FEM-Level Set Techniques for Multiphase Flow

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Some recent results

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Motivation

• **Accurate, robust, flexible and efficient simulation of multiphase problems, particularly in 3D, is still a challenge**

• **Specific Application:** Monodisperse laminar droplets

  **Problem:** Results are due to many parameters, i.e., density (ratio), viscosity (ratio), rheological behaviour, surface tension, flow conditions,…

→ Efficient CFD techniques (**implicit FEM-Multigrid-Level Set** solver in FEATFLOW, dynamically adapted meshes, parallel/HPC techniques)

→ Benchmarking/Validation via experiments
Governing Equations

The incompressible Navier Stokes equation

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) - \nabla \cdot \left( \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) \right) + \nabla p = \mathbf{f}_{\text{st}} + \rho \mathbf{g}
\]

\[ \nabla \cdot \mathbf{v} = 0 \]

Interphase tension force

\[ \mu = \mu(D(\mathbf{v}), \Gamma), \quad \rho = \rho(\Gamma) \cdot \nabla \cdot \mathbf{n} \quad \text{on} \quad \Gamma \]

Dependency of physical quantities

\[ \mu = \mu(D(\mathbf{v})) \]
Discretization:
- a) Navier-Stokes: FEM $Q_2/P_1$
- b) Levelset: DG-FEM $P_1$
- Crank-Nicholson scheme in time

+ stabilization (TVD, EO-FEM)
no stabilization!

Main features of the FeatFlow approach:
- Parallelization based on domain decomposition
- High order discretization schemes
- Use of unstructured meshes
- Multigrid linear solver
- FCT & EO stabilization techniques
- Adaptive grid deformation
- UCHPC
Required: Efficient Interphase Tracking

Levelset method (\(\rightarrow\)“smooth” distance function)

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0
\]

Benefits:
- Provides an accurate representation of the interphase
- Provides other auxiliary quantities (normal, curvature)
- Allows topology changes
- Treatment of viscosity, density and surface tension without explicit representation of the interphase
- Adaptive grid advantageous, but not necessary

Problems:
- It is not conservative \(\rightarrow\) mass loss
- Needs to be reinitialized to maintain its distance property
- Higher order discretization?
Problems and Challenges

• Steep gradients of the velocity field and of physical properties near the interphase (oscillations!)

• Reinitialization (smoothed sign function, artificial movement of the interphase (→ mass loss), how often to perform?)

• Mass conservation (during levelset advection and reinitialization)

• Representation of interphacial tension: CSF, Line Integral, Laplace-Beltrami, Phasefield, etc., explicit or implicit treatment?
**Stabilization Techniques**

**Steep changes of physical quantities:**

1) Elementwise averaging of the physical properties (prevents oscillations):
   \[ \rho_e = x\rho_1 + (1-x)\rho_2, \quad \mu_e = x\mu_1 + (1-x)\mu_2 \]
   \( x \) is the volume fraction

2) Flow part: Extension of nonlinear stabilization schemes (AFC, TVD) for the momentum equation for LBB stable element pairs.

3) Interphase tracking part with DG-FEM: Flux limiters satisfying LED requirements.
Reinitialisation

Alternatives

• Brute force (introducing new points at the zero level surfaces)
• Fast sweeping (applying „advancing front“ upwind type formulas)
• Fast marching
• Algebraic Newton method
• Hyperbolic PDE approach
• many more…..

Maintaining the signed distance function by PDE reinitialization

\[
\frac{\partial \phi}{\partial \tau} + u \cdot \nabla \phi = S(\phi) \quad u = S(\phi) \frac{\nabla \phi}{|\nabla \phi|} \quad \Leftrightarrow \quad |\nabla \phi| = 1
\]

Problems:

• What to do with the sign function at the interphase? (smoothing?)
• How often to perform? (expensive \(\rightarrow \) steady state)
Our reinitialization is performed in combination of 2 ingredients:

1) Elements intersected by the interphase are modified w.r.t. the slope of the distance distribution ("Parolini trick") such that
\[ \left| \nabla \phi \right| = 1 \]

2) Far field reinitialization: realization is based on the PDE approach ("FBM"), but it does not require smoothening of the distance function!

In addition: continuous projection of the interphase (smoothening of the discontinuous $P_1$ based distance function)

\[ \phi_{P_1} \xrightarrow{L_2 \text{ projection}} \phi_{Q_1} \xrightarrow{L_2 \text{ projection}} \phi_{P_1} \]
**Mass conservation**

Must be satisfied on the continuous and discrete level as well!

(In work) Replacement of:

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0, \quad \text{by} \quad \frac{\partial \rho(\phi)}{\partial t} + \nabla \cdot (\rho(\phi)\mathbf{v}) = 0 \quad \text{Nonlinear PDE!}
\]

**Remark**: No stabilization! (to avoid numerical diffusion)

→ distance function should be smooth anyway

Good agreement with experimental measurements
(in terms of droplet size, frequency)
Benefits of DG-FEM for Levelset

- possibility of reduction of the computational domain (only for levelset)
- mass preserving (interphase preserving!) reinitialization
- exact localization of the interphase (polygons)
- exact evaluation of volume fractions
- relatively simple parallelization

Layering concept

Parallelization based on domain decomposition

Interphase representation by polygons
Surface Tension

Continuum Surface Force (CSF):
- Transformation of the surface integrals to volume integrals with the help of a regularized Dirac delta function \( \delta \)
- Requires globally defined normals and curvature
- Reduction of spurious oscillations

\[
f_{\text{ST}} = \sigma \kappa n \delta(x, \varepsilon)
\]

\[
f = \int \nabla \cdot n \, dx
\]

\[
\kappa_Q = \frac{\int \nabla \cdot n \, dx}{\int dx}
\]

Levelset distribution

Distribution of the smoothed interphacial tension force \( (\sigma \kappa \delta)_{Q_i} \)

Resulting pressure distribution

Continuous normal field

Continuous curvature field
Phase Field (PF) approach

\[ f_{\text{ST}} = \sigma \nabla \cdot \left( \nabla \phi_{PF} \times \nabla \phi_{PF} \right) \]

- No reconstruction of normals and curvature needed
- Fully implicit treatment is possible
- Also possible for LS (?)
**Surface Tension - Alternative Treatments**

**Semi implicit CSF** formulation based on Laplace-Beltrami

\[
\mathbf{f}_{st} = \int_{\Omega} \sigma \mathbf{n} \cdot \mathbf{v} \delta(\Gamma, \mathbf{x}) \, d\mathbf{x} = \int_{\Omega} \sigma (\Delta x|_{\Gamma}) \cdot (\mathbf{v} \delta(\Gamma, \mathbf{x})) \, d\mathbf{x}
\]

\[
= -\int_{\Omega} \sigma \mathbf{n} \cdot \nabla (\mathbf{v} \delta(\Gamma, \mathbf{x})) \, d\mathbf{x} = -\int_{\Omega} \sigma \mathbf{n} \cdot \nabla \mathbf{v} \delta(\Gamma, \mathbf{x}) \, d\mathbf{x}
\]

Application of the semi-implicit time integration yields

\[
\mathbf{x}_{\Gamma}^{n+1} = \mathbf{x}_{\Gamma}^{n} + \Delta t \mathbf{u}^{n+1} \quad \rightarrow \quad \mathbf{f}_{st} = -\int_{\Omega} \sigma \delta_{\varepsilon} (\text{dist}(\Gamma^n, \mathbf{x})) \nabla \mathbf{x}|_{\Gamma}^{n} \cdot \mathbf{v} \, d\mathbf{x}
\]

\[
- \Delta t^{n+1} \int_{\Omega} \sigma \delta_{\varepsilon} (\text{dist}(\Gamma^n, \mathbf{x})) \mathbf{u}^{n+1} \cdot \nabla \mathbf{v} \, d\mathbf{x}
\]

**Advantages**
- Relaxes capillary time step restriction
- „Optimal“ for FEM-Levelset approach
Bubble Benchmarks

http://www.featflow.de/beta/en/benchmarks/

Benchmark quantities

Center of mass

\[ x_c = \frac{\int_{\Omega_2} x \, dx}{\int_{\Omega_2} 1 \, dx} \]

Mean rise velocity

\[ U_c = \frac{\int_{\Omega_2} u \, dx}{\int_{\Omega_2} 1 \, dx} \]

Circularity

\[ \phi = \frac{P_a}{P_b} = \frac{\pi d_a}{P_b} \]

Adaptive HPC Techniques

CELL processor (PS3), 218 GFLOP/s, Memory @ 3.2 GHz

GPU (NVIDIA GTX 285): 240 cores @ 1.476 GHz, 1.242 GHz memory bus (160 GB/s) ≈ 1.06 TFLOP/s

40 GFLOP/s, 140 GB/s on GeForce GTX 280

0.7 (1.4) GFLOP/s on 1 core of Xeon E5450
Droplet Jetting Application

Next step: Extension to liquid-gas systems