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

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Outline

- Governing Equations & Numerical Method
- Current State of Work
- Cut-Cell Details
- Levelset
- Pressure Boundary Condition
- Surface PDE (preliminary work regarding 2nd phase)
- Outlook
  - Rest of 1st Phase
  - 2nd Phase (Rupert Klein)
  - 2nd Phase (Michael Oevermann)
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 \( \lim_{Ma \to 0} \)

\[ \nabla p^{(0)} = 0 \quad \Rightarrow \quad p^{(0)} = p^{(0)}(t) \]

\[ \nabla p^{(1)} = 0 \quad \Rightarrow \quad p^{(1)} = p^{(1)}(t) \]

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: \[
\frac{d}{dt} \int_{\Omega} \rho \, dV = - \int_{\partial\Omega} \rho \, \mathbf{v} \cdot \mathbf{n} \, dS
\]

spec: \[
\frac{d}{dt} \int_{\Omega} \rho Y_s \, dV = - \int_{\partial\Omega} \rho Y_s \, \mathbf{v} \cdot \mathbf{n} \, dS - \int_{\partial\Omega} \mathbf{j}_s \cdot \mathbf{n} \, dS + \int_{\Omega} \dot{\sigma}_s \, dV
\]

mom: \[
\frac{d}{dt} \int_{\Omega} \rho \, \mathbf{v} \, dV = - \int_{\partial\Omega} \rho \, \mathbf{v} \, (\mathbf{v} \cdot \mathbf{n}) \, dS - \int_{\partial\Omega} \rho^{(2)} \, n \, dS + \int_{\Omega} \rho \, g \, dV
\]
\[
+ \int_{\partial\Omega} \mathbf{T} \cdot \mathbf{n} \, dS + \int_{\partial\Omega \cap \partial\Sigma} \sigma t \, d\Gamma
\]

energy (to be integrated):

\[
(\nabla \cdot \mathbf{v}) = -\frac{1}{\rho c^2} \frac{d \rho^{(0)}}{dt} + \frac{1}{\rho c^2} \equiv \left[ \nabla \cdot \mathbf{q} + \sum_s \mathbf{j}_s \cdot \nabla h_s + \sum_s \Delta h_s \dot{\sigma}_s \right]
\]

\[\text{SPP 1506 Page 4}\]
Finite Volume Projection Method

Overview

- **Predictor** (2-stage Strong Stability Preserving Runge-Kutta scheme; Gottlieb et al. 2001)
  - scalars $2^{nd}$ order accurate (density, species ...)
  - old time level pressure in momentum equation
  - momentum $1^{st}$ order accurate
  - no divergence constraint imposed
  - tracking of divergence error using one more transport equation

- **Corrector**
  - $1^{st}$ projection (cell centered Poisson problem)
    - correction of advective fluxes using tracked divergence error
      → scalars done after this step
  - $2^{nd}$ projection (nodal Poisson problem)
    - correction of pressure term in momentum equation
      → momentum $2^{nd}$ order accurate
      → divergence constraint satisfied
**Finite Volume Projection Method**

**Divergence Control**

\[
\nabla \cdot (\rho \theta \mathbf{u}) = D \quad \rho \theta = \text{const.} \quad \rightarrow \quad \nabla \cdot \mathbf{u} = \frac{D}{\rho \theta} \quad \rightarrow \quad \nabla \cdot \mathbf{u} = 0
\]

\[
(\rho \theta)_t + \nabla \cdot (\rho \theta \mathbf{u}) = D
\]

\[
(\rho \theta)_t = D - \nabla \cdot (\rho \theta \mathbf{u})
\]

\[
(\rho \theta)_t^{\text{ex.}} + (\rho \theta)_t^{\text{err.}} = D - \nabla \cdot (\rho \theta \mathbf{u})^{\text{ex.}} - \nabla \cdot (\rho \theta \mathbf{u})^{\text{err.}} = 0
\]

\[
- \int_{\partial \Omega} (\rho \theta \mathbf{u})^{\text{err.}} \cdot \mathbf{n} \, dS = \int_{\Omega} (\rho \theta)^{\text{err.}} \, dV = \int_{\Omega} (\rho \theta)_t \, dV
\]

\[
- \left( \int_{\partial \Omega} (\rho \theta \mathbf{u})^{\text{err.}} \cdot \mathbf{n} \, dS \right)^{(n+\frac{1}{2})} = \frac{\Delta V}{\Delta t} \left( \frac{\rho \theta^{(n+1,*)}}{n} - \frac{\rho \theta^{(n)}}{n} \right)
\]
\[
\int_{\partial \Omega} \theta \nabla \partial p^{(2)} \cdot \mathbf{n} \, dS = \left( \int_{\partial \Omega} (\rho \theta \mathbf{u})^{\text{err.}} \cdot \mathbf{n} \, dS \right)^{(n + \frac{1}{2})}
\]
\[
= -\frac{\Delta V}{\Delta t} \left( \bar{\rho} \theta^{(n+1,*)} - \bar{\rho} \theta^{(n)} \right)
\]
\[
\int_{\partial \Omega} F_{\rho \theta}^{\text{corr.}} \cdot \mathbf{n} \, dS = \int_{\partial \Omega} \theta \nabla \partial p^{(2)} \cdot \mathbf{n} \, dS
\]

\[
F_{\rho \theta}^{\text{corr.}} = \theta \nabla \partial p^{(2)} = (\rho \theta \mathbf{u})^{\text{err.}}
\]
\[
F_{\rho \phi}^{\text{corr.}} = \left( \frac{\rho \phi}{\rho \theta} \right)_{\text{upwind}} F_{\rho \theta}^{\text{corr.}}
\]
Current State of Work

- combined level set with single phase flow solver
- extended periodic boundary conditions
- implemented cut-cell features (2d, all code segments)
- currently debugging & extension to 3d
Cut Cell Details
Predictor - Advection - Stencil Selection
Cut Cell Details

Predictor - Advection - Stencil Selection

[Diagram of a grid with a red 'x' indicating a cut cell]
Cut Cell Details

Predictor - Advection - Stencil Selection

- Diagram showing different configurations of cut cells with 'o' and 'x' markers.
- Each diagram represents a different stencil selection for different predictor methods.
Cut Cell Details

Predictor - Advection - Stencil Selection
Cut Cell Details

Predictor - Advection - Interface Movement

```
0 0 0 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0
```

```
0 0 0 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0
```

```
0 0 0 0 0 0
0 0 0 0 0 0
0 0 0 0 0 0
```
Cut Cell Details
Predictor - Advection - Interface Movement

Interface **moves** on cell face during time step

Interface **leaves** cell face during time step

Interface **enters** cell face during time step
Zeppelin: pseudo-incompressible Euler
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Jump conditions

\[
[u] = 0
\]

\[
[p] - n \cdot [\mu D] \cdot n = \sigma_k
\]

\[
\frac{1}{\rho} \nabla \rho \cdot n = [\nu \Delta u]
\]

\[
t \cdot [\mu D] \cdot n = \nabla \Sigma \sigma
\]

Problems involving interphase mass transfer, e.g.

\[
[D_c \nabla Y \cdot n] = 0
\]

\[
H Y_2 = Y_1
\]
Evaluation of jump conditions I

- first order derivatives:

\[
\frac{\partial \phi}{\partial x} = \frac{\phi_{x+dx} - \phi_{x-dx}}{2 \, dx} + \mathcal{O}(dx^2)
\]

- second order derivatives:

\[
\frac{\partial^2 \phi}{\partial x^2} = \frac{\phi_{x+dx} - 2 \phi_x + \phi_{x-dx}}{dx^2} + \mathcal{O}(dx^2)
\]

- first approximation:

\[
[\nu \Delta u] \approx [\nu] \Delta u
\]

- final approximation: second order approximation via one sided stencil or cell value reconstruction
Evaluation of jump conditions I

- evaluation of jump conditions on corners of control volume
- second order interpolation to interface
- done for jump conditions (stress tensor, laplacian) and tangential force (momentum balance)
First / Second Projection correction

▶ evaluation of integrals for bilinear ansatz functions (Oevermann, Klein, JCP Vol. 219 (2), 2006)

▶ first projection: correction flux from addition of two inner integrals

▶ second projection: correction flux from averaged outer integrals

▶ currently no flux splitting for correction flux
Levelset approaches available

- HCR2 method D. Hartmann (2010, Diss. RWTH Aachen) WENO–3/Upstream-Central–3 in space and SPP RK-2
- bi/tri-cubic interpolation from Chopp, D.L.
- combined levelset advection and reinitialisation Klein,R.
Levelset method currently in application

\[ \frac{\partial \phi}{\partial t} + f_n |\nabla \phi| + \phi^m(|\nabla \phi| - 1)^n = 0 \]

- with odd m,n and \( f_n = -u_{\text{levelset}} \cdot n \)
- Combination of advection, conservation of signed distance property and minimized zero level displacement
- new narrow band cells by first order fast marching method
Chopp’s reinitialization method

\[ p(x, y) = \sum_{m=0}^{3} \sum_{n=0}^{3} a_{m,n} x^m y^n \]

\( a_{m,n} \) by four corner values of \( \phi(x, y) \), \( \frac{\partial \phi}{\partial x} \), \( \frac{\partial \phi}{\partial y} \), \( \frac{\partial^2 \phi}{\partial x \partial y} \)

explicit reconstruction of corner values by modified Newton Iteration:

\[ p(y) = 0 \]
\[ \nabla p(y) \cdot (x_0 - y_0) = 0 \]
Pressure Boundary Condition

Incompressible Momentum Equation

\[ u_t + u \cdot \nabla u - \nu \nabla \cdot \nabla u + \frac{1}{\rho} \nabla p^{(2)} = g \]

Divergence (considering \( \nabla \cdot u = 0 \)):

\[ \nabla \cdot \frac{1}{\rho} \nabla p^{(2)} = -\nabla \cdot (u \cdot \nabla u) \]

Boundary normal component at the no-slip boundary (\( u = 0 \)):

\[ \frac{1}{\rho} \nabla p^{(2)} \cdot n = g \cdot n - (\nu \nabla \cdot \nabla u) \cdot n \]

Boundary tangential component:

\[ \frac{1}{\rho} \nabla p^{(2)} \cdot t = g \cdot t - (\nu \nabla \cdot \nabla u) \cdot t \]
Pressure Boundary Condition

1st Issue

\[ u_t + u \cdot \nabla u - \nu \nabla \cdot \nabla u + \frac{1}{\rho} \nabla p^{(2)} = g \]

Divergence (considering \( \nabla \cdot u = 0 \)):

\[ \nabla \cdot \frac{1}{\rho} \nabla p^{(2)} = -\nabla \cdot (u \cdot \nabla u) \]

Boundary normal component at the no-slip boundary (\( u=0 \)) with piecewise constant normal vector:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial N} = g \cdot n - \nu \frac{\partial}{\partial N} \frac{\partial}{\partial N} (u \cdot n) - \nu \frac{\partial}{\partial T} \frac{\partial}{\partial T} (u \cdot n) \]

Boundary tangential component:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial T} = g \cdot t - \nu \frac{\partial}{\partial N} \frac{\partial}{\partial N} (u \cdot t) - \nu \frac{\partial}{\partial T} \frac{\partial}{\partial T} (u \cdot t) \]
Pressure Boundary Condition

1st Issue

\[ \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p^{(2)} = \mathbf{g} \]

Divergence (considering \( \nabla \cdot \mathbf{u} = 0 \)):

\[ \nabla \cdot \frac{1}{\rho} \nabla p^{(2)} = -\nabla \cdot (\mathbf{u} \cdot \nabla \mathbf{u}) \]

Boundary normal component at the no-slip boundary \( \mathbf{u}=0 \) with piecewise constant normal vector:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial N} = \mathbf{g} \cdot \mathbf{n} - \nu \frac{\partial}{\partial N} \frac{\partial}{\partial N} (\mathbf{u} \cdot \mathbf{n}) \]

Boundary tangential component:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial T} = \mathbf{g} \cdot \mathbf{t} - \nu \frac{\partial}{\partial N} \frac{\partial}{\partial N} (\mathbf{u} \cdot \mathbf{t}) \]
Pressure Boundary Condition

1st Issue

\[ u_t + u \cdot \nabla u - \nu \nabla \cdot \nabla u + \frac{1}{\rho} \nabla p^{(2)} = g \]

Divergence (considering \( \nabla \cdot u = 0 \)):

\[ \nabla \cdot \frac{1}{\rho} \nabla p^{(2)} = -\nabla \cdot (u \cdot \nabla u) \]

Boundary normal component at the no-slip boundary (\( u=0 \)) with piecewise constant normal vector:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial N} = g \cdot n + \nu \frac{\partial}{\partial N} \frac{\partial}{\partial T} (u \cdot t) \]

Boundary tangential component:

\[ \frac{1}{\rho} \frac{\partial p^{(2)}}{\partial T} = g \cdot t - \nu \frac{\partial}{\partial N} \frac{\partial}{\partial N} (u \cdot t) \]
Pressure Boundary Condition

1st Issue

Predictor-Corrector-Numerics:

\[ u = u^* - \frac{\Delta t}{\rho} \nabla p^{(2)} \]

Boundary normal component at the no-slip boundary \((u=0)\) with piecewise constant normal vector:

\[
\frac{1}{\rho} \frac{\partial p^{(2)}}{\partial N} = g \cdot n + \nu \frac{\partial}{\partial N} \frac{\partial}{\partial T} (u \cdot t)
\]

\[
\frac{1}{\rho} \frac{\partial p^{(2)}}{\partial N} = g \cdot n + \nu \frac{\partial}{\partial T} \frac{\partial}{\partial N} (u^* \cdot t) - \Delta t \nu \frac{\partial}{\rho \partial T} \frac{\partial}{\partial T} \left( \frac{\partial p^{(2)}}{\partial N} \right)
\]
Helmholtz-type equation on the outer boundary:

\[
(\Delta t\nu) \frac{\partial}{\partial T} \frac{\partial}{\partial T} \left( \frac{\partial p^{(2)}}{\partial N} \right) - \frac{\partial p^{(2)}}{\partial N} = \rho g \cdot n + \rho \nu \frac{\partial}{\partial T} \frac{\partial}{\partial N} (u^* \cdot t) \neq 0
\]

Assumptions:

- \( \nu = \text{const.} \)
- \( \rho = \text{const.} \)
- \( \nabla \cdot \mathbf{u} = 0 \)
- 2 space dimensions
- no-slip boundaries
- piecewise constant normal/tangential vector
Pressure Boundary Condition

\[ u_t + u \cdot \nabla u - \nu \nabla \cdot \nabla u + \frac{1}{\rho} \nabla p^{(2)} = g \]

Divergence (considering \( \nabla \cdot u = 0 \)):

\[ \nabla \cdot \frac{1}{\rho} \nabla p^{(2)} = -\nabla \cdot (u \cdot \nabla u) \]

Boundary normal component at the no-slip boundary \((u=0)\) with piecewise constant normal vector:

\[ \frac{1}{\rho} \nabla p^{(2)} \cdot n = g \cdot n - \nu \nabla \cdot \nabla (u \cdot n) \]

Boundary tangential component:

\[ \frac{1}{\rho} \nabla p^{(2)} \cdot t = g \cdot t - \nu \nabla \cdot \nabla (u \cdot t) \]
divergence-free velocity field

\[ u(x, y) = \frac{1}{2} \left( -\sin^2(2\pi x) \sin(4\pi y) \right) \left( \frac{\sin(4\pi x) \sin^2(2\pi y)}{\sin(4\pi y)} \right) \]

error of wall-tangential component of pressure gradient

\[ \frac{1}{\rho} \left( \nabla p^{(2)} \cdot t \right) - \left[ \mathbf{g} \cdot t - \nu \nabla \cdot \nabla (u \cdot t) \right] \]
Advection-diffusion problem on an interface $\Gamma \subset \mathbb{R}^n$:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0 \\
\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (\rho u \phi) &= \nabla \cdot (\rho D \nabla \phi)
\end{align*}
\]

Instead of solving (1) on $\Gamma$ we solve for $\rho, \phi \in \mathbb{R}^n$:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0 \\
\frac{\partial \rho \phi}{\partial t} + \nabla (\rho u \phi) &= \nabla \cdot (\rho D \nabla \phi)
\end{align*}
\]

in the embedding Euclidian space. where
$\nabla \Gamma$, $\Delta \phi \Gamma$ in (1) have been replaced in (2) by standard Cartesian operators.
Surface surfactant equation

Embedding method

Solution procedure:

1. Extend solution from surface \( \Gamma \) into the embedding space under the constraints \( \nabla \phi \cdot n = 0, \phi(x) = \phi_\Gamma(x_\Gamma) \) via closest point method (Ruuth, Merriman, JCP 227, 2008)

2. Solve (2) in \( \Omega_\Gamma \) for timestep \( \Delta t \)

3. Interpolate solution \( u(x) \) back onto the closest points (CP) on the surface

4. Repeat 1.-3. until end of simulation time
**Example:** Scalar advection on an ellipse ($\rho_\Gamma = 1$):

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

Initial condition: $\phi(s, 0) = \cos^2(2\pi s/L)$

Embedding PDE:

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = 0
\]

where $\phi$ and $\mathbf{u}$ are closest point representations of $\phi_\Gamma$ and $u_\Gamma$.
Surface surfactant equation
Embedding method

**Example:** Scalar advection on an ellipse:

\[
\frac{\partial \phi}{\partial t} + \frac{\partial (\phi u)}{\partial s} = 0
\]

Error in the \(L_\infty\)-norm using three-step Runge-Kutta time integration and a 2nd order finite volume discretisation in space

<table>
<thead>
<tr>
<th>(\Delta x)</th>
<th>Error</th>
<th>Conv. rate</th>
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<td>1.11e-03</td>
<td>–</td>
</tr>
<tr>
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</tr>
<tr>
<td>0.003125</td>
<td>4.29e-06</td>
<td>2.07</td>
</tr>
</tbody>
</table>
Surface Advection by Divergent Velocity

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_{\Gamma}}{\partial s_{\Gamma}} = 0 \]

\[ \frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho \phi u_{\Gamma}}{\partial s_{\Gamma}} = 0 \]
Outlook - Rest of 1st Phase

- debugging cut-cell 2d → Taylor flow 2d (scenario 1)
- extension cut-cell 3d → TBSC, TFSC
- improve code efficiency and speed
- finalize AMR capability
- full 2nd order
Outlook second phase
Rupert Klein & Ralf Kornhuber + Michael Oevermann (external)

- Continuation of first phase developments
  - asymptotic preconditioner for $\rho_1 / \rho_2 \to \infty$
  - variable density flow
  - full-space conservative solver for surface transport
  - mass transfer problems

- Open challenges for second phase
  - nonlocal Navier-Stokes pressure/projection B.C.s
  - in-surface conservative solver for surface transport
Outlook - 2nd Phase
Michael Oevermann

- Application for an external project funded by the Swedish Science Foundation attached to the SPP (application deadline: March/April 2013)
- Continuation of first phase developments towards
  - mass transfer problems
  - variable density flow
  - cavitation problems
- Application interests
  - evaporating fuel sprays
  - primary jet break-up
  - cavitation induced jet break-up