On higher order FEM techniques for multiphase flow

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Overview & Motivation:

Accurate, robust, flexible and efficient simulation of multiphase problems with dynamic interfaces and complex geometries, particularly in 3D, is still a challenge!

- Mathematical Modelling
- Numerics / CFD Techniques
- Validation / Benchmarking
- HPC Techniques / Software

Vision: Highly efficient, flexible and accurate „real life“ simulation tools based on modern Numerics and algorithms while exploiting modern hardware!

Realization: FeatFlow
Typical applications require efficient basic flow solvers and techniques for liquid-liquid & liquid-solid interfaces in complex (time-dependent) domains.
Basic Flow Solver: FeatFlow

**Numerical features:**
- High order FEM (Q2/P1) discretization schemes
- FCT & EO stabilization techniques
- Use of unstructured meshes
- Fictitious Boundary (FBM) methods
- Adaptive grid deformation
- Newton-Multigrid solvers

**HPC features:**
- Massive parallel
- GPUs/ARMs
- Open source

Hardware-oriented Numerics
Two phase flow (I-I) with resolved interfaces

The incompressible Navier Stokes equations

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

$$\nabla \cdot \mathbf{v} = 0$$

Interface tension force

$$\mathbf{f}_{ST} = \sigma \kappa \mathbf{n}, \quad \kappa = -\nabla \cdot \mathbf{n} \quad \text{on} \quad \Gamma$$

Dependency of physical quantities

$$\mu = \mu(D(\mathbf{v}), \Gamma), \quad \rho = \rho(\Gamma)$$

Interface capturing realized by Level Set method

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

- Exact representation of the interface
- Natural treatment of topological changes
- Provides derived geometrical quantities ($\mathbf{n}, \kappa$)
Two phase flow (I-I) with resolved interfaces

<table>
<thead>
<tr>
<th>Problems and Challenges</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Steep gradients</strong> of the velocity field and of other physical quantities near the interface (oscillations!)</td>
</tr>
<tr>
<td><strong>Reinitialization</strong> w.r.t. distance field (artificial movement of the interface → mass loss, how often to perform?)</td>
</tr>
<tr>
<td><strong>Mass conservation</strong> (during advection and reinitialization of the Level Set function)</td>
</tr>
<tr>
<td>Representation of <strong>surface tension</strong>: CSF, Line Integral, Laplace-Beltrami, Phasefield, etc.</td>
</tr>
<tr>
<td><strong>Explicit</strong> or <strong>implicit</strong> treatment (→ <em>Capillary Time Step</em> restriction?)</td>
</tr>
<tr>
<td><strong>Fast multigrid solvers</strong> for Q2/P1 via Discrete Projection Method</td>
</tr>
</tbody>
</table>
Two phase flow (I-I) with resolved interfaces

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 (FCT, TVD, EO-FEM) for the momentum equation for LBB stable element pairs with discontinuous pressure (Q2/P1)

3) Interface tracking part with DG(1)-FEM: Flux limiters satisfying LED requirements
Two phase flow (I-I) with resolved interfaces

Reinitialization
- Mainly required in the vicinity of the interface
- How often to perform?
- Which realization to implement?
- Efficient parallelization (3D!)

Alternatives
- Brute force (introducing new points at the zero level set)
- Fast sweeping ("advancing front" upwind type formulas)
- Fast marching
- Algebraic Newton method
- Hyperbolic PDE approach
- many more…..

Maintaining the signed distance function by PDE reinitialization
\[
\frac{\partial \phi}{\partial \tau} + \mathbf{u} \cdot \nabla \phi = S(\phi) \quad \mathbf{u} = S(\phi) \frac{\nabla \phi}{|\nabla \phi|} \quad \Leftrightarrow \quad |\nabla \phi| = 1
\]

Problems:
- What to do with the sign function at the interface? (smoothing?)
- How to handle the underlying non-linearity?
- How often to perform? (expensive \(\rightarrow\) steady state)
## Fine-tuned reinitialization

**Our reinitialization is performed in combination of 2 ingredients:**

1) Elements intersected by the interface are modified w.r.t. the slope of the distance distribution ("Parolini trick" for DG-P1) such that $|\nabla \phi| = 1$

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 interface (smoothening of the discontinuous P₁ based distance function)

\[
\phi_{P₁} \xrightarrow{L₂ \text{ projection}} \phi_{Q₁} \xrightarrow{L₂ \text{ projection}} \phi_{P₁}
\]

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### Two phase flow (I-I) with resolved interfaces

![Image](image.png)
Two phase flow (I-I) with resolved interfaces

**Continuum**

**Surface**

**Force**

- 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

$$ f_{ST} = \sigma \kappa \mathbf{n} \delta(x, \varepsilon) $$

$$ \kappa_{Q_i} = \frac{\int_{\Omega} \nabla \cdot \mathbf{n}_{Q_i} \, dx}{\int_{\Omega} dx} $$

**Level Set distribution**

**Distribution of the smoothed surface tension force**

**Resulting pressure distribution**
Two phase flow (l-l) with resolved interfaces

Surface Tension: Semi-implicit CSF formulation based on Laplace-Beltrami

\[ f_{ST} = \int_{\Omega} \sigma \hat{n} \cdot v \, \delta(\Gamma, x) \, dx = \int_{\Omega} \sigma (\nabla x_{\Gamma}) \cdot (v \, \delta(\Gamma, x)) \, dx \]

\[ = -\int_{\Omega} \sigma \nabla x_{\Gamma} \cdot \nabla (v \, \delta(\Gamma, x)) \, dx = -\int_{\Omega} \sigma \nabla x_{\Gamma} \cdot \nabla v \delta(\Gamma, x) \, dx \]

Application of the semi-implicit time integration yields

\[ x|_{\Gamma^{n+1}} = x|_{\Gamma^n} + \Delta t \, u^{n+1} \]

\[ f_{ST} = -\int_{\Omega} \sigma \, \delta_{\varepsilon} \left( \text{dist}(\Gamma^n, x) \right) \nabla \tilde{x}_{\Gamma}^n \cdot \nabla v \, dx \]

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

Advantages

- Relaxes Capillary Time Step restriction
- „Optimal“ for FEM-Level Set approach due to global information
Data Layout for Q2/P1 FEM

1 cell/4 dofs

P₁ – stencil
27 cells/108 (4x27) dofs

1 cell/27 dofs

Q₂ – stencil
8 cells/125 (5x5x5) dofs

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### Numerical Analysis of the Multigrid Solvers

#### dt = 0.001 | nOfSmstepP(SOR) = 8,F,rlx = 1.0 | nOfSmstepV(SOR+JAC) = 4,V,rlx = 0.5

<table>
<thead>
<tr>
<th>Level</th>
<th># MG steps P</th>
<th>MG rates P</th>
<th># NonLin/MG steps V</th>
<th>MG rates V</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.4</td>
<td>0.0425</td>
<td>2/1</td>
<td>3.6e-4</td>
</tr>
<tr>
<td>3</td>
<td>3.7</td>
<td>0.1324</td>
<td>2/1</td>
<td>1.3e-3</td>
</tr>
<tr>
<td>4</td>
<td>3.0</td>
<td>0.0947</td>
<td>2/1</td>
<td>2.2e-3</td>
</tr>
</tbody>
</table>

#### dt = 0.010 | nOfSmstepP(SOR) = 8,F, rlx = 1.0 | nOfSmstepV(SOR+JAC) = 4,V,rlx = 0.5

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<tr>
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<th>MG rates P</th>
<th># NonLin/MG steps V</th>
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<tr>
<td>2</td>
<td>2.2</td>
<td>0.0330</td>
<td>2/1</td>
<td>1.3e-3</td>
</tr>
<tr>
<td>3</td>
<td>3.9</td>
<td>0.1439</td>
<td>2/1</td>
<td>6.4e-3</td>
</tr>
<tr>
<td>4</td>
<td>3.2</td>
<td>0.1064</td>
<td>2/1</td>
<td>8.5e-3</td>
</tr>
</tbody>
</table>

#### Convergence criterions
- LinearDefectReductionP=1e-3
- NonLinearDefectReductionV=1e-4
- LinearDefectReductionV=1e-1
Known benchmark problem (DFG) in the CFD community

- Comparison of CFX 12.0, OpenFoam 1.6 andFeatFlow
- Drag and lift coefficients behave very sensitive to mesh resolution
- Ideal indicator for computational accuracy
- Five consequently refined meshes L1 (coarse), …, L5 (fine)
- Same meshes and physical models used in all three codes

\[
F_L = \frac{1}{2} \rho v^2 A C_L \\
F_D = \frac{1}{2} \rho v^2 A C_D
\]

<table>
<thead>
<tr>
<th>Mesh Level</th>
<th># Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>L2</td>
<td>6,144</td>
</tr>
<tr>
<td>L3</td>
<td>49,152</td>
</tr>
<tr>
<td>L4</td>
<td>393,216</td>
</tr>
<tr>
<td>L5</td>
<td>3,145,728</td>
</tr>
</tbody>
</table>
Flow Simulation with CFD software available on the market

**Benchmarking**

<table>
<thead>
<tr>
<th>Case</th>
<th>L2 error</th>
<th>timing</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$c_D$</td>
<td>$c_L$</td>
</tr>
<tr>
<td>CFX L3</td>
<td>0.0152</td>
<td>0.0781</td>
</tr>
<tr>
<td>CFX L4</td>
<td>0.0098</td>
<td>0.0631</td>
</tr>
<tr>
<td>CFX L5</td>
<td>0.0029</td>
<td>0.0224</td>
</tr>
</tbody>
</table>

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<tr>
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<th>Timing</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$c_D$</td>
<td>$c_L$</td>
</tr>
<tr>
<td>OF L3</td>
<td>0.0261</td>
<td>0.1449</td>
</tr>
<tr>
<td>OF L4</td>
<td>0.0067</td>
<td>0.0591</td>
</tr>
<tr>
<td>OF L5</td>
<td>0.0016</td>
<td>0.0147</td>
</tr>
</tbody>
</table>
Flow Simulation with **FEATFLOW**

**Comparison**

- Same order of accuracy with **FEATFLOW** on L3 as L5 with **CFX** and **OpenFOAM** on L5!
- High order Q2/P1 FEM + (parallel) Multigrid Solver

### Case L2 error Timing

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<tr>
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<th>L2 error</th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$c_D$</td>
<td>$c_L$</td>
</tr>
<tr>
<td>FF L2</td>
<td>0.0209</td>
<td>0.1378</td>
</tr>
<tr>
<td>FF L3</td>
<td>0.0029</td>
<td>0.0109</td>
</tr>
<tr>
<td>FF L4</td>
<td>0.0005</td>
<td>0.0015</td>
</tr>
<tr>
<td>FF L5</td>
<td>(ref)</td>
<td>(ref)</td>
</tr>
</tbody>
</table>

Less than 2 hours sim. time with adaptive time stepping on 3+1 processors

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 \( \phi = \frac{P_a}{P_b} = \frac{\pi d_a}{P_b} \)
3D convergence analysis for large density jumps

Rising bubble problem for $Eo = 60, \ Re = 34$
Density jump 1:100
Benchmarking with experimental results

Continuous phase:

Glucose-Water mixture
\[ \mu_D = 500 \text{ mPa s} \]
\[ \rho_D = 972 \text{ kg m}^{-3} \]
\[ \dot{V}_D = 3,64 \text{ ml min}^{-1} \]
\[ \sigma_{CD} = 0,034 \text{ N m}^{-1} \]

Silicon oil
\[ \mu_C = 500 \text{ mPa s} \]
\[ \rho_C = 1340 \text{ kg m}^{-3} \]
\[ \dot{V}_C = 99,04 \text{ ml min}^{-1} \]

Dispersed phase:

Validation parameters:
- frequency of droplet generation
- droplet size
- stream length

Experimental setup with AG Walzel (BCI/Dortmund)
Benchmarking with experimental results

<table>
<thead>
<tr>
<th></th>
<th>Separation frequency [Hz]</th>
<th>Droplet size [dm]</th>
<th>Stream Length [dm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp</td>
<td>0.58</td>
<td>0.062</td>
<td>0.122</td>
</tr>
<tr>
<td>Sim</td>
<td>0.6</td>
<td>0.058</td>
<td>0.102</td>
</tr>
</tbody>
</table>

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In case of monodisperse droplet generation:

\[ \dot{V}_D = fV_{\text{droplet}} \]

**Influencable variables**

On the level of the process:
- Flowrates
- Modulation frequency
- Modulation amplitude

Geometrical changes:
- Capillary size
- Contraction angle
- Contraction ratio

**Resulting operation envelope:**
- Size: 4.5 mm – 5.7 mm
- Volume: 0.38 cm³ – 0.77 cm³
Preliminary Studies: Coupling FBM-LSFEM
Next Steps for Multiphase Flow

- Adaptive time stepping + adaptive grid alignment/ALE.
- Coupling with turbulence models.
- Coupling with rigid particles.
- Analysis of viscoelastic effects.
- **Benchmarking** and experimental validation for many particles/bubbles.