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

\[
\begin{align*}
\text{mass: } & \quad \frac{d}{dt} \rho \theta = \int \left( \rho \mathbf{u} \cdot \mathbf{n} \right) dS \\
\text{spec: } & \quad \frac{d}{dt} \rho \nabla \cdot \mathbf{u} = \int \left( \rho (\mathbf{u} \cdot \mathbf{n}) - \mathbf{u} \cdot \mathbf{n} \right) dS - \int \left( \frac{\partial}{\partial n} \rho \mathbf{u} \cdot \mathbf{n} + \frac{\partial}{\partial t} \rho \mathbf{u} \cdot \mathbf{n} + \mathbf{j}_m \cdot \mathbf{n} \right) dS \\
\text{mom: } & \quad \frac{d}{dt} \rho \mathbf{u} = \int \left( \rho (\mathbf{u} \cdot \mathbf{n}) \mathbf{n} - \mathbf{u} \cdot \mathbf{n} \mathbf{n} \right) dS - \int \left( \frac{\partial}{\partial t} \rho \mathbf{u} + \mathbf{j}_m \cdot \mathbf{n} - \mathbf{j}_m \mathbf{n} \right) dS + \int \mathbf{T} \cdot \mathbf{n} dS \\
\text{en: } & \quad \frac{d}{dt} \rho \theta = \int \left( \rho (\mathbf{u} \cdot \mathbf{n}) \theta - \mathbf{u} \cdot \mathbf{n} \theta \right) dS - \int \left( \frac{\partial}{\partial t} \rho \theta + \mathbf{j}_m \cdot \theta \mathbf{n} - \mathbf{j}_m \theta \mathbf{n} \right) dS + \int \mathbf{T} \cdot \theta dS.
\end{align*}
\]

Discretisation of a surface surfactant equation with an embedding method

Prototype of an advection-diffusion equation on an interface

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = - \nabla \cdot \mathbf{j}_m - \nabla \cdot \mathbf{D} \nabla \phi,
\]

with solution \( \phi \in \mathbb{R} \) and surface gradient \( \nabla \phi \). Instead of solving (1) on the surface \( \Gamma \) we solve a PDE for \( \phi \in \mathbb{R} \) in the surface embedding domain \( \Omega \subset \mathbb{R}^2 \).

Solution procedure:

1. Extend solution from surface \( \Gamma \) into the embedding space under the constraints \( \nabla \cdot \mathbf{v} \mathbf{n} = 0 \) via a closest point method (Rushton, Memering, JCP 227, 2008). Fig. 3

2. Solve (2) in \( \Omega \) for timestep \( \Delta t \).

3. Interpolate solution \( \phi(x) \) back onto the closest points \( \{ \mathbf{C} \} \) on the surface.

4. Repeat 1–3 until end of simulation time.

Example: Scalar advection on an ellipse:

\[
\begin{align*}
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi &= 0 \\
\mathbf{v} &= \mathbf{v}(x),
\end{align*}
\]

where \( \phi \) and \( \mathbf{v} \) are closest point representations of \( \phi \) and \( \mathbf{v} \).

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

Introducing the asymptotic expansion

\[
\begin{align*}
u^+ &\sim u^+ + \epsilon u^+ \frac{1}{1 + \epsilon^2} \\
u^- &\sim u^- + \epsilon u^- \frac{1}{1 + \epsilon^2}
\end{align*}
\]

into (3) leads to the following

Solution strategy for the perturbation equations:

1. Solve

\[
\nabla \cdot \left( \frac{\partial}{\partial x^i} \mathbf{v} \right) = \frac{\partial^2}{\partial x^i \partial x^j} \phi(x), \quad x \in \Omega^+
\]

in \( \Omega^+ \) with boundary condition \( u^+ = 0 \) on \( \Gamma \cap \Omega \) and interface condition \( u^+ = u^- \) on \( \Gamma \).

2. Solve the coupled problem

\[
\nabla \cdot \left( \frac{\partial}{\partial x^i} \mathbf{v} \right) = 0, \quad x \in \Omega^+
\]

with

\[
\begin{align*}
u^+ &= u^- = 0 \\
\mathbf{j}_m &= \frac{\partial}{\partial n} \mathbf{u} \cdot \mathbf{n} \mathbf{n} \nabla \phi
\end{align*}
\]

1D example:

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

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 discretisation
- single piecewise be-2D (or) tri-linear (3D) ansatz functions on normal cells,
- dual piecewise be-2D (or) tri-linear (3D) ansatz functions on cut-cells with explicit incorporation of the known interface jump conditions \( [u] \) and \( [\mathbf{j}_m] \).
- locally second order accurate,
- interface representation using standard 2nd order levels.

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

The accurate and efficient solution of elliptic equations

\[
\begin{align*}
\nabla \cdot \left( \left( \mathbf{A} \right) \nabla \phi \right) &= f(x), \quad x \in \Omega
\end{align*}
\]

with variable coefficients and prescribed interface jump conditions

\[
\begin{align*}
\left[ \phi \right] &= \phi^+ - \phi^- \\
\left[ \left( \frac{\partial}{\partial n} \mathbf{A} \mathbf{n} \right) \phi \right] &= \left( \mathbf{A} \right) \mathbf{n} \cdot \mathbf{n} \nabla \phi
\end{align*}
\]

across an interface \( \Gamma \) 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. \( \lambda = \rho_2 / \rho_1 \)).

Asymptotic solution approach

On each side of the interface we have

\[
\nabla \cdot \left( \left( \mathbf{A} \right) \nabla \phi^+ \right) = f^+(x), \quad x \in \Omega^+
\]

\[
\nabla \cdot \left( \left( \mathbf{A} \right) \nabla \phi^- \right) = f^-(x), \quad x \in \Omega^-
\]

with interface jump conditions

\[
\begin{align*}
\left[ \phi \right] &= \phi^+ - \phi^- \quad \text{and} \quad 
\left[ \left( \frac{\partial}{\partial n} \mathbf{A} \mathbf{n} \right) \phi \right] &= \mathbf{A} \mathbf{n} \cdot \mathbf{n} \nabla \phi
\end{align*}
\]

We are interested in small ratios

\[
\frac{\lambda}{\lambda^3} = \epsilon \ll 1
\]

and write

\[
\nabla \cdot \left( \mathbf{A}^\epsilon \nabla \phi^\epsilon \right) = f^\epsilon, \quad x \in \Omega^+ \\
\nabla \cdot \left( \mathbf{A}^\epsilon \nabla \phi^\epsilon \right) = f^\epsilon, \quad x \in \Omega^-
\]

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

Fig. 2: bubbles (density) in horizontal channel at zero gravity

(* not implemented yet *)