Finite Element-Fictitious Boundary Methods (FEM-FBM) for time-dependent mixing processes in complex geometries

Stefan Turek, Otto Mierka, Raphael Münster
Institut für Angewandte Mathematik, LS III
Technische Universität Dortmund
ture@featflow.de

http://www.featflow.de
http://www.mathematik.tu-dortmund.de/LS3
Motivation: Numerical & Algorithmic Challenges

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

- Mathematical Modelling of Dynamic Interfaces
- Numerics / CFD Techniques
- HPC Techniques / Software
- Validation / Benchmarking

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

Realization: FEATFLOW
Motivation: Target Application I

- Numerical simulation of *micro-fluidic drug encapsulation* ("monodisperse compound droplets") for application in lab-on-chip and bio-medical devices
- Polymeric "bio-degradable" outer fluid with *viscoelastic* effects
- Optimization of chip design w.r.t. boundary conditions, flow rates, droplet size, geometry
Motivation: Target Application II

- Non-Newtonian rheological models (shear & temperature dependent)
- Non-isothermal flow conditions (cooling from outside, heat production)
- Evaluation of torque acting on the screws, resulting energy consumption
- Influence of local characteristics on global product quality
- Influence of gaps on back-mixing
**Basic Flow Solver: FEATFLOW**

**Numerical features:**
- Parallelization based on domain decomposition
- FCT & EO stabilization techniques
- High order FEM (Q2/P1) discretization
- Use of unstructured meshes
- Adaptive grid deformation
- Newton-Multigrid solvers

**HPC features**
- Massive parallel
- GPU computing
- Open source

**Hardware-oriented Numerics**

*Stefan Turek*
The incompressible Navier Stokes equation

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

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

Interphase tension force

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

Dependency of physical quantities

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

**Interphase capturing** realized by **Level Set method**

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

\[ + \quad \frac{\partial \phi}{\partial \tau} + \mathbf{n} \cdot \nabla \phi = S(\phi) \quad \mathbf{n} = S(\phi) \frac{\nabla \phi}{|\nabla \phi|} \]

- Exact representation of the interphase
- Natural treatment of topological changes
- Provides derived geometrical quantities \((\mathbf{n}, \kappa)\)
- Requires reinitialization w.r.t. distance field
- Can lead to mass loss \(\rightarrow\) dG(1) discretization!
Two phase flow (s-l) with resolved interphases

- **Fluid** motion is governed by the **Navier-Stokes equations**
- **Particle** motion is described by **Newton-Euler equations**

\[
M_p \frac{dU_p}{dt} = F_p + F_{\text{ex, col}} + \left( \Delta M_p \right) g,
\]

\[
I_p \frac{d\omega_p}{dt} = T_p - \omega_p \times \left( I_p \omega_p \right).
\]

Hydrodynamic force

\[
F_p = -\int_{\Gamma_p} \sigma \cdot n_p \, d\Gamma_p
\]

Postprocessing the actual flow field

\[
T_p = -\int_{\Gamma_p} \left( X - X_p \right) \times \left( \sigma \cdot n_p \right) \, d\Gamma_p
\]

**Fictitious Boundary Method**

- Surface integral is replaced by volume integral
- Use of monitor function (liquid/solid)

\[
\alpha_p(X) = \begin{cases} 
1 & \text{for } X \in \Omega_p \\
0 & \text{for } X \in \Omega_f 
\end{cases}
\]

- Normal to particle surface vector is non-zero only at the surface of particles

\[
n_p = \nabla \alpha_p
\]

\[
F_p = -\int_{\Gamma_p} \sigma \cdot n_p \, d\Gamma_p = -\int_{\Omega_T} \sigma \cdot \nabla \alpha_p \, d\Omega_T
\]

\[
T_p = -\int_{\Gamma_p} \left( X - X_p \right) \times \left( \sigma \cdot n_p \right) \, d\Gamma_p = -\int_{\Omega_T} \left( X - X_p \right) \times \left( \sigma \cdot \nabla \alpha_p \right) \, d\Omega_T
\]
**Two phase flow (s-l) with resolved interphases**

- Supports HPC concepts (no computational overhead, constant data structures, optimal load balancing)
- Reduces dramatically requirements put on the computational mesh
- Relatively low resolution

Velocity “boundary condition” imposed for particles:

\[
\mathbf{u}(X) = \mathbf{U}_p + \mathbf{\omega}_p \times (X - X_p)
\]

- For computed
  
  \[
  \mathbf{U}^{n+1}_p, \, \mathbf{\omega}^{n+1}_p
  \]

- Position update:
  
  \[
  \frac{dX_p}{dt} = \mathbf{U}_p
  \]

- Angle update:
  
  \[
  \frac{d\theta_p}{dt} = \mathbf{\omega}_p
  \]

- Grid deformation (via Level-Set function)

- Brute force → Finer mesh resolution
- High resolution interpolation functions

Stefan Turek
Grid Deformation Method

**idea**: construct transformation \( \phi \), \( x = \phi (\xi, t) \) with \( \det \nabla \phi = f \)

\[ \text{local mesh area} \approx f \]

1. Compute monitor function \( f(x, t) > 0, f \in C^1 \)

\[ \int_{\Omega} f^{-1}(x, t) dx = |\Omega|, \quad \forall t \in [0,1] \]

2. Solve (\( t \in [0,1] \))

\[ \Delta v(\xi, t) = - \frac{\partial}{\partial t} \left( \frac{1}{f(\xi, t)} \right), \quad \frac{\partial v}{\partial n}\bigg|_{\partial \Omega} = 0 \]

3. Solve the ODE system

\[ \frac{\partial}{\partial t} \phi (\xi, t) = f (\phi (\xi, t), t) \nabla v (\phi (\xi, t), t) \]

new grid points: \( x_i = \phi (\xi_i, 1) \)

Grid deformation preserves the (local) logical structure of the grid

Stefan Turek
Generalized Tensorproduct Meshes

Stefan Turek
Sedimentation of many Particles

Stefan Turek

tu technische universität dortmund
**Benchmarking and Validation**

**Flow Simulation for the Flow Around Cylinder problem**

Known benchmark problem (DFG) in the CFD community

- Comparison of **CFX 12.0, OpenFoam 1.6** and **FeatFlow**
- 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

\[
\begin{align*}
F_L &= \frac{1}{2} \rho v^2 A C_L \\
F_D &= \frac{1}{2} \rho v^2 A C_D
\end{align*}
\]

<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>
**Benchmarking and Validation**

**CFX**

<table>
<thead>
<tr>
<th>Case</th>
<th>L_2 Err</th>
<th>c_D</th>
<th>c_L</th>
</tr>
</thead>
<tbody>
<tr>
<td>cfxL3</td>
<td>0.0152</td>
<td>0.0781</td>
<td></td>
</tr>
<tr>
<td>cfxL4</td>
<td>0.0098</td>
<td>0.0631</td>
<td></td>
</tr>
<tr>
<td>cfxL5</td>
<td>0.0029</td>
<td>0.0224</td>
<td></td>
</tr>
</tbody>
</table>

**OpenFOAM**

<table>
<thead>
<tr>
<th>Case</th>
<th>L_2 Err</th>
<th>c_D</th>
<th>c_L</th>
</tr>
</thead>
<tbody>
<tr>
<td>OFL3</td>
<td>0.0261</td>
<td>0.1449</td>
<td></td>
</tr>
<tr>
<td>OFL4</td>
<td>0.0067</td>
<td>0.0591</td>
<td></td>
</tr>
<tr>
<td>OFL5</td>
<td>0.0016</td>
<td>0.0147</td>
<td></td>
</tr>
</tbody>
</table>
Benchmarking and Validation

\[ \text{FeatFlow} \]

\[ \text{Comparison} \]

<table>
<thead>
<tr>
<th>Case</th>
<th>( c_D )</th>
<th>( c_L )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q2P1L3</td>
<td>0.0029</td>
<td>0.0109</td>
</tr>
<tr>
<td>Q2P1L4</td>
<td>0.0005</td>
<td>0.0015</td>
</tr>
</tbody>
</table>

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

\[ \rightarrow \text{Same order of accuracy with FeatFlow on L3 as L5 with CFX and OpenFOAM on L5!} \]
\[ \rightarrow \text{High order Q2/P1 FEM + (parallel) Multigrid Solver} \]

\text{Stefan Turek}

\text{tu technische universität dortmund}
Benchmarking and Validation

Free fall of particles:
• Terminal velocity
• Different physical parameters
• Different geometrical parameters

\[ \begin{array}{cccc}
\nu & U_{\text{featflow}} & U_{\text{exp}} & \text{Relative error (\%)} \\
0.02 & 5.885 & 6.283 & 6.33 \\
0.05 & 4.133 & 3.972 & 4.05 \\
0.1 & 2.588 & 2.426 & 6.66 \\
0.2 & 1.492 & 1.401 & 6.50 \\
\end{array} \]

\[ \begin{array}{cccc}
\nu & U_{\text{featflow}} & U_{\text{exp}} & \text{Relative error (\%)} \\
0.02 & 4.370 & 4.334 & 0.83 \\
0.05 & 2.699 & 2.489 & 8.44 \\
0.1 & 1.649 & 1.552 & 6.25 \\
0.2 & 0.946 & 0.870 & 8.74 \\
\end{array} \]

\[ \begin{array}{cccc}
\nu & U_{\text{featflow}} & U_{\text{exp}} & \text{Relative error (\%)} \\
0.01 & 1.4660 & 1.4110 & 3.90 \\
0.02 & 0.9998 & 0.9129 & 9.52 \\
0.05 & 0.4917 & 0.4603 & 6.82 \\
0.1 & 0.2637 & 0.2571 & 2.57 \\
0.2 & 0.1335 & 0.1317 & 1.37 \\
\end{array} \]

Münster, R.; Mierka, O.; Turek, S.: Finite Element Fictitious Boundary Methods (FEM-FBM) for 3D particulate flow, IJNMF, 2010, accepted

Stefan Turek
3D simulations with complex shapes

‘Kissing, Drafting, Thumbling’

Sedimentation of particles in a complex domain
Absorber packing simulations

Velocity distribution

Pressure distribution

\[ v_{\text{mean}} = (1 \pm 0.1 \pm 0.01) \text{ms}^{-1} \]
\[ \rho = 1.25 \text{ g cm}^{-3} \]
\[ \mu = 17.57 \times 10^{-6} \text{ Pa s} \]
Absorber packing simulations

<table>
<thead>
<tr>
<th>Level</th>
<th>Mesh points</th>
<th>Velocity DOFs</th>
<th>Pressure DOFs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$n_x$</td>
<td>$n_{yz}$</td>
<td>$n_{xyz}$</td>
</tr>
<tr>
<td>2</td>
<td>155</td>
<td>109</td>
<td>16,895</td>
</tr>
<tr>
<td>3</td>
<td>309</td>
<td>409</td>
<td>126,381</td>
</tr>
<tr>
<td>4</td>
<td>617</td>
<td>1,585</td>
<td>977,945</td>
</tr>
</tbody>
</table>

Stefan Turek
Twinscrew Flow Simulations

Geometrical representation of the twinscrews → **Fictitious Boundary Method**

- Fast and accurate description of the rotating geometry (screws)
- Applicable for conveying and kneading elements
- Mathematical description available for single, double- or triplet-flighted screws
- Surface and body of the screws are known at any time
- Mathematical formulation replaces external CAD-description

*In cooperation with:*

[UNIVERSITÄT PADERBORN](mailto:)

[IANUS Simulation](mailto:)

[Stefan Turek](mailto:)
Twinscrew Flow Simulations

Meshing strategy – Hierarchical mesh refinement

Pre-refined regions in the vicinity of gaps

2D mesh extrusion into 3D
Twinscrew Flow Simulations

Stefan Turek
Vielen Dank!
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 Set-up 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>

Exp. results → Group of Prof. Walzel BCI/Dortmund

Stefan Turek