A sharp interface finite volume method for variable density zero Mach number two–phase flow with soluble surfactants

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Zero-Mach number variable density finite volume scheme

Leading order system in dimensional (space-)integral form

$$mass: \quad \frac{d}{dt}\int_{\Omega} \rho \, dV = -\int_{\partial\Omega} (\rho\theta\, \mathbf{u}\cdot\mathbf{n}) \left(\frac{1}{\theta}\right) dS$$

$$spec: \quad \frac{d}{dt}\int_{\Omega} \rho Y_s \, dV = -\int_{\partial\Omega} (\rho\theta\, \mathbf{u}\cdot\mathbf{n}) \left(\frac{Y_s}{\theta}\right) dS - \int_{\partial\Omega} \mathbf{j}_s\cdot\mathbf{n}\, dS + \int_{\Omega} \dot{\sigma}_s \, dV$$

$$mom: \quad \frac{d}{dt}\int_{\Omega} \rho \mathbf{u} \, dV = -\int_{\partial\Omega} (\rho\theta\, \mathbf{u}\cdot\mathbf{n}) \left(\frac{\mathbf{u}}{\theta}\right) dS - \int_{\partial\Omega} p^{(2)}\mathbf{n}\, dS + \int_{\Omega} \rho\mathbf{g}\, dV + \int_{\partial\Omega} \mathbf{T}\cdot\mathbf{n}\, dS + \int_{\partial\Omega\cap\Gamma} \sigma\mathbf{t}\, dl$$

$$en: \quad \frac{d}{dt}\int_{\Omega} \rho\theta \, dV = -\int_{\partial\Omega} (\rho\theta\mathbf{u}\cdot\mathbf{n}) \, dS + \int_{\Omega} \rho\theta D\, dV \qquad \textit{with}$$

$$\int_{\Omega} \rho\theta D\, dV = -\frac{dp^{(0)}}{dt}\int_{\Omega}\frac{\theta}{c^2}\, dV + \int_{\Omega}\left(\frac{\theta}{c^2\Xi}\left[\nabla\cdot\mathbf{q} + \sum_s \mathbf{j}_s\cdot\nabla h_s + \sum_s \Delta h_s \dot{\sigma}_s\right]\right) dV$$

black: implemented as predictor (2nd order Runge-Kutta) - corrector (2 projection steps) method (yet single-phase) with
fluxes based on fluxes of $\rho\theta$ where θ is the entropy
red: not implemented yet

1^{st} projection step: Poisson equation to enforce divergence constraint via flux corrections

$$\int_{\partial\Omega} \left[\frac{\Delta t}{2}\theta^{(n+\frac{1}{2})}\right] \left(\nabla\pi^{(2)}\right)^{(n+\frac{1}{4})} \cdot \mathbf{n}\, dS = -\left(\frac{d}{dt}\int_{\Omega}\rho\theta\, dV\right)^{(*)} \quad \textit{where} \quad \left(\nabla\pi^{(2)}\right)^{(n+\frac{1}{4})} = \left(\nabla\pi^{(2)}\right)^{(n+\frac{1}{2})}$$

2^{nd} projection step: Poisson equation to correct pressure via momentum flux correction

$$\int_{\partial\overline{\Omega}} \left[\Delta t\theta^{(n+1)}\right] \left(\nabla\partial p^{(2)}\right)^{(n+\frac{1}{2})} \cdot \mathbf{n}\, dS = \int_{\partial\overline{\Omega}} (\rho\theta\mathbf{u})^{(n+1,**)}\cdot\mathbf{n}\, dS - \int_{\overline{\Omega}} (\rho\theta D)^{(n+1,**)}\, dV$$

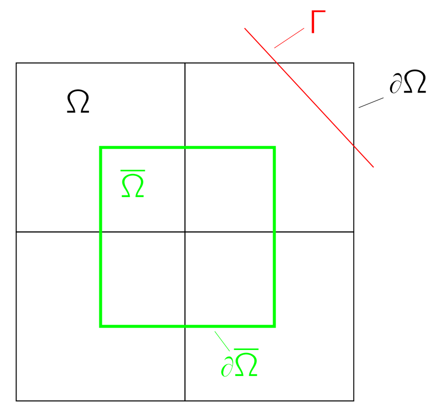


Fig 1: interface (red), primal (black) and dual (green) cells

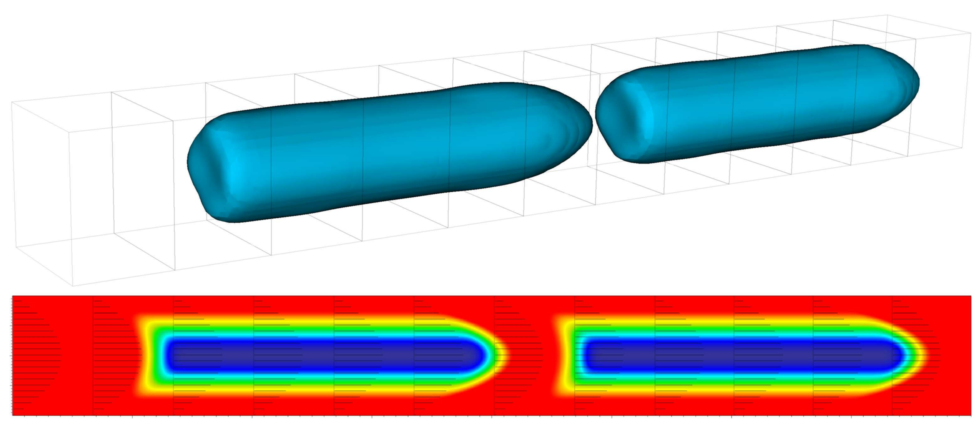


Fig 2: bubbles (density) in horizontal channel at zero gravity (yet no interface / phase separation included)

Discretisation of a surface surfactant equation with an embedding method*

Prototype of an advection-diffusion equation on an interface $\Gamma \subset \mathbb{R}^n$:

$$\frac{\partial\phi_\Gamma}{\partial t} = F(\phi_\Gamma, \nabla_\Gamma\phi_\Gamma, \Delta_\Gamma\phi_\Gamma), \qquad (1)$$

with solution $\phi_\Gamma \in \mathbb{R}$, surface gradient ∇_Γ and Laplace-Beltrami operator $\Delta_\Gamma = \nabla_\Gamma\cdot\nabla_\Gamma$.

Instead of solving (1) on the surface Γ we solve a PDE for $\phi \in \mathbb{R}^d$ in the surface embedding domain $\Omega_\Gamma \in \mathbb{R}^d$:

$$\frac{\partial\phi}{\partial t} = F(\phi, \nabla\phi, \Delta\phi), \qquad (2)$$

where $\phi_\Gamma, \nabla_\Gamma, \Delta\phi_\Gamma$ in (1) have been replaced by Cartesian operators in the embedding Euclidian space.

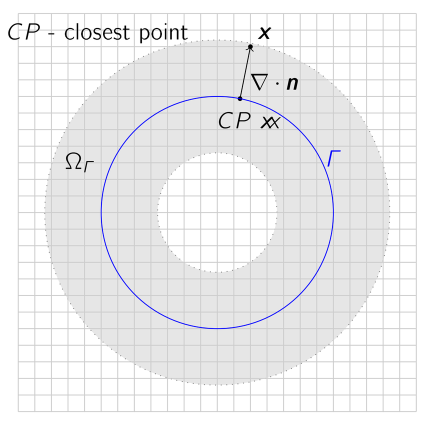


Fig 3: Closest point representation

Solution procedure:

1. Extend solution from surface Γ into the embedding space under the constraints $\nabla u\cdot\mathbf{n} = 0$, $u(\mathbf{x}_\Gamma) = u_\Gamma(\mathbf{x}_\Gamma)$ via closest point method (Ruuth, Merriman, JCP 227, 2008), Fig. 3
2. Solve (2) in Ω_Γ for timestep Δt
3. Interpolate solution $u(\mathbf{x})$ back onto the closest points (CP) on the surface
4. Repeat 1.-3. until end of simulation time

Example: Scalar advection on an ellipse:

$$\frac{\partial\phi_\Gamma}{\partial t} + \frac{\partial(\phi_\Gamma u_\Gamma)}{\partial s} = 0$$

with arclength s and initial condition $\phi(s, 0) = \cos^2(2\pi\, s/L)$.
The embedding PDE is

$$\frac{\partial\phi}{\partial t} + \nabla\cdot(\phi\,\boldsymbol{u}) = 0$$

where ϕ and $\boldsymbol{u}$ are closest point representations of ϕ_Γ and u_Γ.

Δx	Error	Conv. rate
0.05	1.11e-03	–
0.025	2.76e-04	2.01
0.0125	6.90e-05	2.00
0.00625	1.80e-05	1.94
0.003125	4.29e-06	2.07

Tab. 1: Error in the L_∞-norm using three-step Runge-Kutta time integration and 2nd order finite volume discretisation in space.

* Kathrin Mellert, Diploma thesis, TU Berlin, to appear

Sharp interface Poisson solver

We have implemented our locally second order Poisson solvers (JCP 2006, 2009) for node-centered and cell-centered problems into the LLNL AMR framework SAMRAI, Fig. 4. Key features

- finite volume discretization
  $\int_{\partial\Omega}\beta\,(\nabla u\cdot\boldsymbol{n})\, dS = \int_{\Omega^+} f^+\, dV + \int_{\Omega^-} f^-\, dV - \int_{\Gamma_\Omega} [\![\beta u_n]\!]\, dS$,
- single piecewise bi- (2D) or tri-linear (3D) ansatz functions on normal cells,
- dual piecewise bi- (2D) or tri-linear (3D) ansatz functions on cut-cells with explicit incorporation of the known interface jump conditions $[\![u]\!]_\Gamma$ and $[\![\beta u_n]\!]_\Gamma$,
- 9- (2D) and 27-point (3D) compact stencils,
- locally second order accurate,
- interface representation using standard 2nd order levelsets.

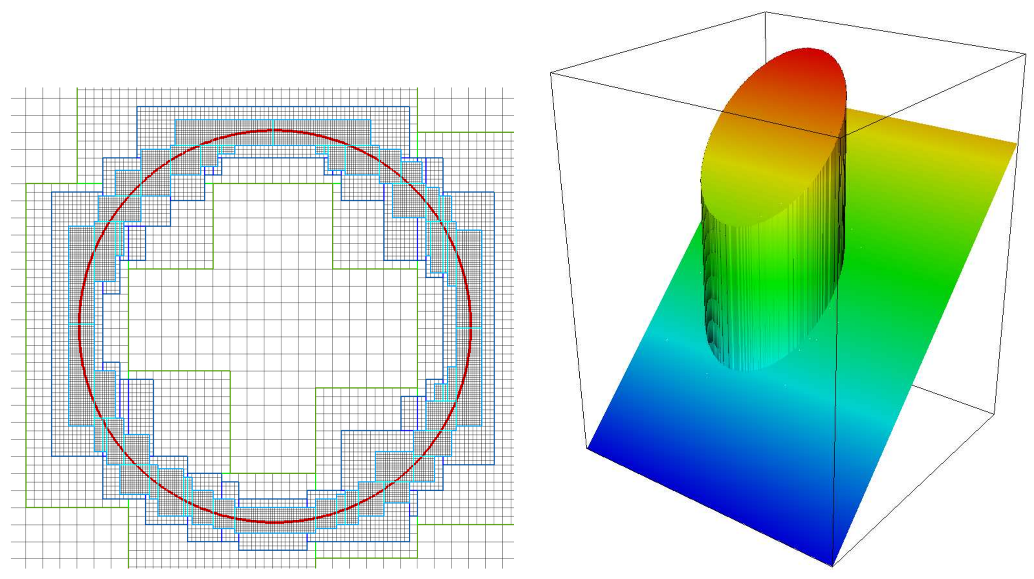


Fig. 4: Adapted Cartesian grid and initial hydrostatic pressure with density ratio 1.

Asymptotics based sharp interface Poisson solver for arbitrary ratios of the coefficients

The accurate and efficient solution of elliptic equations

$$\nabla\cdot\left(\beta(\mathbf{x})\,\nabla u(\mathbf{x})\right) = f(\mathbf{x})$$

with variable coefficients and prescribed interface jump conditions

$$[\![u]\!]_\Gamma \quad \text{and} \quad [\![\beta u_n]\!]_\Gamma$$

across an interface Γ is a key component in modeling incompressible two phase flow. One associated numerical problem is the robust solution in the case of a **large ratio of the coefficient** (e.g. $\beta = \rho, \mu, D$).

Asymptotic solution approach
On each side of the interface we have

$$\begin{aligned} \nabla\cdot(\beta^+\,\nabla u^+(\mathbf{x})) &= f^+(\mathbf{x}), \quad \mathbf{x}\in\Omega^+ \\ \nabla\cdot(\beta^-\,\nabla u^-(\mathbf{x})) &= f^-(\mathbf{x}), \quad \mathbf{x}\in\Omega^- \end{aligned} \qquad (3)$$

with interface jump conditions

$$[\![u]\!]_\Gamma = g(\mathbf{x}_\Gamma) \quad \text{and} \quad [\![\beta u_n]\!]_\Gamma = h(\mathbf{x}_\Gamma).$$

We are interested in small ratios

$$\beta^-/\beta^+ = \varepsilon \ll 1$$

and write

$$\begin{aligned} \nabla\cdot(\varepsilon^{-1}\beta^-\,\nabla u^+(\mathbf{x})) &= f^+(\mathbf{x}), \quad \mathbf{x}\in\Omega^+ \\ \nabla\cdot(\beta^-\,\nabla u^-(\mathbf{x})) &= f^-(\mathbf{x}), \quad \mathbf{x}\in\Omega^- \end{aligned}$$

Introducing the asymptotic expansion

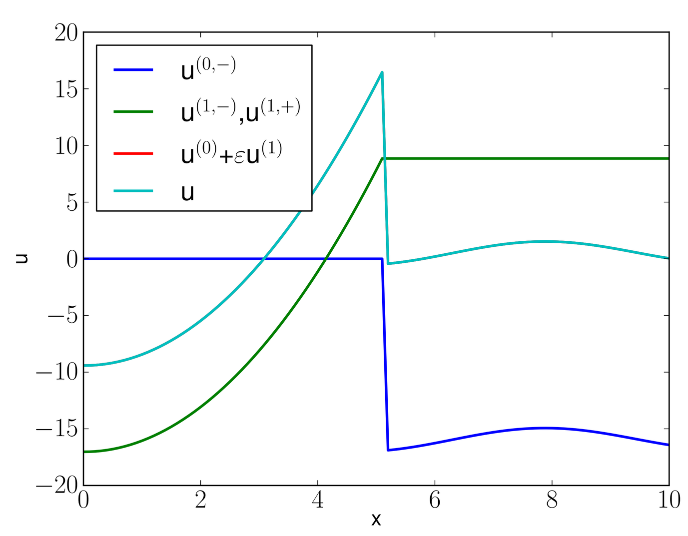
$$\begin{aligned} u^+(\mathbf{x}) &= u^{(0,+)}(\mathbf{x}) + \varepsilon\, u^{(1,+)}(\mathbf{x}) \\ u^-(\mathbf{x}) &= u^{(0,-)}(\mathbf{x}) + \varepsilon\, u^{(1,-)}(\mathbf{x}) \end{aligned}$$

into (3) leads to the following
Solution strategy for the perturbation equations:

1. Solve $$\nabla\cdot\left(\beta^-\,\nabla u^{(0,-)}(\mathbf{x})\right) = f^-(\mathbf{x})$$
   in Ω^- with boundary condition $u_n^{(0,-)} = u_{n,w}^-$ on $\partial\Omega^-\backslash\Gamma$ and interface condition $u^{(0,-)} = -g$ on Γ.
2. Solve the coupled problem
   $$\begin{aligned} \nabla\cdot\left(\beta^-\,\nabla u^{(1,+)}(\mathbf{x})\right) &= f^+(\mathbf{x}), \quad \mathbf{x}\in\Omega^+ \\ \nabla\cdot\left(\beta^-\,\nabla u^{(1,-)}(\mathbf{x})\right) &= 0, \quad \mathbf{x}\in\Omega^- \end{aligned}$$
   with
   $$\begin{aligned} &[\![u^{(1)}]\!]_\Gamma = u^{(1,+)} - u^{(1,-)} = 0, \\ &\beta^- u_n^{(1,+)} - \varepsilon\beta^- u_n^{(1,-)} = h + \beta^- u_n^{(0,-)} \text{ on } \Gamma, \\ &u_n^{(1,-)} = 0,\ u_n^{(1,+)} = \varepsilon^{-1}u_{n,w}^+ \text{ on } \partial\Omega. \end{aligned}$$

1D example:

$$\begin{aligned} u^+ &= x^2,\ x\in(0, 5.14] \\ u^- &= 10 + \sin(x),\ x\in[5.14, 10) \end{aligned}$$



	condition number		
$\varepsilon = \beta^-/\beta^+$	$u^{(0,-)}$	$u^{(1)}$	u (single step)
1	3.9e3	8.2e4	8.2e4
1e-3	3.9e3	6.3e4	6.3e7
1e-6	3.9e3	6.3e4	6.3e10
1e-9	3.9e3	6.3e4	6.3e13