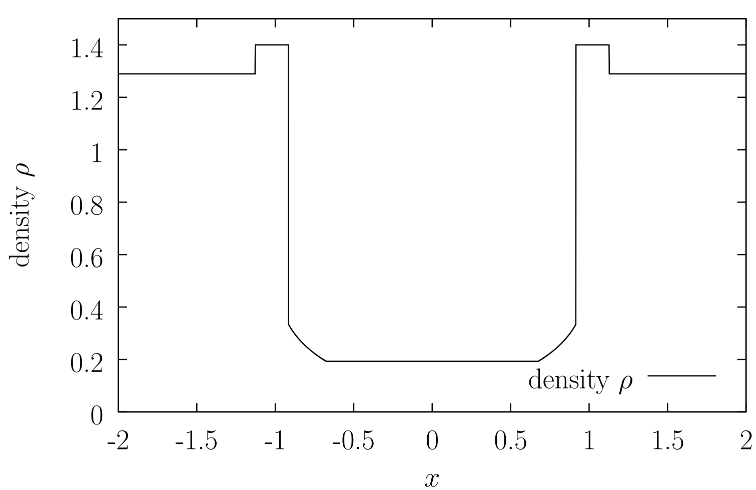


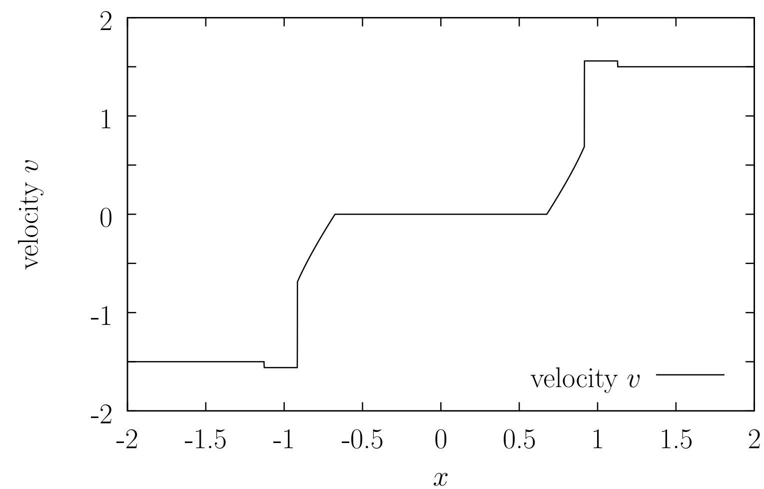
Graphs for density and velocity.

Analysis: Wave Curves and Solution for a Nucleation Case



Generalized one-forward and two-backward curves





Graphs for density and velocity.

Some (Eulerian) Methods for Subsonic Waves/Mixed-Type Systems

- LeFloch: Glimm-type scheme
- Hou&Rosakis&LeFloch '99, Merkle&R.'06: level-set appoach for (trilinear) pressure function,
- LeFloch, Hayes, Mercier, R. '98-'01: artificial dissipation approach for scalar equations,
- Abgrall&Saurel '03, Le Metayer&Massoni& Saurel '05: discrete equations method for evaporation fronts,
- Chalons, Coquel, Goatin, LeFloch,.. '06-: random-choice methods, transport-equilibrium approach

...

$\rightsquigarrow$ Keep phase boundary sharp (whatever it costs)

$\rightsquigarrow$ Do not use (hidden) phase field coupling

1D Finite-Volume Ghostfluid Approach (Merkle&R. M2AN 07)

Note: ghostfluid idea by Fedkiw,Aslam,Merriman,Osher, JCP 99.

Step 0: (data initialization)
For $t^0 := 0$ we define

$$u_j^0 := (\rho_j^0, m_j^0) := \frac{1}{h} \int_{I_j} (\rho_0, \rho_0 v_0)(x)\, dx \qquad (j \in \mathbb{Z}).$$

Assume that for time $t^n > 0$ the sequence

$$u_j^n := \{(\rho_j^n, m_j^n)\}_{j \in \mathbb{Z}}$$

with density values **not** in the elliptic region is given.
Let pairwise distinct phase boundary positions $\{p_k^n\}_{k=1,\ldots,K} \in$ be given.

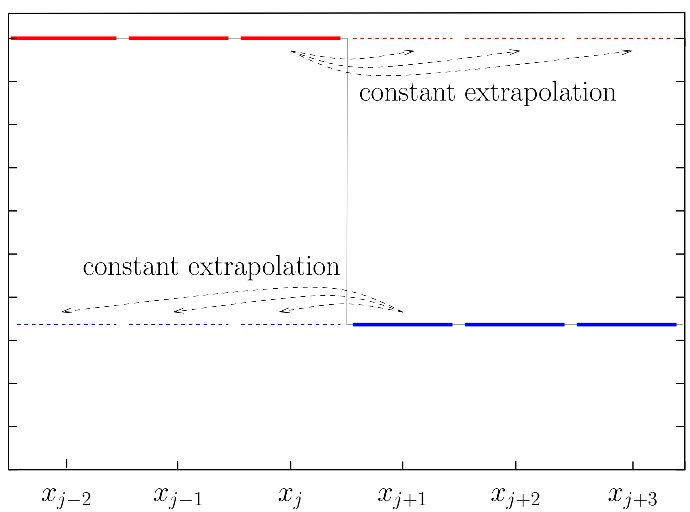
Step 1: (Construction of two preliminary one-phase data sets)

For $j \in \mathbb{Z}$ define the **vapour data set** $\{u\text{vap}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ by

$$u\text{vap}_j^n := \begin{cases} u_j^n & : \quad u_j^n \text{ is vapour state,} \\ u_{k(j)}^n & : \quad u_j^n \text{ is liquid state.} \end{cases}$$

Here $u_{k(j)}^n$ denotes the values of the vapour state in the cell $I_{k(j)}$ which is most close to the cell I_j.

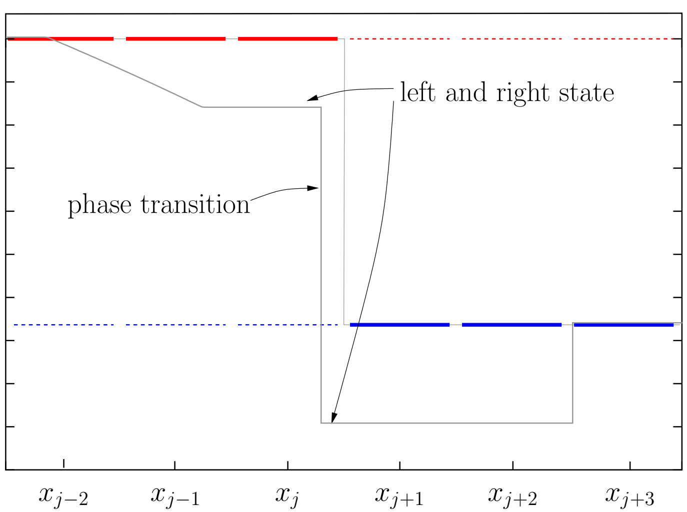
The **liquid data set** $\{u\text{liq}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ is defined analogously.



Step 2: (Solution of Riemann problems)

For $j \in \mathbb{Z}$ determine the unique weak solution $u^{(j,n)} : \mathbb{R} \times [0,\infty) \to (0,\infty) \times \mathbb{R}$ of the Riemann problem with initial data

$$u^{(j,n)}(x,0) \quad := \quad \begin{cases} \begin{cases} u_{\text{liq}}{}_j^n & : \quad x < 0 \\ u_{\text{vap}}{}_j^n & : \quad x > 0 \end{cases} & (u_{\text{vap}}{}_j^n = u_j^n), \\ \begin{cases} u_{\text{vap}}{}_j^n & : \quad x < 0 \\ u_{\text{liq}}{}_j^n & : \quad x > 0 \end{cases} & (u_{\text{liq}}{}_j^n = u_j^n). \end{cases}$$



$w_{\text{liq}}{}_j^n$: liquid state at phase boundary

$w_{\text{vap}}{}_j^n$: vapour state at phase boundary

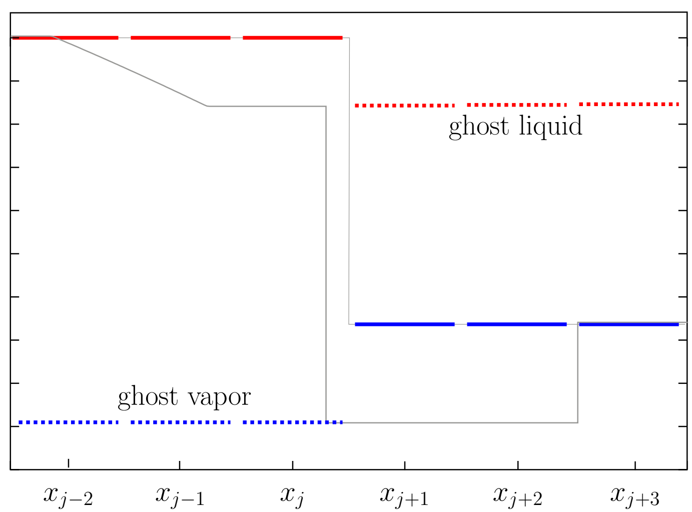
s_j^n : speed of phase boundary

Step 3: (Construction of two final one-phase data sets)

Define the **final vapour data set** $\{u\text{vap}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ by

$$u\textbf{vap}_j^n := \begin{cases} u_j^n & : \quad u_j^n \text{ is vapour state} \\ w\text{vap}_j^n & : \quad u_j^n \text{ is liquid state} \end{cases} \qquad (j \in \mathbb{Z})$$

The **final liquid data set** $\{u\text{liq}_j^n\}_{j\in\mathbb{Z}}$ is defined analogously.



Step 4: (Time evolution by finite-volume scheme)

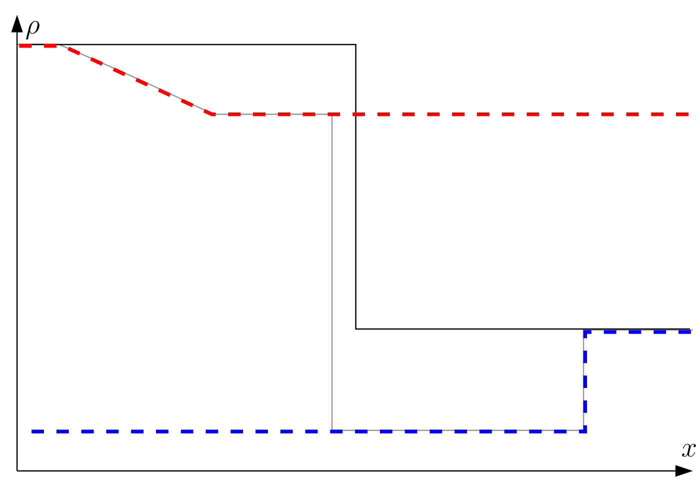
For $j \in \mathbb{Z}$ define $\{u_{\text{liq}}{}_j^{n+1}\}_{j\in\mathbb{Z}}$

$$u_{\text{liq}}{}_j^{n+1} \quad := \quad u_{\text{liq}}{}_j^{n} - \frac{\Delta t^n}{h}\left[g(u_{\text{liq}}{}_j^{n}, u_{\text{liq}}{}_{j+1}^{n}) - g(u_{\text{liq}}{}_{j-1}^{n}, u_{\text{liq}}{}_j^{n})\right]$$

Here g be a standard numerical flux function for the Euler equations.

The data set $\{u_{\text{vap}}{}_j^{n+1}\}_{j\in\mathbb{Z}}$ is defined analogously.

The phase boundary positions are updated using $\{s_j^n\}_{j\in\mathbb{Z}}$: $\{p_k^{n+1}\}_{k=1,\ldots,K}$.

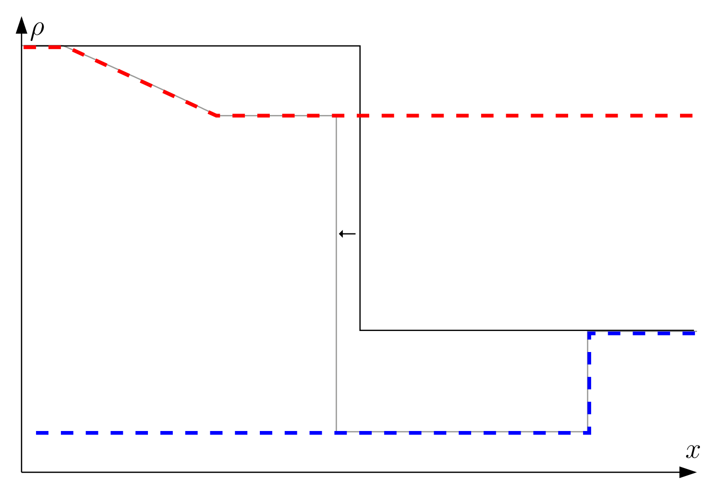


Step 5: (Finalization)

Determine from $\{u_j^n\}_{j\in\mathbb{Z}}$ and $\{p_k^{n+1}\}_{k=1,\ldots,K}$ a new phase distribution.

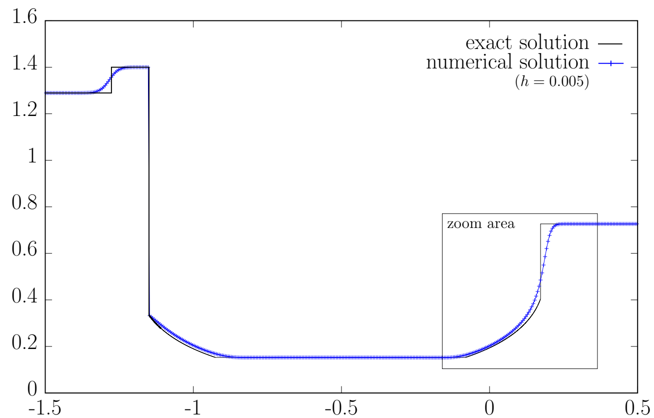
For $j \in \mathbb{Z}$ define $\{u_j^{n+1}\}_{j\in\mathbb{Z}}$ by

$$u_j^{n+1} := \begin{cases} u_{\text{vap}}{}_j^{n+1} & : \quad \text{state in } I_j \text{ is vapour state} \\ u_{\text{liq}}{}_j^{n+1} & : \quad \text{state in } I_j \text{ is liquid state} \end{cases}$$

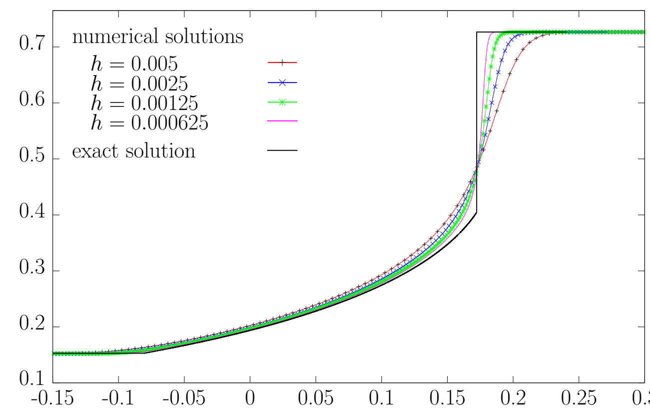


Sharp Interface II

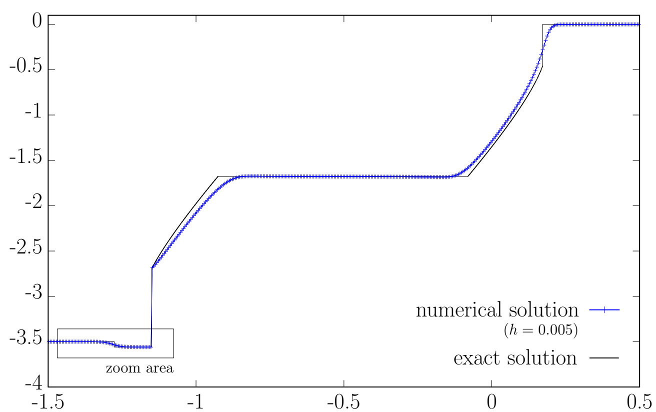
A 1D-Numerical Experiment:



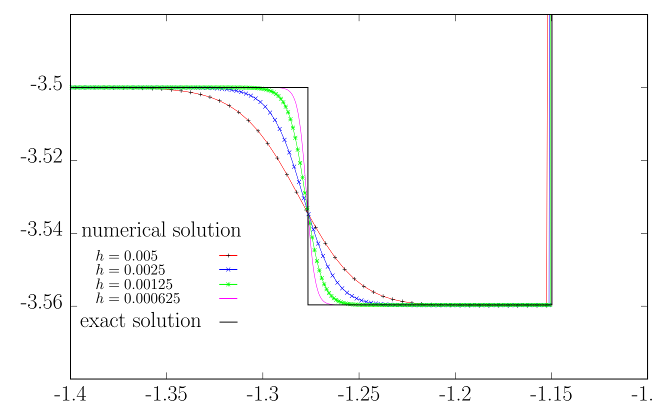
Density



Density: Detailed view.



Velocity



Velocity: Detailed view.

A 1D-Numerical Experiment:

grid size	L^1–error of ρ	EOC	L^1–error of v	EOC
0.04	0.08953370		0.22612267	
		0.85		1.03
0.02	0.04975303		0.11056125	
		0.48		0.39
0.01	0.03562381		0.08429837	
		0.75		0.84
0.005	0.02126755		0.04722471	
		0.77		0.88
0.0025	0.01247926		0.02572075	
		0.79		0.90
0.00125	0.00721779		0.01378924	
		0.83		0.97
0.000625	0.00406572		0.00702086	
		0.87		1.08
0.0003125	0.00222163		0.00332194	
		0.77		0.77
0.00015625	0.00130720		0.00195002	
		0.77		0.75
0.000078125	0.00076604		0.00115614	
		0.76		0.70
0.0000390625	0.00045315		0.00071321	
		0.85		0.89
0.00001953125	0.00025183		0.00038543	

L^1–error and EOC rate for subsequent refinement levels of the grid.

A Convergence Result:

Proposition: (Traveling phase boundary)
Assume that states $u_{l/r}$ are given such that the phase boundary connecting u_l and u_r is G-admissible. Let u be the traveling wave solution for initial datum

$$u_0(x) := \begin{cases} u_l & : \quad x - h/2 < 0, \\ u_r & : \quad x - h/2 > 0, \end{cases}$$

and let u_h denote the numerical solution obtained by the ghostfluid algorithm.
Then we have for all $S, t > 0$

$$\|u(.,t) - u_h(.,t)\|_{L^1([-S,S])} = \mathcal{O}(h), \qquad \int_{\mathbb{R}} u(x,t) - u_h(x,t)\, dx = \mathcal{O}(h).$$

Remarks on the 2D-Algorithm:

- Construct e.g. the preliminary liquid density data set by solving

$$u_t - \mathbf{n}(\mathbf{x},t^n)\cdot\nabla u = 0, \quad u(\mathbf{x},t^n) = \begin{cases} \rho(\mathbf{x},t^n) & : \quad \mathbf{x}\in D_{\text{liq}}(t^n), \\ 0 & : \quad \mathbf{x}\in D_{\text{vap}}(t^n) \end{cases}$$

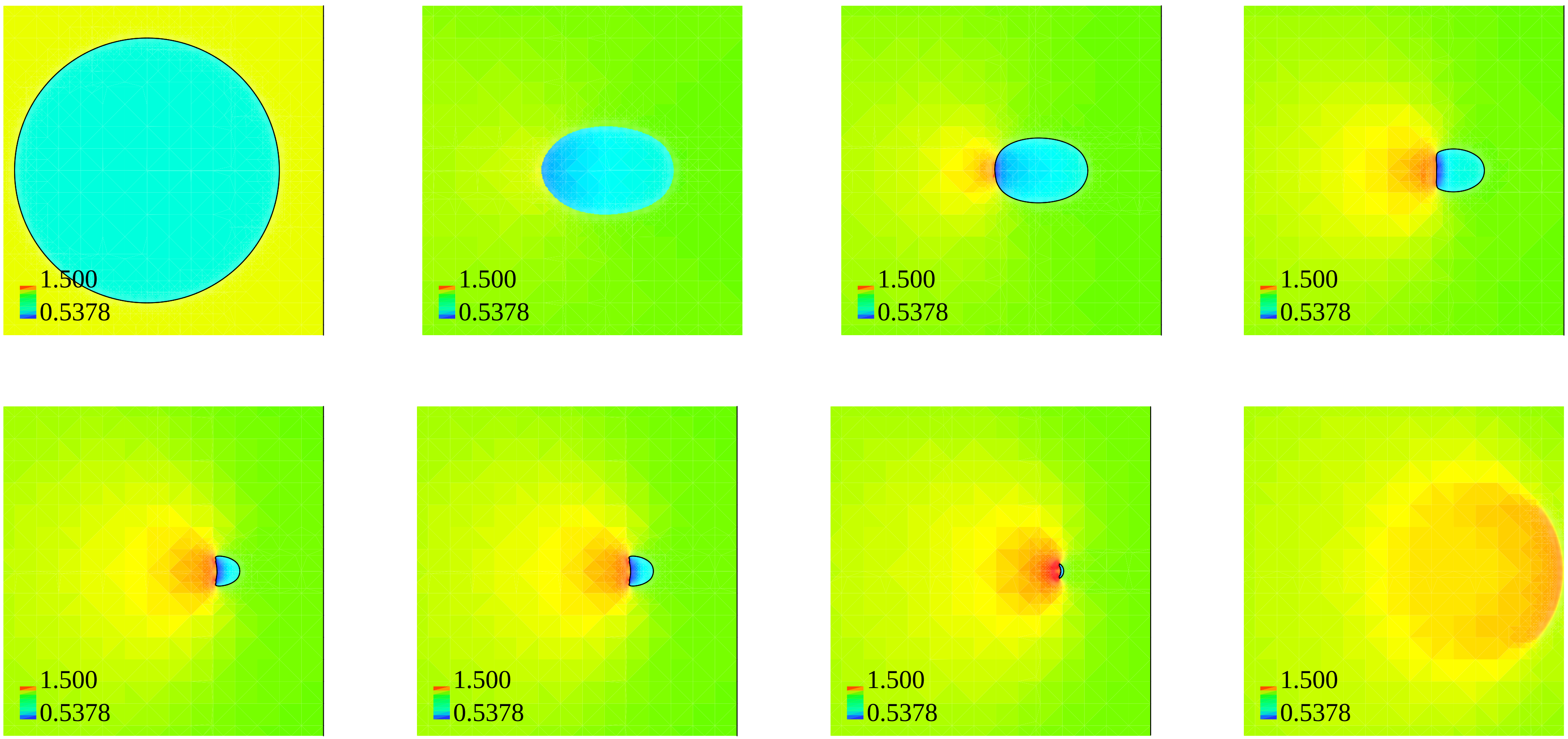
  in $D \times [t^n, t^{n+1}]$.

- The evolution of the discrete phase boundary Γ_h is tracked by solving

$$\varphi_t + V_h(\mathbf{x},t^n)|\nabla\varphi| = 0, \quad \varphi(\mathbf{x},t^n) = \text{signed dist}(\mathbf{x},\Gamma_h(t^n))$$

  in $D \times [t^n, t^{n+1}]$.
  Here $V_h(.,t^n)$ is the speed of the phase boundary obtained by Riemann problem solutions at time $t = t^n$.

2D Experiment without curvature: (PhD-thesis C. Merkle ’06)



5) Conclusions and Outlook

- Development of approximate nonclassical Riemann solvers
- Extension to the curvature-dependent case
  (Generalized Riemann solution: Dressel&Rohde 08)
- Tests for realistic density regimes
- Multiscale coupling of Navier-Stokes equations with Euler equations