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

Stephan Gerber[1], Matthias Waidmann[2]
Warren O'Neill[2]

Dr. Michael Oevermann[1], Prof. Dr. Rupert Klein[2]

[1] Konrad-Zuse-Zentrum
für Informationstechnik Berlin

[2] Freie Universität Berlin
Institut für Mathematik
AG Geophysical Fluid Dynamics

SPP 1506 Transport Processes at Fluidic Interfaces

DFG Priority Programm SPP 1506

Team at FU Berlin

Stephan Gerber
(Berlin Institute of Technology)

- diploma in energy- and chemical engineering
- diploma in physical engineering science (thermodynamics, numerics, simulation)
- Ph.D. (almost done) in reactive multi-phase flows

Warren O'Neill

- B.Sc.: Mathematics
  (Trinity College Dublin, Ireland)
- M.Sc: Mathematical Modeling
  (University College London, England)
- Ph.D. (just started) in geophysical fluid dynamics

Matthias Waidmann

- diploma in aerospace engineering
  (University of Stuttgart / University of Colorado)
- Ph.D. (right in the middle) in cut-cell methods for hyperbolic flows

ZIB

Berlin Mathematical School

Freie Universität Berlin

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)

$\Rightarrow$

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

- sharp resolution of discontinuities
- variable, surfactant dependent surface tension
- conservative discretisation for the surface surfactant equation
- asymptotics based Poisson solver

Our project objective within the SPP

Work packages

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

plus

everything in an AMR framework

Adaptive Mesh Refinement framework

DNS: several million grid cells

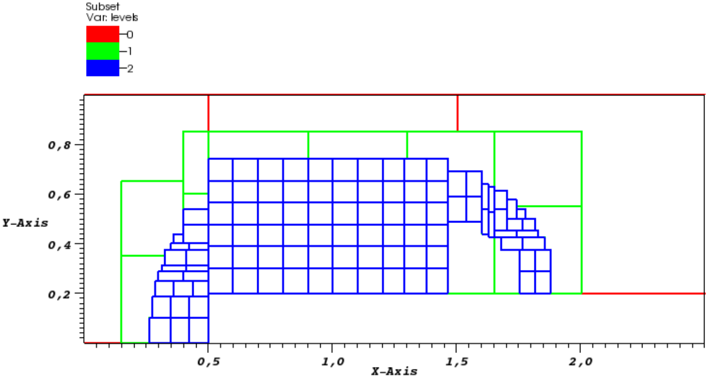
AMR framework to be used for

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

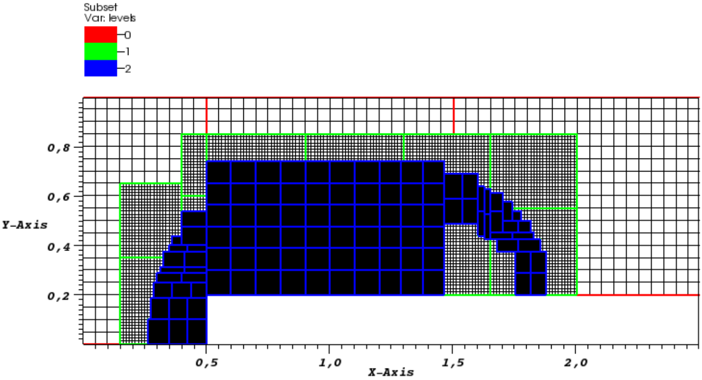
$\Rightarrow$ SAMRAI (Lawrence Livermore National Labs)

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

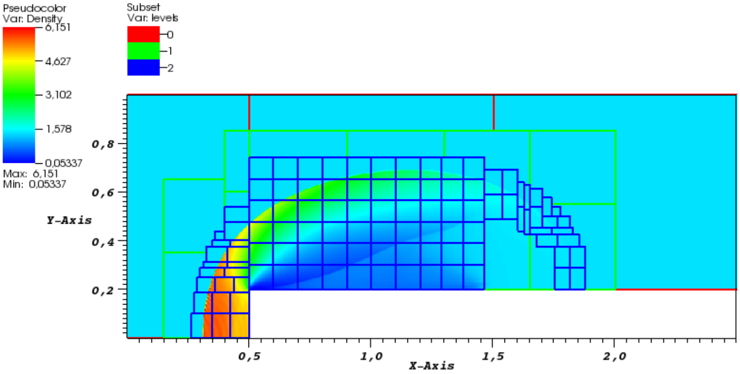
Adaptive Mesh Refinement framework



Adaptive Mesh Refinement framework



Adaptive Mesh Refinement framework



Expansions in Mach number

- introduction of expansion for p etc. (in Ma number): $p = p^{(0)} + Ma \cdot p^{(1)} + Ma^2 \cdot p^{(2)} + ...$
- reformulation of balance equations in dimensionless form
- $Re = \frac{\rho v_{ref} l_{ref}}{\mu}$ $\quad Sr = \frac{l_{ref}}{t_{ref} v_{ref}}$ etc. for Pe, Sc, Da
- equating the corresponding coefficients in Ma

Consequences of Mach number expansions

- $\nabla p^{(0)} = 0$ and $\nabla p^{(1)} = 0$
- no coupling via EOS with pressure term in NVS
- substitution of pressure state variable via EOS
- divergence constraint involves naturally terms like heat exchange, reaction influences etc.
- divergence constraint instead of energy balance
- explicit decoupling from acoustic phenomena

Governing equations

Zero Mach-number variable density equations

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

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

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

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

Governing equations

Isothermal zero Mach number two-phase flow

Interface conditions

$$\begin{aligned} [\![\boldsymbol{u}]\!] &= 0 \\ [\![p]\!] - \boldsymbol{n} \cdot [\![\mu \mathbf{D}]\!] \cdot \boldsymbol{n} &= \sigma \kappa \\ \boldsymbol{t} \cdot [\![\mu \mathbf{D}]\!] \cdot \boldsymbol{n} &= \nabla_{\Sigma} \sigma \end{aligned} \tag{1}$$

(1) + momentum equation

$$\left[\!\!\left[\frac{1}{\rho} \nabla p \cdot \boldsymbol{n} \right]\!\!\right] = [\![\nu \Delta \boldsymbol{u}]\!].$$

Problems involving interphase mass transfer, e.g.

$$[\![D_c \nabla Y \cdot \boldsymbol{n}]\!] = 0$$

$$Y_1 = H \, Y_2$$

Generating equations for phase coupling

Different paths to achieve phase coupling:

- physical reasons (e.g. no-slip)
- difference of two sets of phase equations for Ω^+ and Ω^-
- usage of integral balances which include the interface (with $dV \to 0$)

Work package 1:

Sharp interface FV projection method

FV Projection method

Predictor step

(2nd-ord.: Schneider et al., JCP '99)

Solve over Δt by second-order (upwind FV) scheme:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho \,\mathrm{d}V = \dots$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho Y_s \,\mathrm{d}V = \dots$$

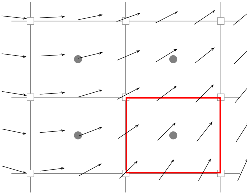
predicted values $\{\rho^*, (\rho \boldsymbol{v})^*, (\rho Y_s)^*\}$ no divergence imposed!

FV Projection method

Projection scheme – MAC-projection

Constraint

$$\nabla \cdot \boldsymbol{v}^{n+\frac{1}{2}} = D \quad \Rightarrow \quad \delta\pi = p^{(2),n+1} - p^{(2),n}$$



Advection velocity correction (at cell interfaces)

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

Divergence control

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

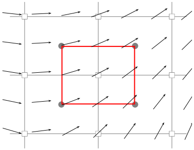
Post-correction of all advective flux contributions

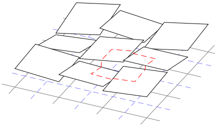
FV Projection method

Inf-sup stable cell-centered exact projection

(Vater, Klein, Num. Math, 2009)

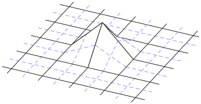
Exact control of divergence on dual cells





Piecewise linear, discontinuous ansatz functions for momentum on primary cells

Bi-/trilinear ansatz functions for the pressure



FV projection method

(Some) features:

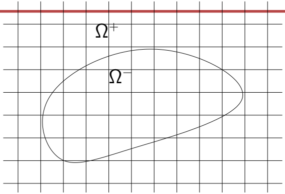
- conservative
- variable density flows; $(\rho_1/\rho_2) = \mathcal{O}(10^3)$
- monotonicity preserving 2nd order version
- interface representation via
  - levelsets
  - mass-preserving combined levelset-VOF approach

Level set method

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

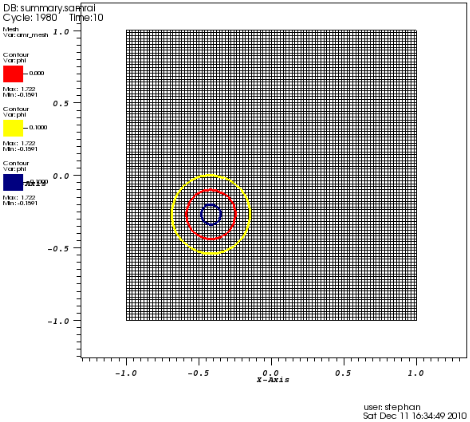
- two steps involved:
  - solving transport pde $\frac{\partial \phi}{\partial t} + \boldsymbol{u}_{levelset} \cdot \nabla \phi = 0$
  - reinitialization: reset the interface by forcing $|\nabla \phi| = 1$
- pde solution via high order ode solver and hyperbolic advection schemes (ENO/WENO/TVD etc.)
-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

Coupling of VOF and level set



- suppose constant density two-phase flow
- cell averaged quantities
- level set and VOF deliver two independent values for the phase fraction
- level set correction via VOF method
- variable density more intricated
- in-cell reconstruction via jump conditions (possibly modified)

Level set example - moving circle



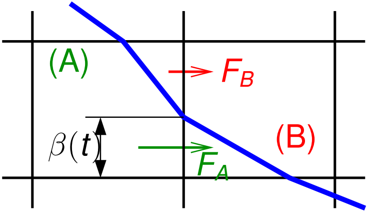
circle with 0.2 m diameter

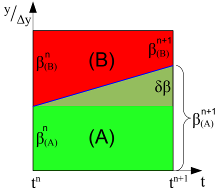
iso-levels for $\phi = \{-0.1, 0, 0.1\}$ shown

FV projection method

Planed extensions:

- sharp representation of all interface discontinuities via
  - (predictor) flux splitting
    two in-cell reconstructions of cell-averaged quantities





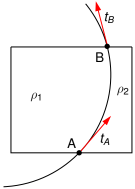
  - (corrector) locally second order elliptic solver
    ⇒ improve present Poisson solver
    ⇒ embed stand-alone Poisson solver into flow solver

FV projection method

Planed extensions:

- FV discr. of surface tension force localized on levelset
  ⇒ pressure jump results from force balance directly

  $$[\![p]\!] - \boldsymbol{n} \cdot [\![\mu \mathbf{D}]\!] \cdot \boldsymbol{n} = \sigma\kappa \qquad \boldsymbol{t} \cdot [\![\mu \mathbf{D}]\!] \cdot \boldsymbol{n} = \nabla_\Sigma \sigma$$

  ⇒ no curvature → no second derivative

  ⇒ no discretization of $\nabla_\Sigma \sigma$
- improve accuracy of viscous terms within the projection approach
- surfactant dependent variable surface tension

Work package 2:

Conservative discretisation of the surface surfactant equation

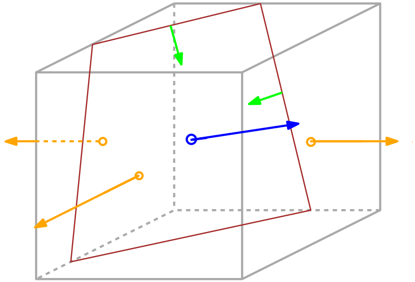
Surface surfactant transport equation

Integral balance for the total surface surfactant mass in a (fixed) computational cell Ω:

$$\frac{\mathrm{d}m_{\Gamma_\Omega}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Sigma_\Omega(t)} \Gamma \,\mathrm{d}S = \underbrace{-\int_{\partial\Omega\cap\Sigma(t)} \Gamma\,(\boldsymbol{u}\cdot\boldsymbol{n})\,\mathrm{d}l}_{\mathcal{L}_{conv}} + \underbrace{\int_{\partial\Omega\cap\Sigma(t)} D_\Gamma\,(\nabla_\Sigma\Gamma\cdot\boldsymbol{t})\,\mathrm{d}l}_{\mathcal{L}_{visc}} - \underbrace{\int_{\Omega\cap\Sigma(t)} (\boldsymbol{j}_\Gamma\cdot\boldsymbol{n}_\Sigma)\,\mathrm{d}S}_{\mathcal{L}_{source}}$$

n normal vector (control vol. surf.)
t tangential vector (interface)
$\mathbf{n}_\Sigma$ normal vector (interface)
Ω control volume
$\partial\Omega$ control volume boundary
Σ interface
Γ concentration
u velocity vector
j surfactant flow

No surface stretching term!



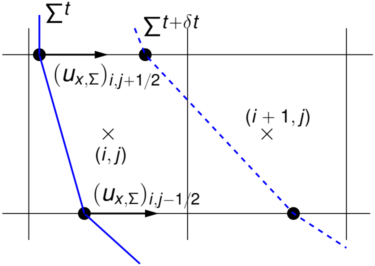
Surface surfactant equation

Solution strategy

- operator splitting for physical processes (convection, diffusion, source terms)

$$m_{\Gamma_\Omega}^{n+1} = \mathcal{L}_{conv}^{\Delta t}\mathcal{L}_{visc}^{\Delta t}\mathcal{L}_{source}^{\Delta t}\, m_{\Gamma_\Omega}^{n}$$

- operator splitting in space for convective transport
  $\Rightarrow$ sequential 1D convective flux calculations,

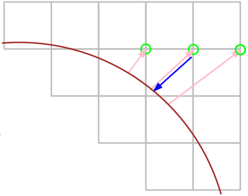


Surface surfactant equation

Solution strategy

- evaluation of surface gradients for diffusive flux calculation via an embedding method

$$\nabla_\Sigma C = \mathbf{P}(\nabla \tilde{C})$$



with the projection operator

$$\mathbf{P} = \mathbf{I} - \nabla\phi \otimes \nabla\phi$$

$\Rightarrow$ three steps involved

1. extrapolation of surface data onto the Cartesian grid ($C \to \tilde{C}$)
2. evaluation of gradients $\nabla \tilde{C}$ on the Cartesian grid
3. interpolation of $\nabla \tilde{C}$ onto the interface ($\nabla \tilde{C} \to \nabla_\Sigma C$)

$\Rightarrow$ no explicit interface reconstruction

(only intersection {interface – cell-boundary})

$\Rightarrow$ conservative with respect to the total surfactant mass

Work package 3:

Sharp interface Poisson solver for arbitrary ratio of coefficients

Poisson Solver – Preliminary work

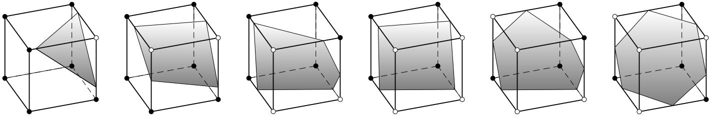
embedded boundary problem

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 for

$$[\![u]\!]_\Gamma = g(\boldsymbol{x}_\Gamma) \quad (\textit{solution values})$$
$$[\![\beta u_n]\!]_\Gamma = h(\boldsymbol{x}_\Gamma) \quad (\textit{normal gradients})$$



Oevermann, Scharfenberg, Klein, JCP Vol. 228 (14), 2009

Poisson Solver – Preliminary work

embedded boundary problem

- double bi-linear (2d) or tri-linear (3d) solution ansatz on cut-boxes (similar to finite elements)
  example bi-linear (2d): $u^- = c_1 + c_2 x + c_3 y + c_4 xy$
  $u^+ = c_5 + c_6 x + c_7 y + c_8 xy$
  $\Rightarrow$ 8 (2d) / 16 (3d) coefficients

- coefficients determined by
  - box corner values $\equiv$ solution values (4 / 8 values)
  - interface jump conditions (4 / 8 conditions necessary)

- singularities from vanishing partial volumes removed by two-step asymptotic approach

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

Oevermann, Scharfenberg, Klein, JCP Vol. 228 (14), 2009

Poisson Solver – Preliminary work

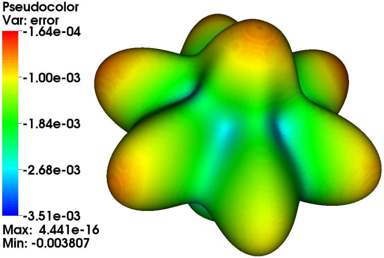
Embedded boundary problem – Example

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

Interface position:

$$r(\phi, \theta) = R + \Delta R_{\phi} \cos^{3}(\theta) \cos(\omega_{\phi} \phi) + \Delta R_{\theta} \cos(\omega_{\theta} \theta),$$

$0 \leqslant \phi \leqslant 2\pi$
$0 \leqslant \theta \leqslant \pi$
$R = 0.65$
$\Delta R_{\phi} = \Delta R_{\theta} = 0.15$
$\omega_{\phi} = 6$
$\omega_{\theta} = 4$

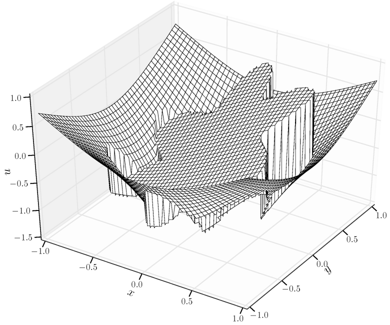


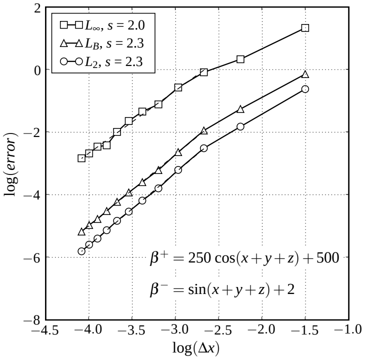
Exact Solution:

$$u^{+} = \ln(x^2 + y^2 + z^2)$$
$$u^{-} = \sin(x + y + z)$$

Poisson Solver – Preliminary work

Embedded boundary problem – Example





Poisson solver for arbitrary ratio of coefficients

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

Limitations up to now:

- no AMR capability
- parallel solving possible, but no parallel matrix assembly (assembly : solving $\approx$ 1 : 1)

\+
Problem:

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

Solution strategy:

- asymptotic approach also for the coefficients