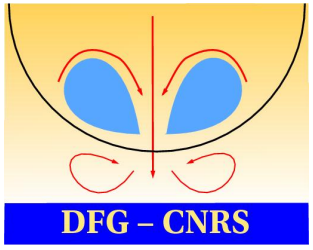


Micro-Macro Modelling and
Simulation of Liquid-Vapour Flow

DFG - CNRS Project RO 2222/4-1

ians

Sharp Interface Approach for Liquid-Vapour Flow with Phase Transition

Christoph Zeiler

Institute for Applied Analysis and Numerical Simulation

February 2014

Free Boundary Value Problem in $\mathbb{R}^d$

Bulk Phases

$$\begin{aligned} \varrho_t + \operatorname{div}(\varrho\, \boldsymbol{v}) &= 0, \\ (\varrho\, \boldsymbol{v})_t + \operatorname{div}\left(\varrho\, \boldsymbol{v} \otimes \boldsymbol{v} + p(\varrho)\, \boldsymbol{I}\right) &= \boldsymbol{0}. \end{aligned}$$

Phase Boundary

$$\begin{aligned} [\![\varrho(\boldsymbol{v}\cdot\boldsymbol{n} - \sigma)]\!] &= 0, \\ [\![\varrho(\boldsymbol{v}\cdot\boldsymbol{n} - \sigma)\, \boldsymbol{v} + p(\varrho)\, \boldsymbol{n}]\!] &= (d-1)\gamma\kappa\, \boldsymbol{n}, \\ [\![g(\varrho) + 0.5\,(\boldsymbol{v}\cdot\boldsymbol{n} - \sigma)^2]\!] &= -k\, j. \end{aligned}$$

Local Well-Posedness Results

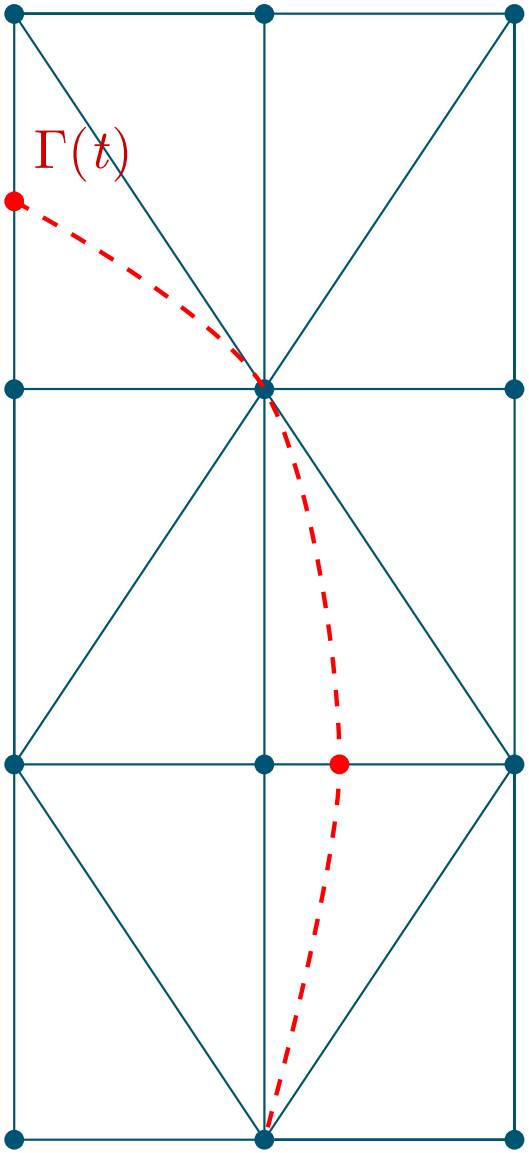
- for $k = 0$ see [Benzoni-Gavage, Freistühler 2004]
- for $k > 0$ see [Kabil, Rohde 2013]

[Binninger et al.]

Outline

Cut Cell Method (joint work with C. Chalons)

Basic Steps



Domain $\Omega \in \mathbb{R}^d$ with fluid in two phases at time $t > 0$

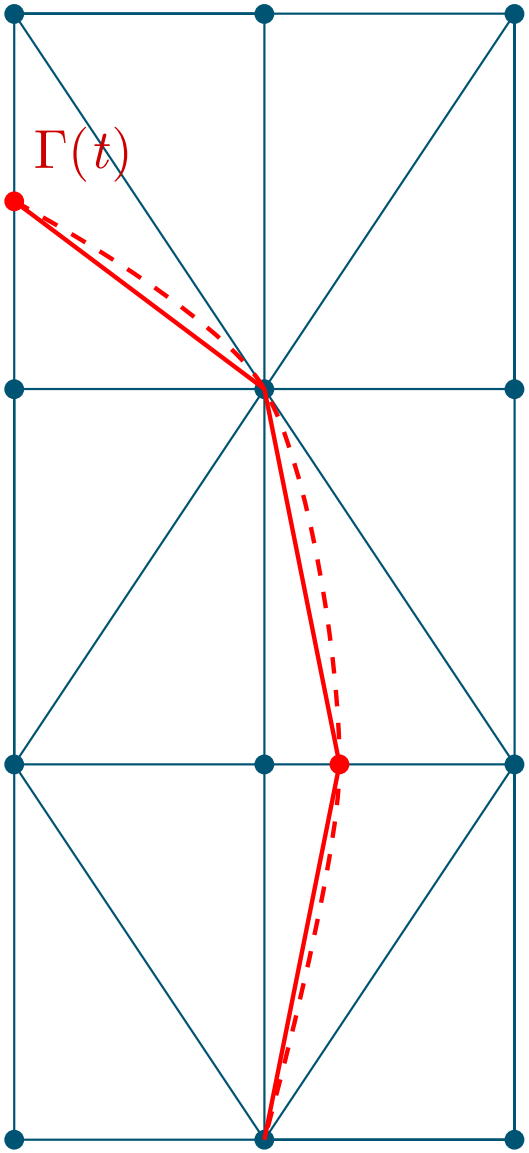
- liquid $\Omega_{\text{liq}}(t)$,
- vapour $\Omega_{\text{vap}}(t)$,
- curved phase boundary $\Gamma(t) = \partial\Omega_{\text{liq}}(t) \cap \partial\Omega_{\text{vap}}(t)$.

We consider physical quantities in Euler coordinates $(\boldsymbol{x}, t)$

- density $\varrho(\boldsymbol{x}, t) > 0$,
- velocity $\boldsymbol{v}(\boldsymbol{x}, t) \in \mathbb{R}^d$.

Cut Cell Method (joint work with C. Chalons)

Basic Steps



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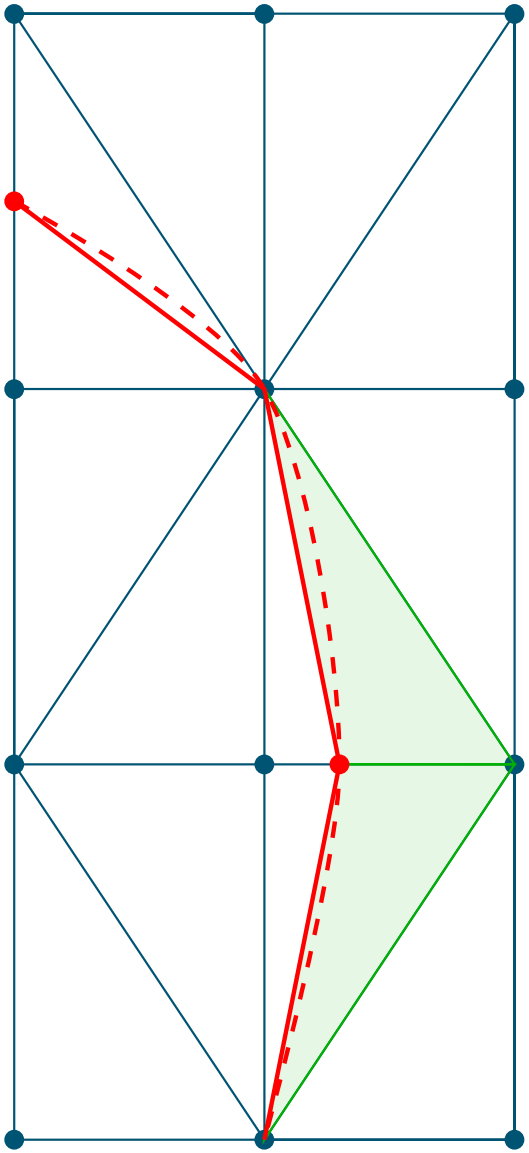
Cut (and Merge) Cell Approach:

- approximate $\Gamma(t) \to \Gamma_h(t)$,

Cut Cell Method (joint work with C. Chalons)

Basic Steps



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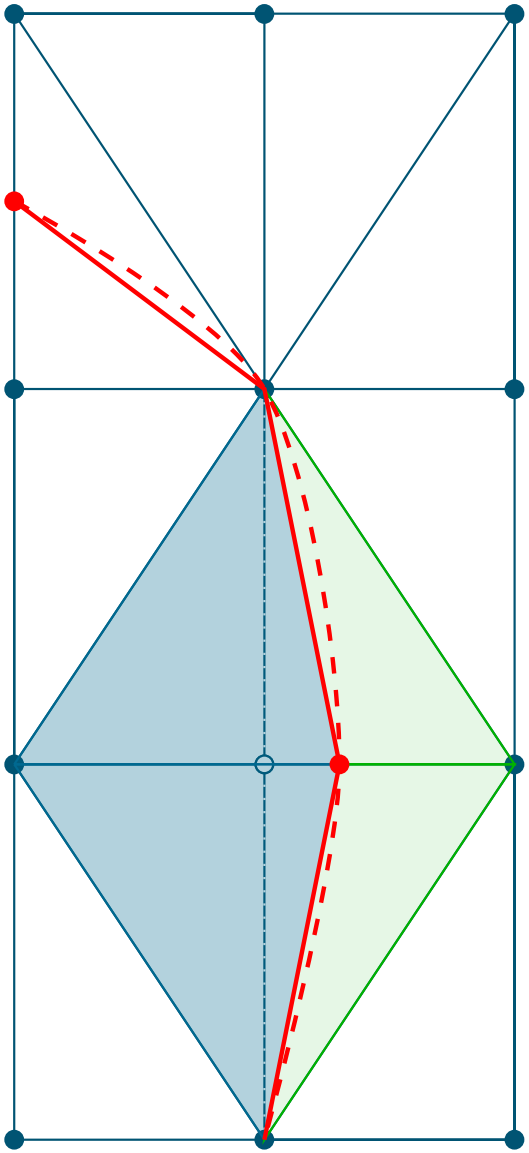
Cut (and Merge) Cell Approach:

- approximate $\Gamma(t) \to \Gamma_h(t)$,
- cut cells

Cut Cell Method (joint work with C. Chalons)

Basic Steps



Domain $\Omega \in \mathbb{R}^d$ with fluid in two phases at time $t > 0$

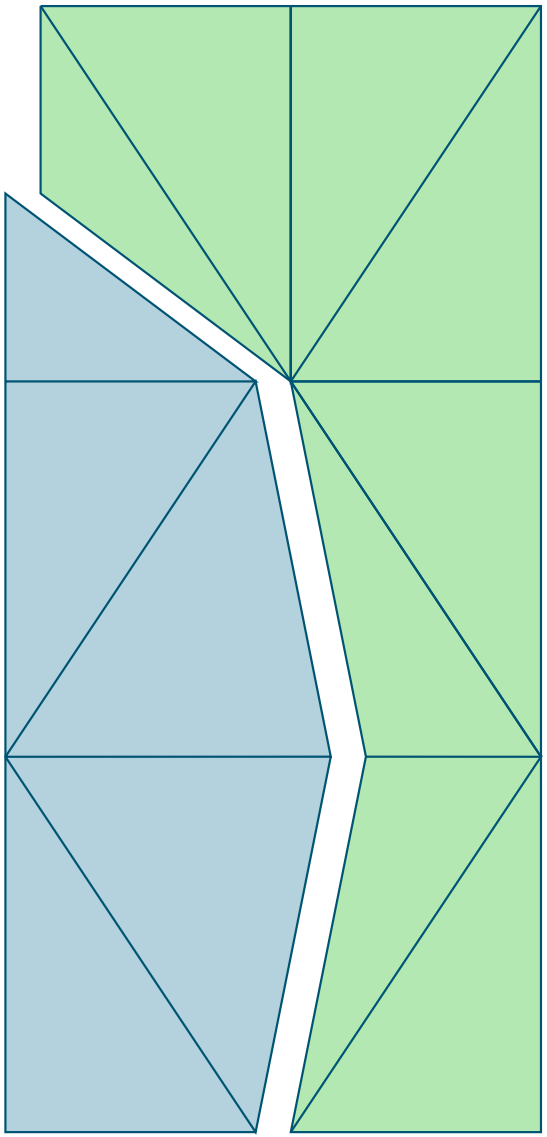
- liquid $\Omega_{\text{liq}}(t)$,
- vapour $\Omega_{\text{vap}}(t)$,
- curved phase boundary $\Gamma(t) = \partial\Omega_{\text{liq}}(t) \cap \partial\Omega_{\text{vap}}(t)$.

Cut (and Merge) Cell Approach:

- approximate $\Gamma(t) \to \Gamma_h(t)$,
- cut cells
- and merge, when cells are to small.

Cut Cell Method

Macroscale



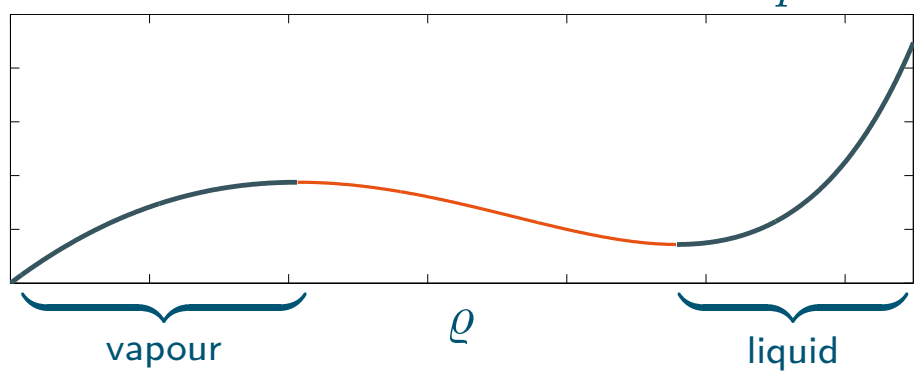
Macroscale

Dynamics of the bulk phases Ω_{liq} and Ω_{vap}.
Model: Isothermal Euler equation

$$\begin{aligned} \varrho_t + \operatorname{div}(\varrho\, \boldsymbol{v}) &= 0, \\ (\varrho\, \boldsymbol{v})_t + \operatorname{div}\left(\varrho\, \boldsymbol{v} \otimes \boldsymbol{v} + p(\varrho)\, \boldsymbol{I}\right) &= \boldsymbol{0}, \end{aligned}$$

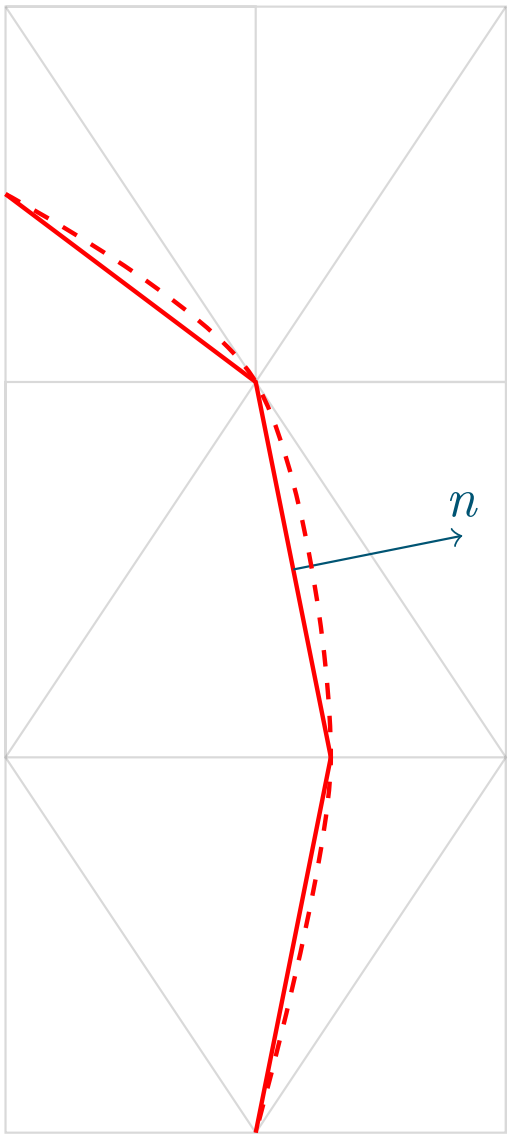
with a pressure function p that covers liquid and vapour phase.

Van-der-Waals like Pressure p



Cut Cell Method

Microscale



Microscale

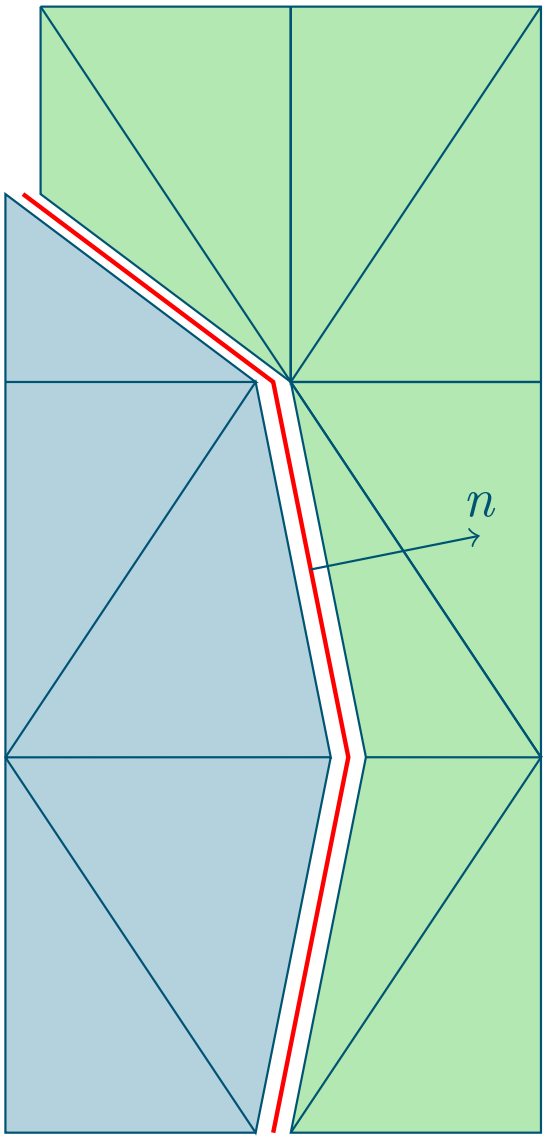
Dynamics at the phase boundary.

We assume that it is sufficient to consider 1D Riemann type problems normal to Γ_h.

- sharp interface models
  - exact (Liu) solver [Jägle, Rohde, Z 2012]
  - approximate (KinRel) solver [Rohde, Z 2013]
  - exact (KinRel) Riemannsolver [today]
- diffuse interface models
- molecular dynamic models

Cut Cell Method

Transfer Operator



Macro- to microscale

- initial states for Riemann type problems

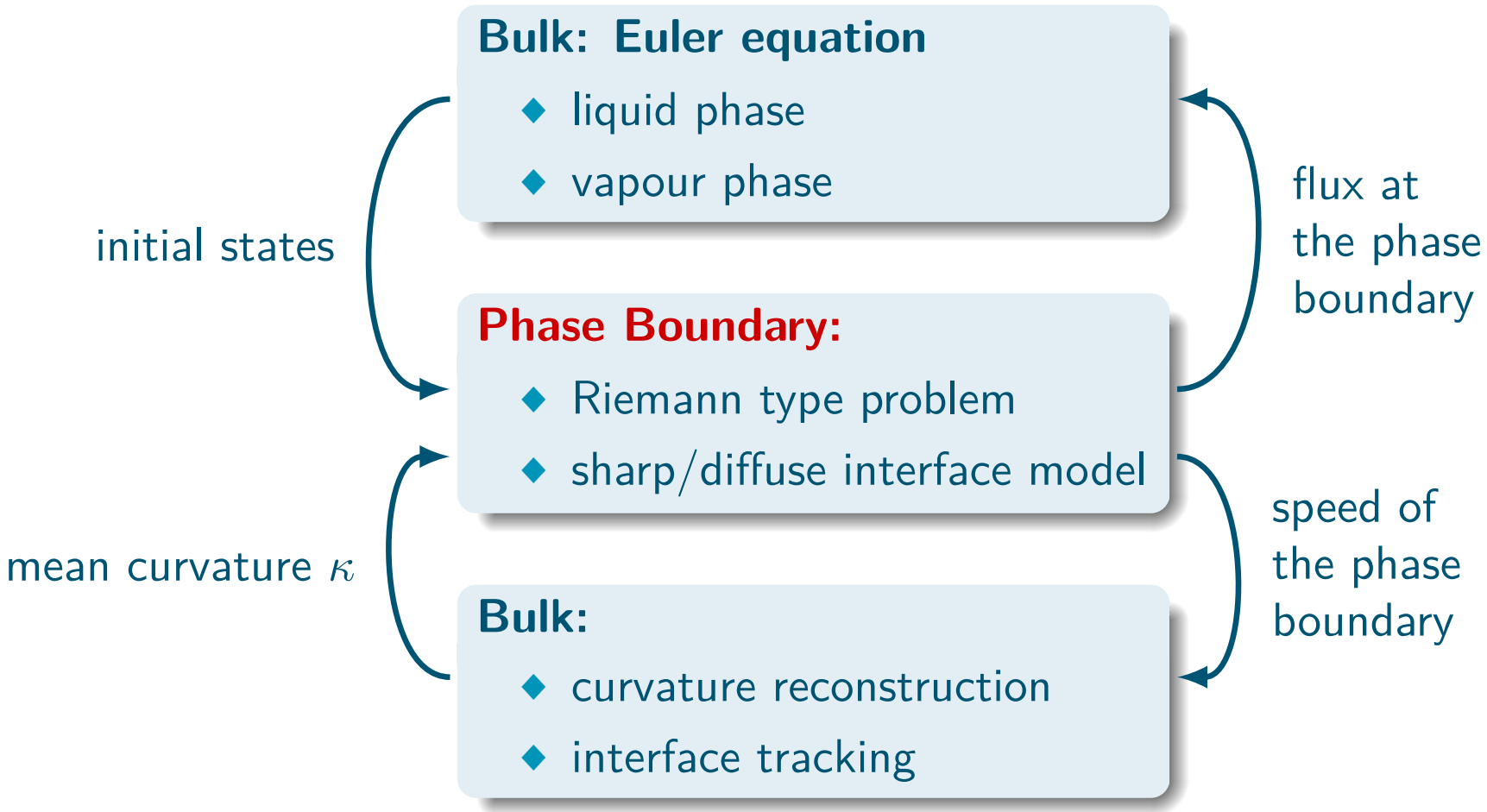
Micro- to macroscale

- fluxes for phase boundary edges

Cut Cell Method

Reconstruction:

Compression:



The cut cell method with Godunov type two phase flux is conservative.

Exact Riemann Solver

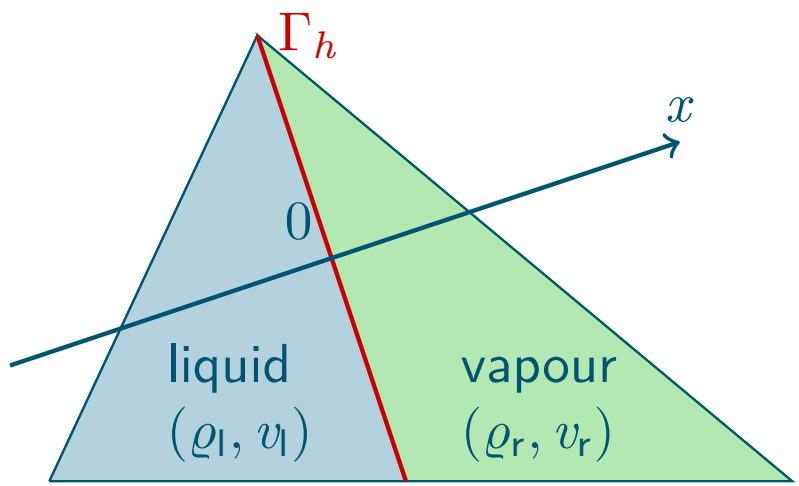
Sharp Interface Model

For each macro time step and any interface segment there is a Riemann problem to solve:

- Initial condition

$$\big(\varrho, v\big)(x,0) := \begin{cases} (\varrho_\mathsf{l}, v_\mathsf{l}) & \text{for } x \leq 0, \\ (\varrho_\mathsf{r}, v_\mathsf{r}) & \text{for } x > 0, \end{cases}$$

  w.l.o.g. ϱ_l in the liquid phase, ϱ_r in the vapour phase.
- $x = \boldsymbol{x} \cdot \boldsymbol{n}$, $v = \boldsymbol{v} \cdot \boldsymbol{n}$.
- Curvature is fixed.
- "Bubble case" with $\kappa > 0$
  "Droplet case" with $\kappa < 0$



Exact Riemann Solver

Sharp Interface Model

$$\begin{pmatrix} \varrho \\ \varrho v \end{pmatrix}_t + \begin{pmatrix} \varrho v \\ \varrho v^2 + p(\varrho) \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{in} \quad \mathbb{R} \times (0, \infty).$$

Riemann Problem

- Classical entropy solution in the bulk phases.
- There exists one phase boundary that satisfies

$$\begin{aligned} -\sigma \, [\![\varrho]\!] + \quad [\![\varrho \, v]\!] \quad &= \quad 0 \\ -\sigma \, [\![\varrho \, v]\!] + [\![\varrho \, v^2 + p(\varrho)]\!] &= (d-1)\gamma\kappa. \end{aligned}$$

- The phase boundary satisfies the kinetic relation

$$[\![g(\varrho) + 0.5 \, (v - \sigma)^2]\!] = -k \, j.$$

σ	speed of the phase boundary	$[\![\varrho]\!]$	$:= \varrho_{\text{vap}} - \varrho_{\text{liq}}$
j	$= \varrho(v - \sigma)$ mass flux	$\tau = 1/\varrho$	specific volume
$\tilde{p}(\tau)$	$:= p(\tau^{-1})$ pressure	$(d-1)\gamma\kappa$	(const.) surface tension
$\tilde{g}(\tau)$	$:= g(\tau^{-1})$ chemical potential	ψ	Helmholz free energy

Exact Riemann Solver

Sharp Interface Model

Exact Riemann Solver

- Classical entropy solution in the bulk phases.
- There exists one phase boundary that satisfies

$$\begin{aligned} -\sigma \left[\!\left[\varrho\right]\!\right] + \quad \left[\!\left[\varrho\, v\right]\!\right] \quad &= \quad 0 \\ -\sigma \left[\!\left[\varrho\, v\right]\!\right] + \left[\!\left[\varrho\, v^2 + p(\varrho)\right]\!\right] &= (d-1)\gamma\kappa. \end{aligned}$$

- The phase boundary satisfies the kinetic relation

$$\left[\!\left[g(\varrho) + 0.5\,(v-\sigma)^2\right]\!\right] = -k\,j.$$

Then, for $k > 0$, follows for the total energy $e = \psi + \frac{1}{2}v^2$:

$$-\sigma\left(\left[\!\left[\varrho e\right]\!\right] + (d-1)\gamma\kappa\right) + \left[\!\left[(\varrho e + p)\, v\right]\!\right] = -k\, j^2 \leq 0$$

Exact solvers are available ([LeFloch et al. (≥ 1991)], [Hantke et a. 2013] . . . , [Jägle, Rohde, Z 2012]), but only for simplified models or kinetic relations.

Exact Riemann Solver

Gibbs-Thomson based Kinetic Relation

Admissible Phase Boundary Wave

- connects liquid state $(\tau_{\text{liq}}, v_{\text{liq}})$ and vapour state $(\tau_{\text{vap}}, v_{\text{vap}})$,
- satisfies

$$\left.\begin{aligned} [\![\varrho(v-\sigma)]\!] &= 0, \\ j\,[\![v]\!] + [\![\tilde{p}(\tau)]\!] &= (d-1)\gamma\kappa \end{aligned}\right\} \quad \Rightarrow \quad j = \pm\sqrt{\frac{(d-1)\gamma\kappa - [\![\tilde{p}(\tau)]\!]}{[\![\tau]\!]}}$$

- and the kinetic relation

$$[\![\tilde{g}(\tau) + 0.5\, j^2\, \tau^2]\!] = -k\, j.$$

σ	speed of the phase boundary	$[\![\varrho]\!]$	$:= \varrho_{\text{vap}} - \varrho_{\text{liq}}$
j	$= \varrho(v-\sigma)$ mass flux	$\tau = 1/\varrho$	specific volume
$\tilde{p}(\tau)$	$:= p(\tau^{-1})$ pressure	$(d-1)\gamma\kappa$	(const.) surface tension
$\tilde{g}(\tau)$	$:= g(\tau^{-1})$ chemical potential	ψ	Helmholz free energy

Exact Riemann Solver

Gibbs-Thomson based Kinetic Relation

Example: Stationary Phase Boundary

- connects liquid state $(\tau_{\text{liq}}^{\text{mw}}, v_{\text{liq}}^{\text{mw}})$ and vapour state $(\tau_{\text{vap}}^{\text{mw}}, v_{\text{vap}}^{\text{mw}})$,
- satisfies

$$j = 0,$$
$$[\![\tilde{p}(\tau)]\!] = (d-1)\gamma\kappa$$

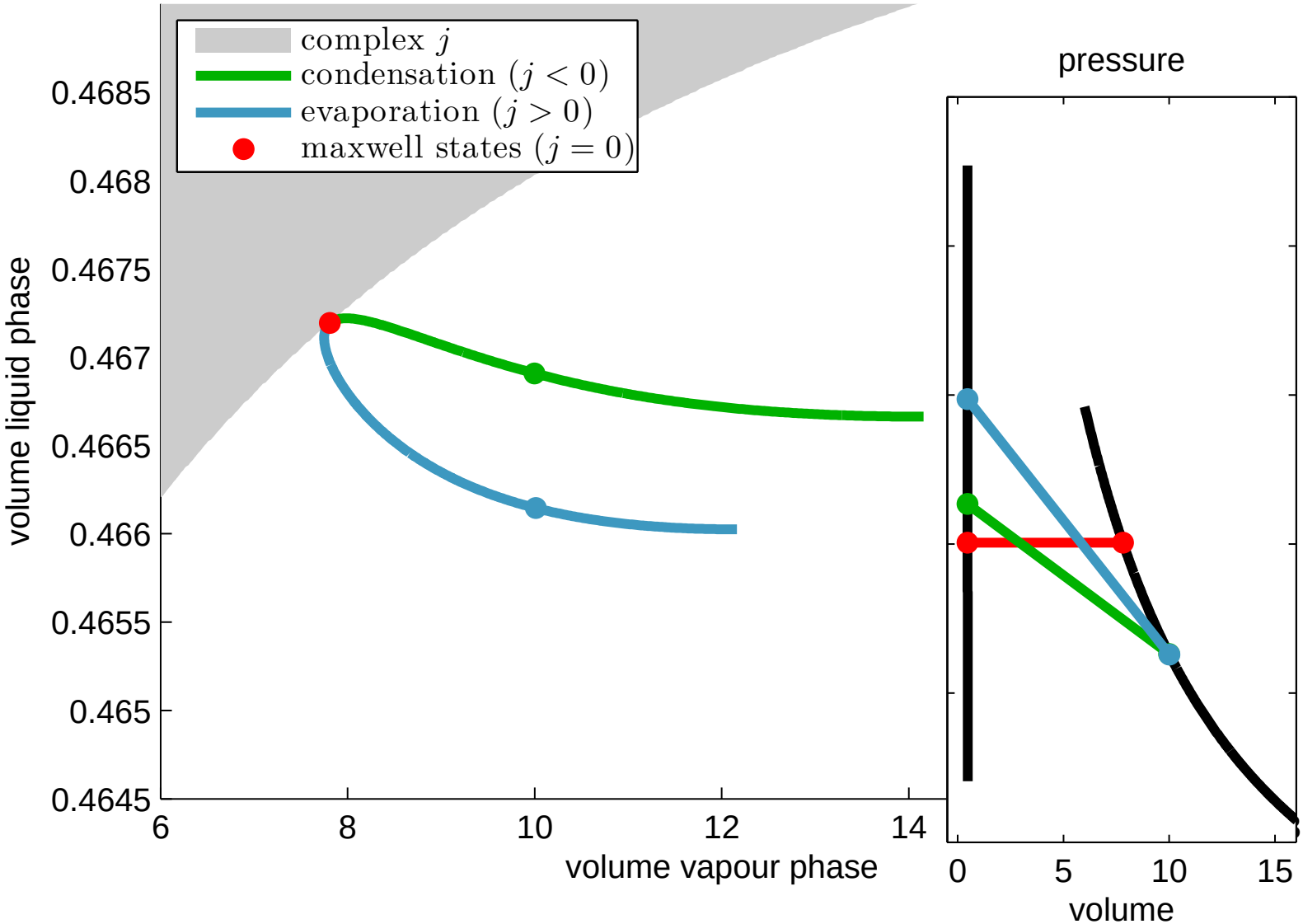
- and the kinetic relation

$$[\![\tilde{g}(\tau)]\!] = 0.$$

σ	speed of the phase boundary	$[\![\varrho]\!]$	$:= \varrho_{\text{vap}} - \varrho_{\text{liq}}$
j	$= \varrho(v-\sigma)$ mass flux	$\tau = 1/\varrho$	specific volume
$\tilde{p}(\tau)$	$:= p(\tau^{-1})$ pressure	$(d-1)\gamma\kappa$	(const.) surface tension
$\tilde{g}(\tau)$	$:= g(\tau^{-1})$ chemical potential	ψ	Helmholz free energy

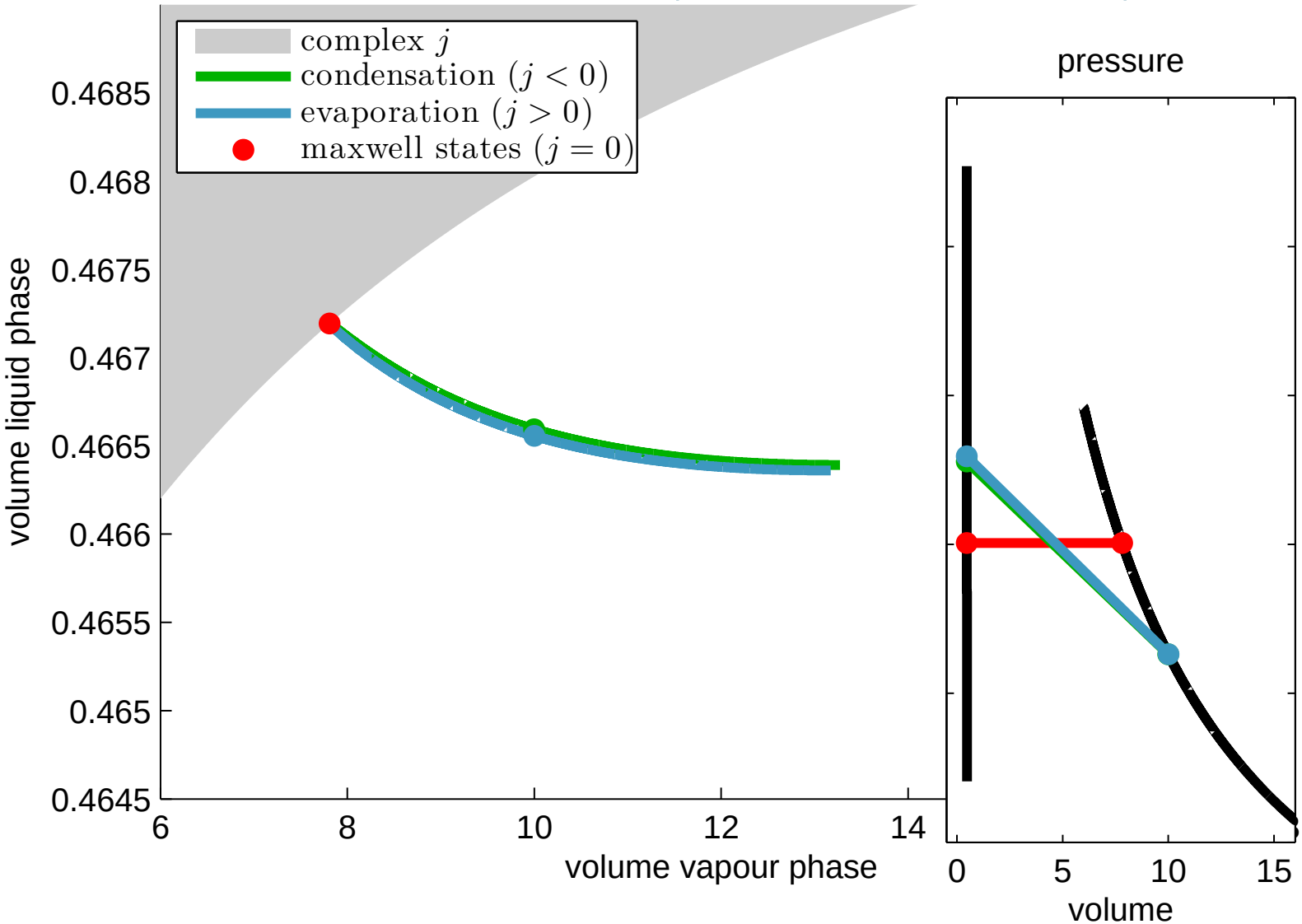
Exact Riemann Solver

Admissible phase boundaries for $k = 1$ (without surface tension)



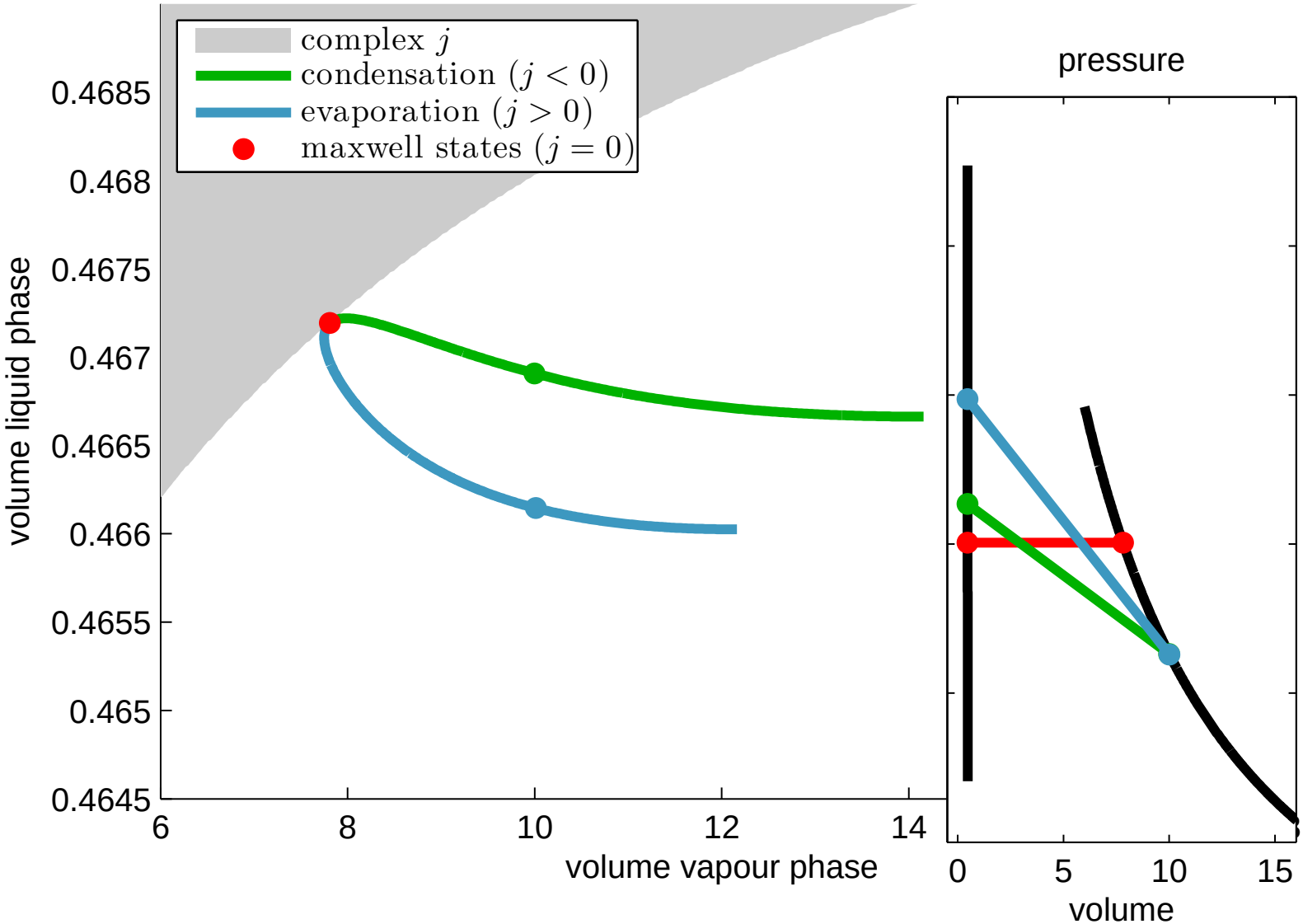
Exact Riemann Solver

Admissible phase boundaries for $k \to 0$ (without surface tension)



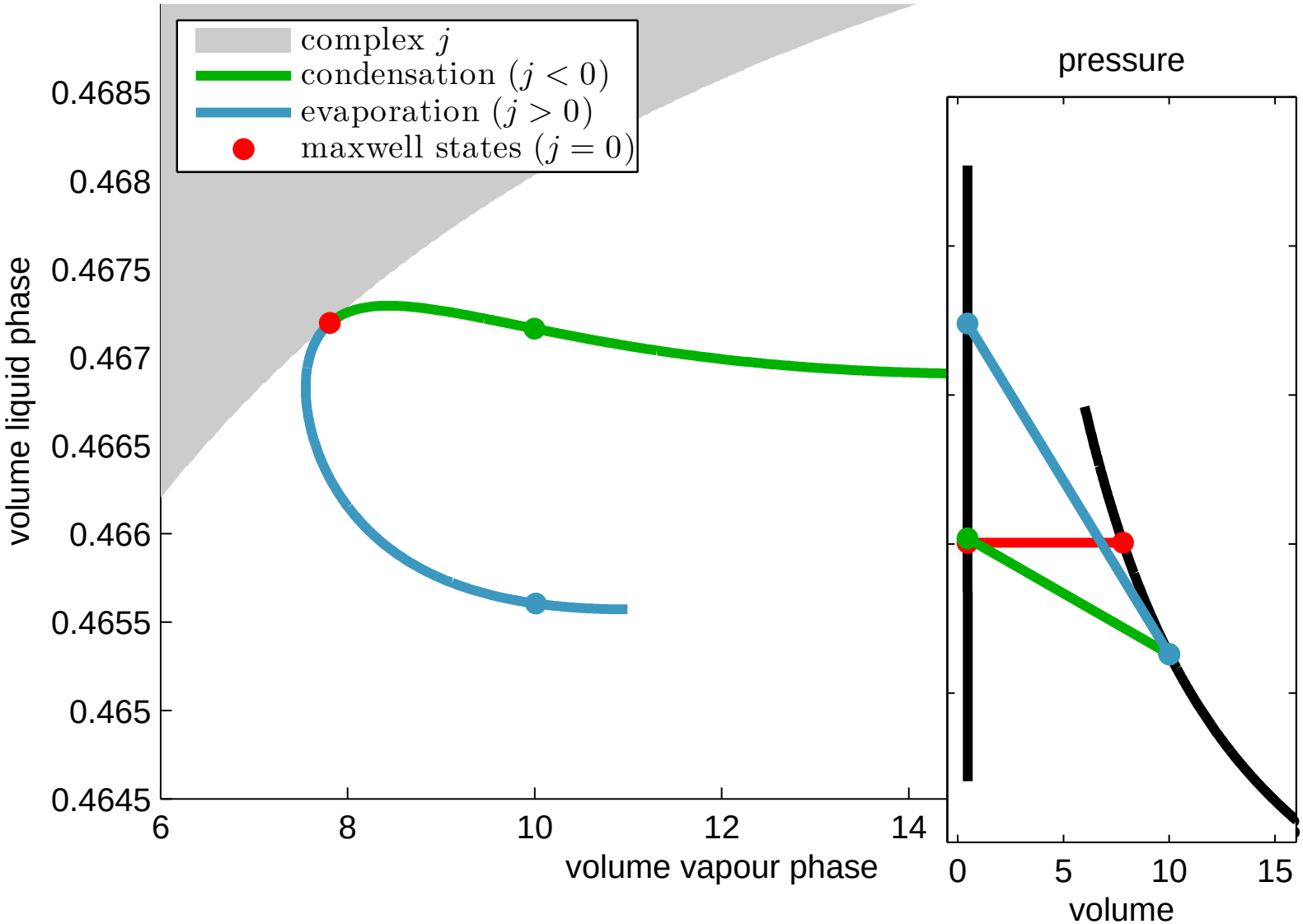
Exact Riemann Solver

Admissible phase boundaries for $k = 1$ (without surface tension)



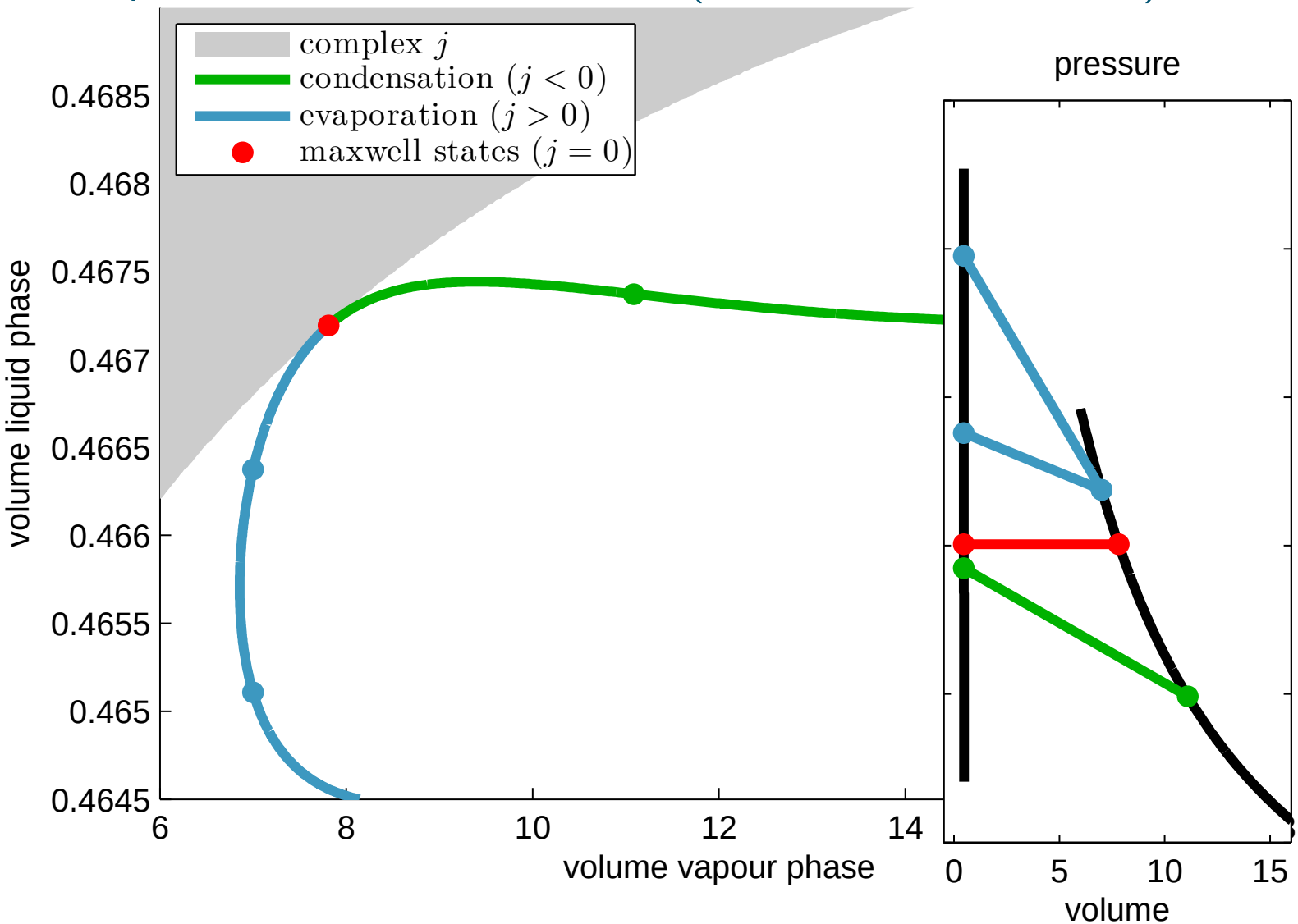
Exact Riemann Solver

Admissible phase boundaries for $k = 2$ (without surface tension)



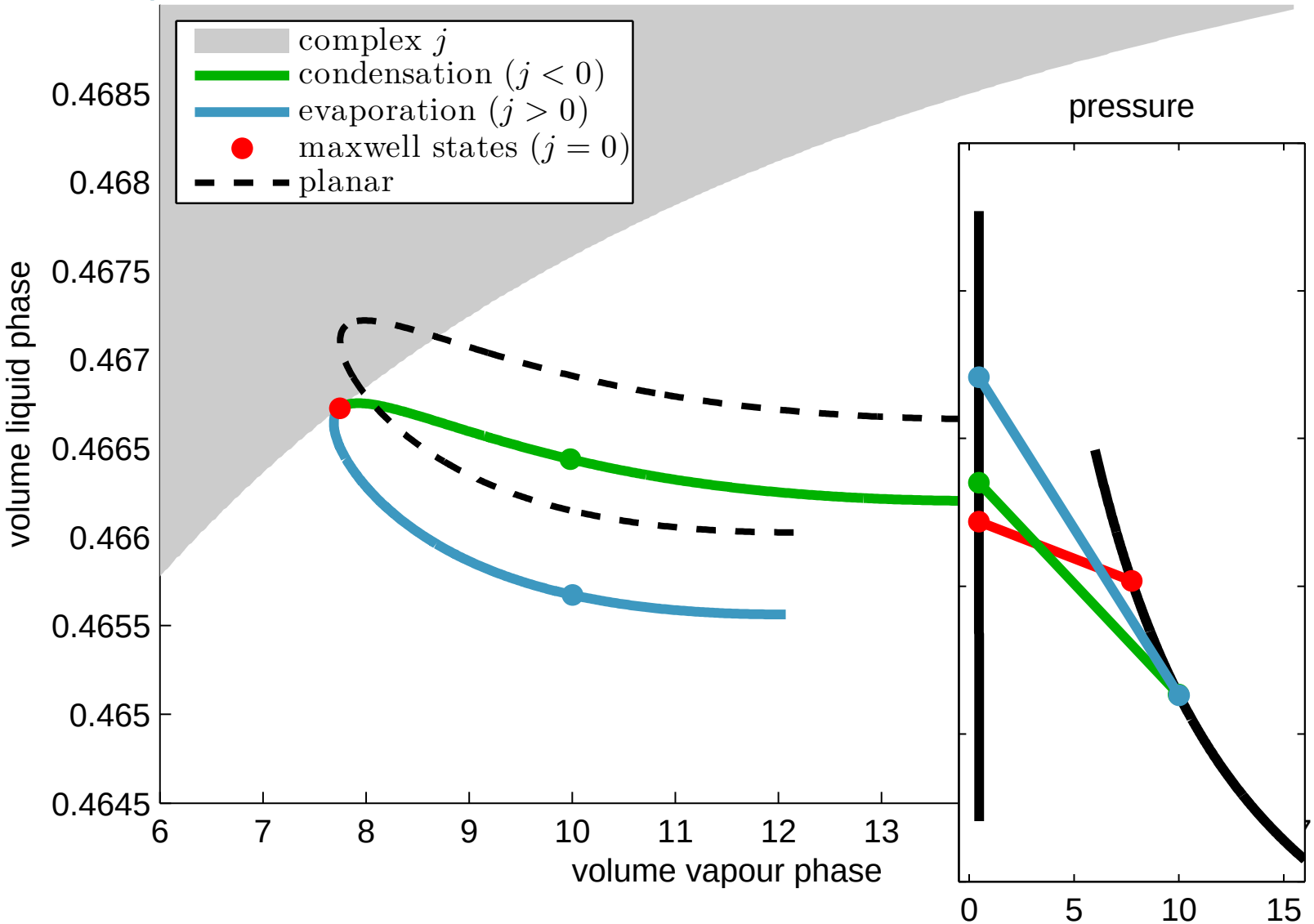
Exact Riemann Solver

Admissible phase boundaries for $k = 3.5$ (without surface tension)



Exact Riemann Solver

Admissible phase boundaries for $k = 1$ with surface tension



Exact Riemann Solver

Kinetic Relation based on the Generalized Gibbs-Thomson Law

There ex. kinetic functions f_c (condensation), f_e (evaporation) such that

$$\left.\begin{array}{rl} & f_c(\tau_{\text{vap}}) = \tau_{\text{liq}} \\ \vee & f_e(\tau_{\text{liq}}) = \tau_{\text{vap}} \end{array}\right\} \Leftrightarrow [\![\tilde{g}(\tau) + 0.5\, j^2\, \tau^2]\!] = -k\, j.$$

$k = 0$ Reversible process $f_c(f_e(\tau_{\text{liq}})) = \tau_{\text{liq}}$.

$0 \leq k < k^*$ Monotone functions $\tau_{\text{vap}} \mapsto f_c$ and $\tau_{\text{liq}} \mapsto f_e$.

$k > k^*$ Phase transition in metastable region.
Loss of monotonicity $\rightarrow$ uniqueness?

Monotone Kinetic Functions with Maximal Entropy Dissipation

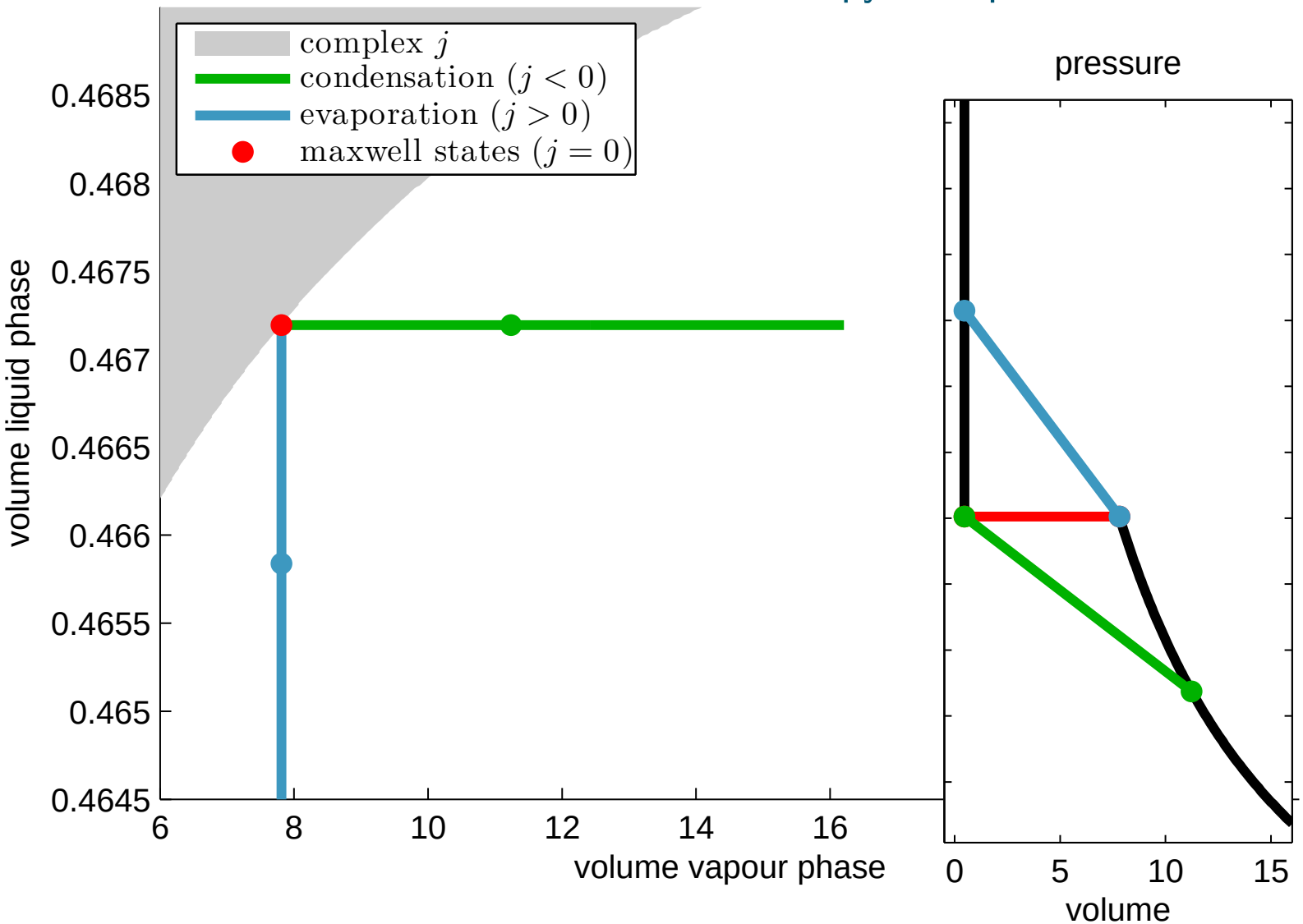
Define $f_c^{\text{m}}(\tau_{\text{vap}}) := \tau_{\text{liq}}^{\text{mw}}$ and $f_e^{\text{m}}(\tau_{\text{liq}}) = \tau_{\text{vap}}^{\text{mw}}$.

Observation:

- The Liu entropy criterion applied on a modified pressure based on the Maxwell equal area rule leads to f_c^{m}, f_e^{m}.

Exact Riemann Solver

Monotone Kinetic Functions with Maximal Entropy Dissipation



Exact Riemann Solver

Based on f_c and f_e we construct the full wave fan. Phase boundaries of Lax type are allowed but undercompresive waves are "preferred".

Theorem [Z 2014]

The Riemann problem for $|\kappa| < C$ and the kinetic relation based on the generalized Gibbs-Thomson law with $0 \leq k < k^*$ or has a unique entropy solution. The solution consist of elementary waves and exactly one phase boundary satisfying

$$-\sigma \left([\![\varrho e]\!] + (d-1)\gamma\kappa \right) + [\![(\varrho e + p)\, v]\!] \leq 0$$

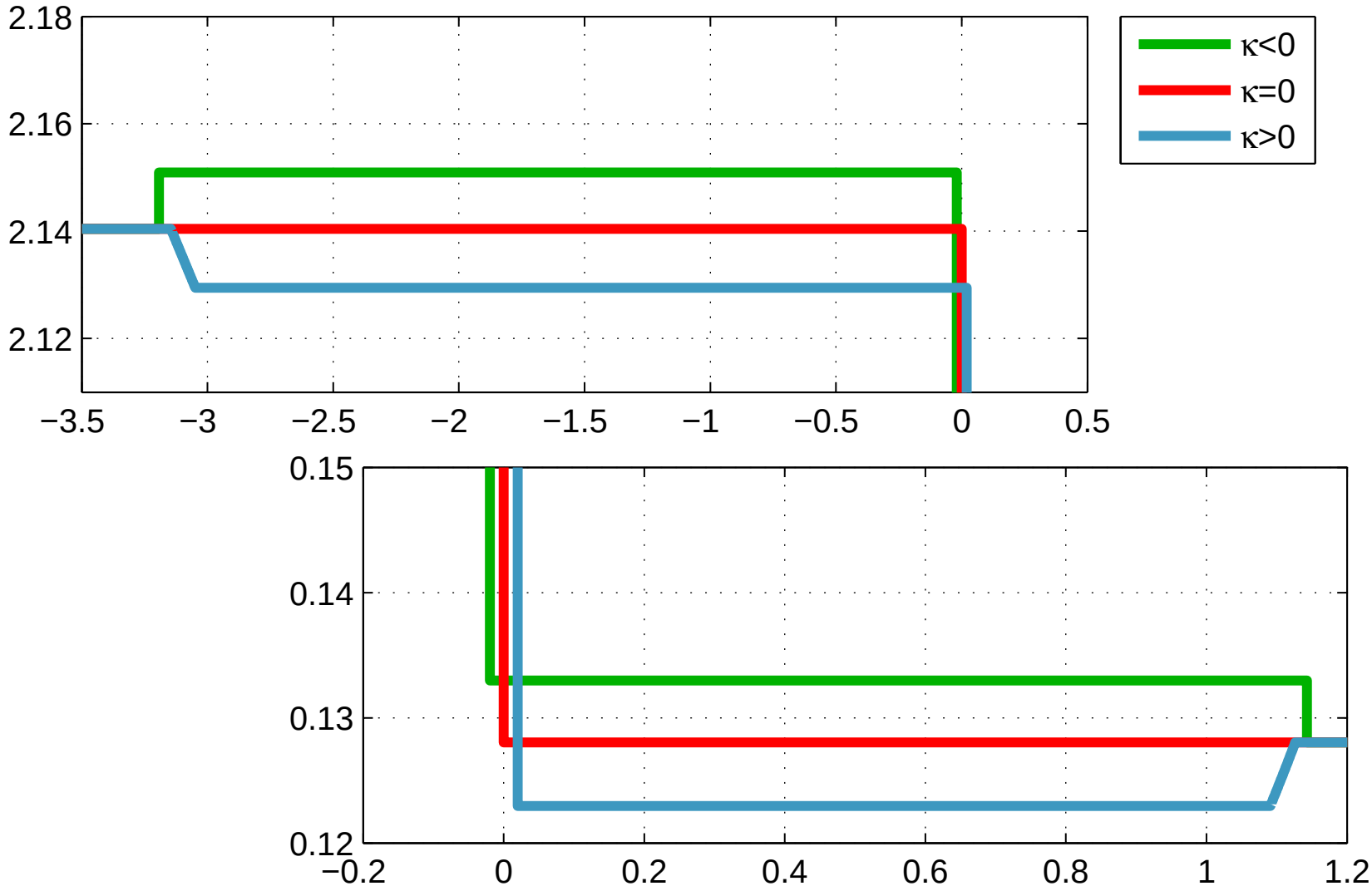
for $e = \psi + \frac{1}{2}v^2$.

For the construction, we follow [LeFloch 2002].

Exact Riemann Solver

Example

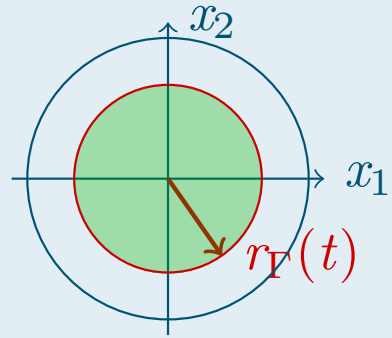
Density of examples with varying surface tension:



Numerical Results

Benchmark Problem for Surface Tension

Cut cell method for radially symmetric solutions on $\Omega = \left\{ \boldsymbol{x} \in \mathbb{R}^d \,\middle|\, 0 < |\boldsymbol{x}| = r < 1 \right\}$ with phase boundary $\Gamma(t) = \left\{ \boldsymbol{x} \in \mathbb{R}^d \,\middle|\, |\boldsymbol{x}| = r_\Gamma(t) \right\}$.



- Bulk system:

$$\begin{pmatrix} \varrho \\ \varrho\, v \end{pmatrix}_t + \begin{pmatrix} \varrho\, v \\ \varrho\, v^2 + p(\varrho) \end{pmatrix}_r = \frac{1-d}{r} \begin{pmatrix} \varrho\, v \\ \varrho\, v^2 \end{pmatrix} \quad \text{for} \quad \begin{array}{c} r \in (0, r_\Gamma) \cup (r_\Gamma, 1), \\ t > 0. \end{array}$$

- Simple interface tracking $\left(r_\Gamma^{n+1} = r_\Gamma^n + \Delta t\, \sigma^n\right)$
  and curvature reconstruction $\left(\kappa^n = 1/r_\Gamma^n\right)$.

$d = 1$: Fully conservative [Chalons, Wiebe]

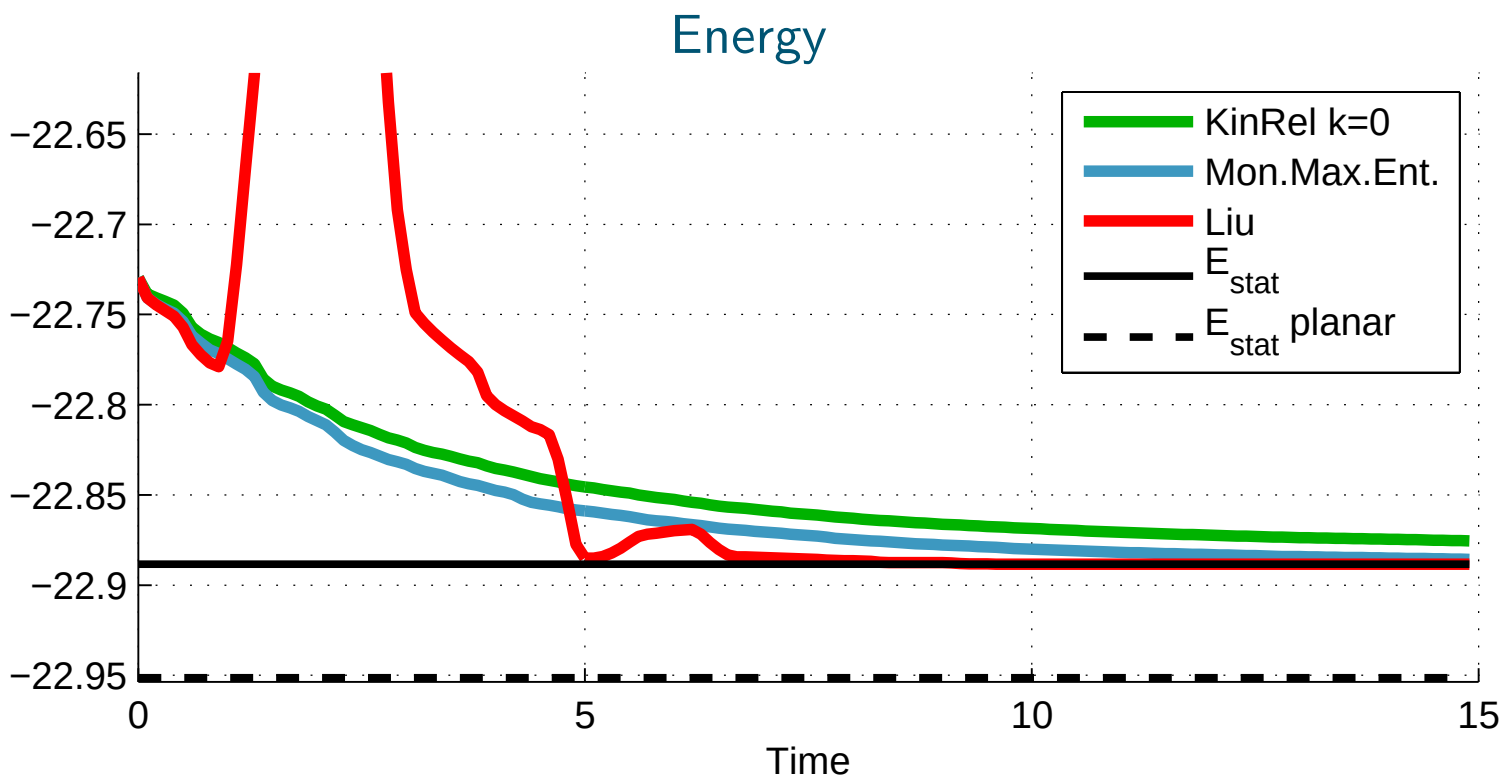
$d > 1$: Mass conservative (multidimensional sence) [Rohde, Z 2013]

Numerical Results

Global Energy (cf. [Gurtin 1985])

$$E(\varrho, \boldsymbol{v}) = \int_\Omega \frac{1}{2}\varrho\,|\boldsymbol{v}|^2 + \varrho\,\psi(\varrho)\,\mathrm{d}x + \gamma\,|\Gamma|\,,$$

$$E_{\text{stat}} = \min\left\{\, E(\varrho, \mathbf{0}) \;\middle|\; \textstyle\int_\Omega \varrho\,\mathrm{d}x = \text{const.} \,\right\}$$

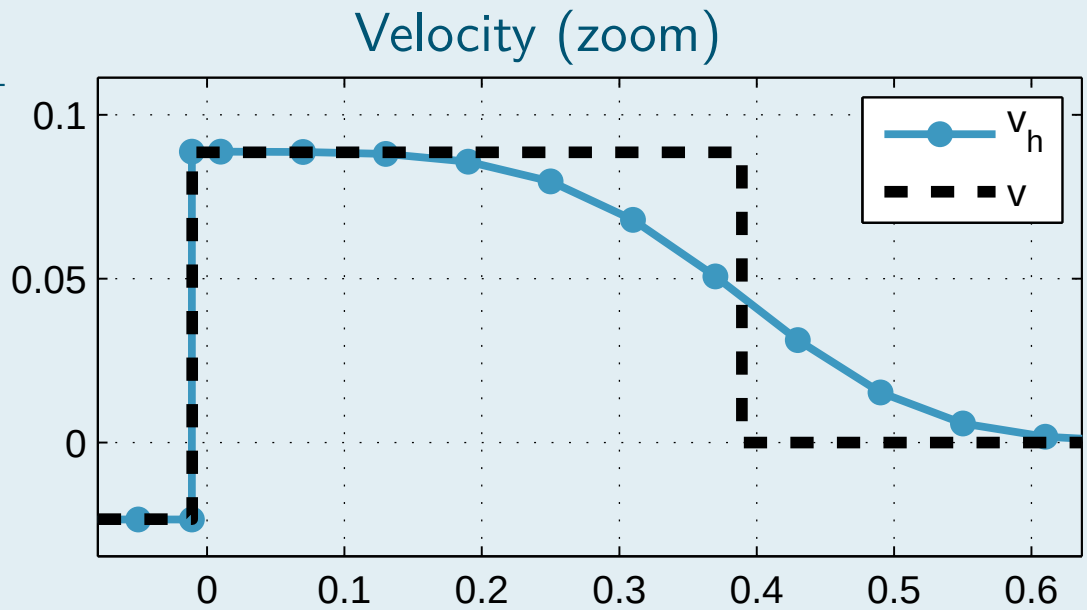


(Initial conditions $\varrho_L = \varrho_{\text{liq}}^{\text{mw}}$, $\varrho_R = \varrho_{\text{vap}}^{\text{mw}}$, $v_R = 0.1$, $v_L = -0.1$, $\gamma = 0.01$, $d = 2$)

Numerical Results

Experimental order of convergence

Cells	Error	Order
100	1.7e-03	
200	1.1e-03	0.68
500	5.7e-04	0.70
1000	3.4e-04	0.74
1500	2.5e-04	0.76
2000	2.0e-04	0.76
2500	1.7e-04	0.75
3000	1.5e-04	0.75



(Initial conditions $\varrho_\mathrm{l} = 2.1368$, $\varrho_\mathrm{r} = 0.0333$, $v = 0$, $k = 0.0001$, reference solution from exact Riemann solver, $d = 1$)

Numerical Results

Application in 2d (with P. Engel)

Pure Liu Riemann solver,

$$\varrho(\boldsymbol{x}, 0) = \begin{cases} 0.319 & : \text{inside}, \\ 1.806 & : \text{outside}, \end{cases}$$

$$\boldsymbol{v}(\boldsymbol{x}, 0) = \mathbf{0},$$

$$\gamma = 0.001.$$

Summary

- Conservative front tracking scheme.
- Exact Riemann solver
  - based on the generalized Gibbs-Thomson law.
  - for arbitrary pressure laws
    (Peng Robinson, external library (FPROPS [IAPWS])).

Outlook

Approximative solver for the full Euler system.

Literature

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