A Sharp Interface Finite Volume Method for Variable Density Zero Mach Number Two–Phase Flow with Soluble Surfactants

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Goals of the Priority Programme:

- derive and expand **mathematical models** that describe relevant physico-chemical interface phenomena,
- improve the understanding of mechanisms and phenomena occuring at fluidic interfaces by means of rigorous **mathematical analysis** of the underlying pde-systems,
- development and analysis of **numerical methods** for the simulation of multiphase flow problems which resolve the local processes at the interface.
- **validation** of the models and numerical simulation methods by means of specifically designed **experiments.**

Our project objective within the SPP

A Sharp Interface Finite Volume Method for Variable Density Zero Mach Number Two–Phase Flow with Soluble Surfactants (= Surface active agent)

⇒

Development of a locally second order conservative finite volume method for immiscible two-phase flow with the following features:

- sharp resolution of discontinuities
  - cut cells
  - combined conservative levelset - volume of fluid approach
- asymptotics based Poisson solver
- variable, surfactant dependent surface tension
- conservative discretization for the surface surfactant equation

Our project objective within the SPP

Work packages

1. *Sharp interface* Finite Volume projection method
2. *Sharp interface* Poisson solver for arbitrary ratio of coefficients
3. Conservative discretization of the surface surfactant equation

plus

everything in an AMR framework

Adaptive Mesh Refinement framework

DNS: several million grid cells

AMR framework to be used for

- Adaptive Mesh Refinement
- Parallelization / Load Balancing
- Grid management
- Structure and handling of data

$\Rightarrow$ SAMRAI (Lawrence Livermore National Labs)

Scaling tests on HLRN with up to 2048 processors
(HLRN: Northern German super-computing center, Berlin/Hannover)

Work package 1:

Sharp Interface
Finite Volume Projection Method

Governing equations

Zero Mach-number variable density equations (Klein et al., 2001)

non-dimensional compressible Navier-Stokes equations

$+$

asymptotic expansion of primitive variables in Mach number
(e.g. $p = p^{(0)} + Ma \cdot p^{(1)} + Ma^2 \cdot p^{(2)} + ...$)

$+$

separately equating only terms of same order of magnitude in Mach number due to $\lim_{Ma \to 0}$

$\Rightarrow$

- $\nabla p^{(0)} = 0 \quad \rightarrow \quad p^{(0)} = p^{(0)}(t)$
- $\nabla p^{(1)} = 0 \quad \rightarrow \quad p^{(1)} = p^{(1)}(t)$
- leading order system ($\rho^{(0)}$, ...) contains $p^{(2)}$ in mom. eq.
- divergence constraint from energy equation
- decoupling from acoustic phenomena

Governing equations

Zero Mach-number variable density equations – leading order system

mass :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s\,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

mom :
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v}\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V$$
$$+\int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = -\frac{1}{\rho c^2}\frac{\mathrm{d}p^{(0)}}{\mathrm{d}t} + \frac{1}{\rho c^2\,\Xi}\left[\nabla\cdot\boldsymbol{q} + \sum_s \boldsymbol{j}_s\cdot\nabla h_s + \sum_s \Delta h_s\dot{\sigma}_s\right]$$

Governing equations

Zero Mach-number variable density equations – leading order system

$$\textit{mass}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho \,\mathrm{d}V = -\int_{\partial\Omega} \rho\, \boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

$$\textit{spec}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho Y_s \,\mathrm{d}V = -\int_{\partial\Omega} \rho Y_s\, \boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega} \boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega} \dot{\sigma}_s\,\mathrm{d}V$$

$$\textit{mom}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho \boldsymbol{v} \,\mathrm{d}V = -\int_{\partial\Omega} \rho\, \boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega} p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega} \rho\boldsymbol{g}\,\mathrm{d}V$$

$$+ \int_{\partial\Omega} \mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma} \sigma\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = 0$$

Governing equations

Zero Mach-number variable density equations – hyperbolic part – advection

mass : $$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho \,\mathrm{d}V = -\int\limits_{\partial\Omega} \rho\, \boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec : $$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho Y_s \,\mathrm{d}V = -\int\limits_{\partial\Omega} \rho Y_s\, \boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int\limits_{\partial\Omega} \boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int\limits_{\Omega} \dot{\sigma}_s\,\mathrm{d}V$$

mom : $$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho\boldsymbol{v} \,\mathrm{d}V = -\int\limits_{\partial\Omega} \rho\, \boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int\limits_{\partial\Omega} p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int\limits_{\Omega} \rho\boldsymbol{g}\,\mathrm{d}V + \int\limits_{\partial\Omega} \mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int\limits_{\partial\Omega\cap\partial\Sigma} \sigma\boldsymbol{t}\,\mathrm{d}l$$

energy (to be integrated):

$$(\nabla\cdot\boldsymbol{v}) = 0$$

Finite Volume Projection Method

Zero Mach-number variable density equations – predictor step (Schneider et al., JCP '99)

mass : $$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

spec : $$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s\,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

mom : $$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v}\,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V$$

$$+\int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\boldsymbol{t}\,\mathrm{d}l$$

$\Rightarrow$ predicted values $\{\bar{\rho}^*, (\rho\bar{\boldsymbol{v}})^*, (\rho\bar{Y}_s)^*\}$ no divergence imposed!

Finite Volume Projection Method

Zero Mach-number variable density equations – predictor step (Klein, 2009)

$$\textit{mass}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho \,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

$$\textit{spec}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho Y_s \,\mathrm{d}V = -\int_{\partial\Omega}\rho Y_s\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S - \int_{\partial\Omega}\boldsymbol{j}_s\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\dot{\sigma}_s\,\mathrm{d}V$$

$$\textit{mom}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}\rho\boldsymbol{v} \,\mathrm{d}V = -\int_{\partial\Omega}\rho\,\boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S - \int_{\partial\Omega}p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int_{\Omega}\rho\boldsymbol{g}\,\mathrm{d}V + \int_{\partial\Omega}\mathbf{T}\cdot\boldsymbol{n}\,\mathrm{d}S + \int_{\partial\Omega\cap\partial\Sigma}\sigma\boldsymbol{t}\,\mathrm{d}l$$

$$\textit{energ}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}(\rho\theta) \,\mathrm{d}V = -\int_{\partial\Omega}(\rho\theta)\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

Finite Volume Projection Method

Zero Mach-number variable density equations – predictor step

$$\boxed{P = \rho\theta = \left(p^{(0)}\right)^{\frac{1}{\gamma}} = const.}$$

energg : $$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega}(\rho\theta)\,\mathrm{d}V = -\int_{\partial\Omega}(\rho\theta)\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S$$

$$P_t = -\nabla(P\boldsymbol{v})$$

exact : $$0 = -P\,\nabla\boldsymbol{v} \quad \rightarrow \quad \boxed{\nabla\boldsymbol{v} = 0}$$

disc : $$\frac{P^{(n+1)} - P^{(n)}}{\Delta t} = -\Big[\nabla(P\boldsymbol{v})\Big]^{(n+\frac{1}{2})} = 0$$

pred : $$\frac{P^{(n+1,*)} - P^{(n)}}{\Delta t} = -\Big[\nabla(P\boldsymbol{v})\Big]^{(n+\frac{1}{2},*)}$$

Finite Volume Projection Method

Zero Mach-number variable density equations – predictor step

$$\textit{mass}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho \,\mathrm{d}V = -\int\limits_{\partial\Omega} (P\,\boldsymbol{v}\cdot\boldsymbol{n}) \left(\frac{1}{\theta}\right) \mathrm{d}S$$

$$\textit{spec}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho Y_s \,\mathrm{d}V = -\int\limits_{\partial\Omega} (P\,\boldsymbol{v}\cdot\boldsymbol{n}) \left(\frac{Y_s}{\theta}\right) \mathrm{d}S$$

$$\textit{mom}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} \rho \boldsymbol{v} \,\mathrm{d}V = -\int\limits_{\partial\Omega} (P\,\boldsymbol{v}\cdot\boldsymbol{n}) \left(\frac{\boldsymbol{v}}{\theta}\right) \mathrm{d}S - \int\limits_{\partial\Omega} p^{(2)}\,\boldsymbol{n}\,\mathrm{d}S + \int\limits_{\Omega} \rho \boldsymbol{g}\,\mathrm{d}V$$

$$\textit{energ}: \quad \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega} (\rho\theta) \,\mathrm{d}V = -\int\limits_{\partial\Omega} (P\,\boldsymbol{v}\cdot\boldsymbol{n})\,\mathrm{d}S$$

Finite Volume Projection Method

Zero Mach-number variable density equations – 1^{st} correction step

Projection scheme – MAC-projection

Advection velocity correction (at cell interfaces) due to use of $p^{(2),n}$ as predictor pressure $\Rightarrow$ $\delta\pi = p^{(2),n+1} - p^{(2),n}$

$$\boldsymbol{v}^{n+\frac{1}{2}} = \boldsymbol{v}^{n+\frac{1}{2},*} - \frac{\Delta t}{2}\left(\frac{1}{\rho}\right)^{n+\frac{1}{2},*} \nabla \delta\pi$$

$$(P\boldsymbol{v})^{n+\frac{1}{2}} = (P\boldsymbol{v})^{n+\frac{1}{2},*} - \frac{\Delta t}{2}\left(\frac{P}{\rho}\right)^{n+\frac{1}{2},*} \nabla \delta\pi$$

$$0 = \nabla\left[(P\boldsymbol{v})^{n+\frac{1}{2}}\right] = \nabla\left[(P\boldsymbol{v})^{n+\frac{1}{2},*}\right] - \nabla\left[\frac{\Delta t}{2}\left(\frac{P}{\rho}\right)^{n+\frac{1}{2},*} \nabla \delta\pi\right]$$

$$\nabla\left[\frac{\Delta t}{2}\left(\frac{P}{\rho}\right)^{n+\frac{1}{2},*} \nabla \delta\pi\right] = \nabla\left[(P\boldsymbol{v})^{n+\frac{1}{2},*}\right] \quad \textit{var. coeff. Poisson eq.}$$

Finite Volume Projection Method

Zero Mach-number variable density equations – 1^{st} correction step

Post-correction of all advective flux contributions

$$\underbrace{\frac{\bar{P}^{(n+1)} - \bar{P}^{(n)}}{\Delta t}}_{=0} = \underbrace{\frac{\bar{P}^{(n+1,*)} - \bar{P}^{(n)}}{\Delta t}}_{\Delta \bar{P}*} + \underbrace{\frac{\bar{P}^{(n+1)} - \bar{P}^{(n+1,*)}}{\Delta t}}_{\Delta \tilde{P} \overset{!}{=} -\Delta \bar{P}*}$$

$$\Delta \tilde{P} = -\frac{1}{\Delta V} \int_{\partial\Omega} \underbrace{\left(-\left[\frac{\Delta t}{2} \left(\frac{P}{\rho} \right)^{n+\frac{1}{2},*} \nabla \delta\pi \right] \cdot \boldsymbol{n} \right)}_{\tilde{F}(P) = P \partial \tilde{\boldsymbol{v}} \cdot \boldsymbol{n}} \mathrm{d}S$$

Finite Volume Projection Method

Zero Mach-number variable density equations – 1^{st} correction step

Post-correction of all advective flux contributions

$$\textit{mass}: \quad \bar{\rho}^{n+1} = \bar{\rho}^{n+1,*} - \frac{\Delta t}{\Delta V} \int\limits_{\partial\Omega} (P\,\partial\tilde{\mathbf{v}}\cdot\mathbf{n}) \left(\frac{1}{\theta}\right) \mathrm{d}S$$

$$\textit{spec}: \quad \overline{\rho Y_s}^{n+1} = \overline{\rho Y_s}^{n+1,*} - \frac{\Delta t}{\Delta V} \int\limits_{\partial\Omega} (P\,\partial\tilde{\mathbf{v}}\cdot\mathbf{n}) \left(\frac{Y_s}{\theta}\right) \mathrm{d}S$$

$$\textit{mom}: \quad \overline{\rho\mathbf{v}}^{n+1,**} = \overline{\rho\mathbf{v}}^{n+1,*} - \frac{\Delta t}{\Delta V} \int\limits_{\partial\Omega} (P\,\partial\tilde{\mathbf{v}}\cdot\mathbf{n}) \left(\frac{\mathbf{v}}{\theta}\right) \mathrm{d}S$$

$$\textit{energ}: \quad \bar{P}^{n+1} = \bar{P}^{n} = \bar{P}^{n+1,*} - \frac{\Delta t}{\Delta V} \int\limits_{\partial\Omega} (P\,\partial\tilde{\mathbf{v}}\cdot\mathbf{n})\, \mathrm{d}S$$

Finite Volume Projection Method

Zero Mach-number variable density equations – 2nd correction step

Post-correction of pressure term in momentum equation

$$(\rho\bar{\boldsymbol{v}})^{n+1} = (\rho\bar{\boldsymbol{v}})^{n+1,**} - \frac{\Delta t}{\Delta V}\int_{\partial\Omega} \boldsymbol{J}\partial p^{(2)} \cdot \boldsymbol{n}\,\mathrm{d}S$$

$$(\rho\boldsymbol{v})^{n+1} = (\rho\boldsymbol{v})^{n+1,**} - \Delta t\nabla\partial p^{(2)}$$

$$\boldsymbol{v}^{n+1} = \boldsymbol{v}^{n+1,**} - \frac{\Delta t}{\rho^{n+1}}\nabla\partial p^{(2)}$$

Finite Volume Projection Method

Zero Mach-number variable density equations – 2nd correction step

Post-correction of pressure term in momentum equation

$$(\bar{\rho \boldsymbol{v}})^{n+1} = (\bar{\rho \boldsymbol{v}})^{n+1,**} - \frac{\Delta t}{\Delta V} \int\limits_{\partial\Omega} \boldsymbol{J} \partial p^{(2)} \cdot \boldsymbol{n} \, \mathrm{d}S$$

$$(\rho \boldsymbol{v})^{n+1} = (\rho \boldsymbol{v})^{n+1,**} - \Delta t \nabla \partial p^{(2)}$$

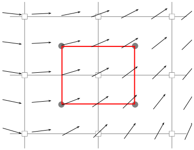
$$0 = \nabla \boldsymbol{v}^{n+1} = \nabla \boldsymbol{v}^{n+1,**} - \nabla \frac{\Delta t}{\rho^{n+1}} \nabla \partial p^{(2)}$$

$$\nabla \frac{\Delta t}{\rho^{n+1}} \nabla \partial p^{(2)} = \Delta t \nabla \boldsymbol{v}^{n+1,**} \qquad \textit{var. coeff. Poisson eq.}$$

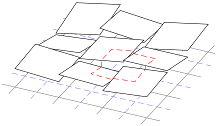
Finite Volume Projection Method

Inf-sup stable cell-centered exact projection

(Vater, Klein, Num. Math, 2009)

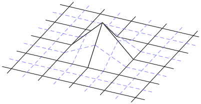


Exact control of divergence on dual cells



Piecewise linear, discontinuous ansatz functions for momentum on primary cells

Bi-/trilinear ansatz functions for the pressure



Finite Volume Projection Method

(Some) features:

- conservative
- variable density flows,
  ratio up to $\left(\rho_1(\boldsymbol{x}, t)/\rho_2(\boldsymbol{x}, t)\right) = \mathcal{O}(10^3)$
- monotonicity preserving 2nd order version
- interface representation via
  - levelsets
  - mass-preserving combined levelset-VOF approach

Finite Volume Projection Method

Next Steps

- optimize present code
- convergence study
  $\Rightarrow$ proof 2^{nd} order accuracy of implementation
- complete AMR capability of Poisson solvers
- include diffusive terms into flow solver
- couple levelset with flow solver $\Rightarrow$ interface
- cut-cell method $\Rightarrow$ sharp interface representation

- discretization of surface tension forces
- solution of the surface surfactant equation
- surfactant dependent variable surface tension

Level set method

Interface tracking not as natural Lagrangian problem but as an Eulerian problem

- two steps involved:
  - solving transport pde $\frac{\partial \phi}{\partial t} + \boldsymbol{u}_{levelset} \cdot \nabla \phi = 0$
  - reinitialization: reset the interface by forcing $|\nabla \phi| = 1$
- pde solution via high order ode solver and hyperbolic advection schemes (WENO)
- reinitialization with fixed ϕ_0
- signed distance function which allows easy distinction between Ω^+ and Ω^-

Level set method - level set transport

local discretization: third order upstream central convection scheme

$$\frac{1}{6\Delta x}\left(\pm\phi_{i\mp 2,j,k} \mp 6\phi_{i\mp 1,j,k} \pm 3\phi_{i,j,k} \pm 2\phi_{i\pm 1,j,k}\right)$$

temporal discretization: third order Runge Kutta scheme

$$\begin{aligned}
u^{(1)} &= u^n + \Delta t\, L(u^n) \\
u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t\, L(u^{(1)}) \\
u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t\, L(u^{(2)})
\end{aligned}$$

Level set method

Implementation of a constrained reinitialization routine by D. Hartmann

Base idea: dividing the narrow band into two sets

- points close to the zero level (Gamma field)
- points adjacent to the Gamma field (given by the width of the narrow band)

different reinitialization equations for Gamma field / narrow band

$$\frac{\partial \phi^\nu}{\partial \tau} + S(\tilde{\phi})\left(|\nabla \phi^\nu| - 1\right) = \beta F^\nu$$

$S(\tilde{\phi}) = \frac{\tilde{\phi}}{\sqrt{\tilde{\phi}^2 + \Delta x^2}}$ with $\tilde{\phi}$ level set before reinitialization

Level set method - constrained approach

- source term only active for Gamma field and ensures minimized zero level displacement

$$F^{\nu}_{i,j,k} = \frac{1}{\Delta x} \left(\tilde{r}^{i,j,k} \sum_{\alpha=1}^{M_{i,j,k}} \phi^{\nu}_{(i,j,k)_\alpha} - \phi^{\nu}_{i,j,k} \right)$$

$\tilde{r}^{i,j,k}$ is calculated once before the reinitialization through

$$\tilde{r}^{i,j,k} = \tilde{\phi}_{i,j,k} \left(\sum_{\alpha=1}^{M_{i,j,k}} \tilde{\phi}_{(i,j,k)_\alpha} \right)^{-1}$$

Level set example - moving circle

circle with 2 m diameter
iso-level for $\phi = 0$ shown with narrow band

Level set example - slotted disk

slotted disk with 2.3 m diameter
iso-level for $\phi = 0$ shown with narrow band

Work package 2:

Sharp Interface

Poisson solver for arbitrary ratio of coefficients

Variable density Poisson solver

Finite volume formulation

$$\int_{\partial\Omega} \beta \, \nabla u \cdot \boldsymbol{n} \, \mathrm{d}S = \int_{\partial\Omega} \nabla \cdot \boldsymbol{v} \, \mathrm{d}S$$

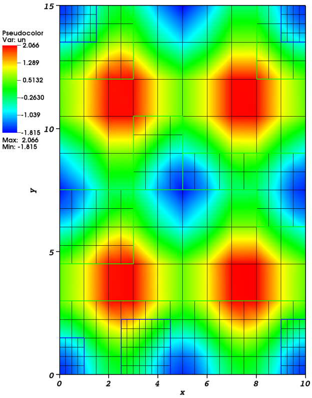
with

$$\nabla u \cdot \boldsymbol{n} = u_n \text{ on } \partial\Omega$$

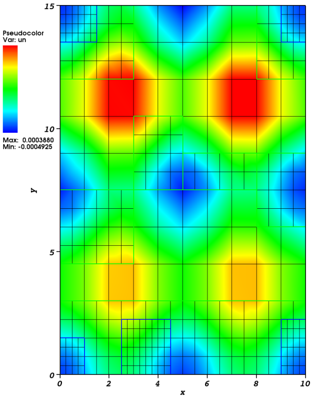
- cell-centered Poisson solver: standard 5-/7-point stencil (2D/3D)
- node-centered Poisson solver: 9-/27-point stencil (bi-/tri-linear ansatz functions on primary cells)
- BiCGSTAB + AMG preconditioner (hypre library, LLNL)

Variable density Poisson solver

2D - example node centered solver
$\boldsymbol{v} = \sin(4\pi \boldsymbol{x}/\boldsymbol{x}_{max}),\ \Delta x : \Delta y = 2 : 3$



$\beta = 1$

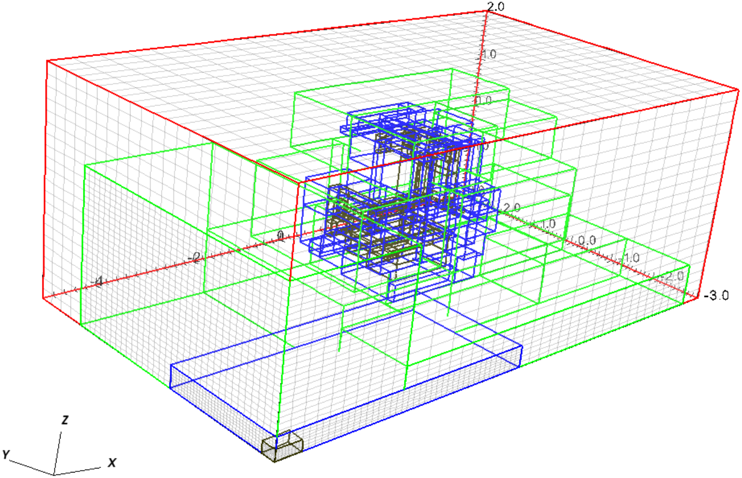


$\beta = 5e3 + 1e3 \sin(2\pi x/x_{max})$

Variable density Poisson solver

3D - example cell centered solver

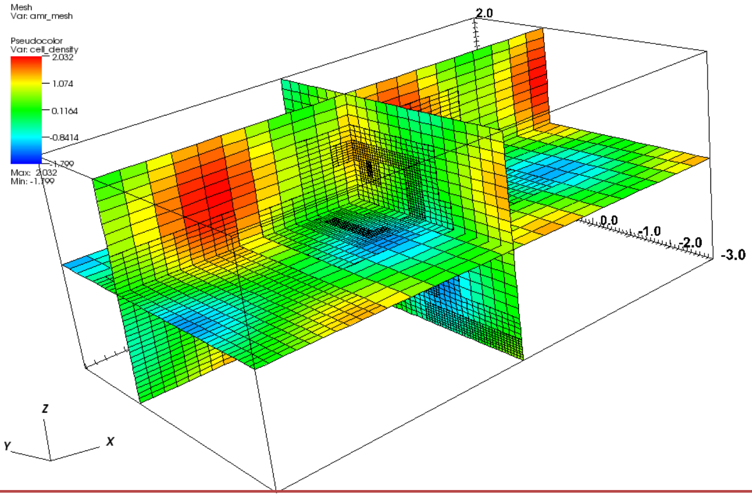
$\boldsymbol{v} = \cos(\boldsymbol{x}\,\pi/2)$, $\beta = 10 + x + y + z$, $\Delta x : \Delta y : \Delta z = 5 : 3 : 2$



Variable density Poisson solver

3D - example cell centered solver

$\boldsymbol{v} = \cos(\boldsymbol{x}\,\pi/2)$, $\beta = 10 + x + y + z$, $\Delta x : \Delta y : \Delta z = 5 : 3 : 2$



Poisson solver for arbitrary ratio of coefficients

Problem:

- large ratio of coefficients (e.g. ρ, μ, D)
- non-symmetric matrix

On each side of the interface we have

$$\nabla \cdot (\beta^+ \nabla u^+(\boldsymbol{x})) = f^+(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega^+$$
$$\nabla \cdot (\beta^- \nabla u^-(\boldsymbol{x})) = f^-(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega^-$$

with interface jump conditions

$$[\![u]\!]_\Gamma = g(\boldsymbol{x}_\Gamma)$$
$$[\![\beta u_n]\!]_\Gamma = h(\boldsymbol{x}_\Gamma)$$

Poisson solver for arbitrary ratio of coefficients

We are interested in small ratios

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

and write

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

Introducing the asymptotic expansion

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

Poisson solver for arbitrary ratio of coefficients

Solution strategie for the perturbation equations

1. Solve

$$\nabla \cdot \left(\beta^- \nabla u^{(0,-)}(\boldsymbol{x})\right) = f^-(\boldsymbol{x})$$

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

$$\begin{aligned} \nabla \cdot \left(\beta^- \nabla u^{(1,+)}(\boldsymbol{x})\right) &= f^+(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega^+ \\ \nabla \cdot \left(\beta^- \nabla u^{(1,-)}(\boldsymbol{x})\right) &= 0, \quad \boldsymbol{x} \in \Omega^- \end{aligned}$$

with

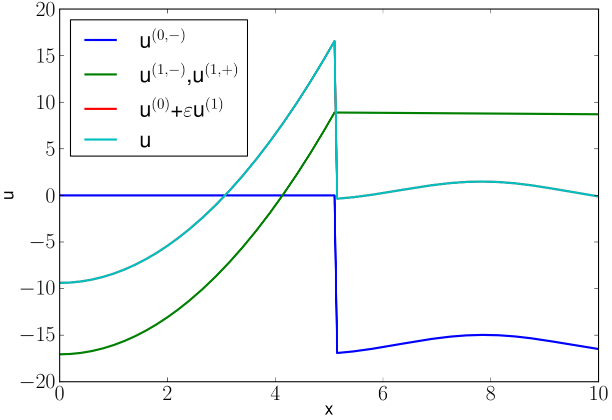
$[\![u^{(1)}]\!]_\Gamma = u^{(1,+)} - u^{(1,-)} = 0$,
$\beta^- u_n^{(1,+)} - \varepsilon \beta^- u_n^{(1,-)} = h + \beta^- u_n^{(0,-)}$ on Γ
$u_n^{(1,-)} = 0$, $u_n^{(1,+)} = \varepsilon^{-1} u_{n,w}^+$ on $\partial\Omega$.

Poisson solver for arbitrary ratio of coefficients

1D example:

$u^{+} = x^2, \; x \in (0, 5.14]$

$u^{-} = 10 + \sin(x), \; x \in [5.14, 10)$



Poisson solver for arbitrary ratio of coefficients

1D example:

	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

Poisson solver for arbitrary ratio of coefficients

Perturbation equations

$$
\begin{aligned}
\varepsilon^{-1} &: & \nabla \cdot (\beta^- \nabla u^{(0,+)}(\boldsymbol{x})) &= 0 \\
\varepsilon^{0} &: & \nabla \cdot (\beta^- \nabla u^{(1,+)}(\boldsymbol{x})) &= f^+(\boldsymbol{x}) \\
& & \nabla \cdot (\beta^- \nabla u^{(0,-)}(\boldsymbol{x})) &= f^-(\boldsymbol{x}) \\
\varepsilon^{n},\ n \geqslant 1 &: & \nabla \cdot (\beta^- \nabla u^{(n+1,+)}(\boldsymbol{x})) &= 0 \\
& & \nabla \cdot (\beta^- \nabla u^{(n,-)}(\boldsymbol{x})) &= 0
\end{aligned}
$$

Interface jump conditions

$$
\begin{aligned}
\varepsilon^{0} &: & [\![u]\!]_\Gamma^{(0)} &= u^{(0,+)} - u^{(0,-)} = g \\
\varepsilon^{n},\ n \geqslant 1 &: & [\![u]\!]_\Gamma^{(n)} &= u^{(n,+)} - u^{(n,-)} = 0
\end{aligned}
$$

$$
\begin{aligned}
\varepsilon^{-1} &: & [\![\beta u_n]\!]^{(0)} &= \beta^- u_n^{(0,+)} &= 0 \\
\varepsilon^{0} &: & [\![\beta u_n]\!]^{(1)} &= \beta^- u_n^{(1,+)} - \beta^- u_n^{(0,-)} &= h \\
\varepsilon^{1} &: & [\![\beta u_n]\!]_\Gamma^{(1)} &= -\beta^- u^{(1,-)} &= 0
\end{aligned}
$$