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

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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 $l-g$, $l-l$, $s-l$ Interfaces
- Numerics / CFD Techniques
- HPC Techniques / Software
- Validation / Benchmarking

Vision: 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

Flow simulations in twinscrew extruders

- 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

Main features of the FeatFlow approach:
- Parallelization based on domain decomposition
- FCT & EO stabilization techniques
- High order FEM discretization schemes
- Use of unstructured meshes
- Adaptive grid deformation
- Newton-Multigrid solvers

HPC features
- Massive parallel
- GPU computing
- Open source

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

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

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

Dependency of physical quantities

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

Interphase capturing realized by the Level Set method

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0 \quad + \quad \frac{\partial \phi}{\partial \tau} + \mathbf{n} \cdot \nabla \phi = S(\phi) \quad \mathbf{n} = S(\phi) \frac{\nabla \phi}{|\nabla \phi|}
\]

- Exact representation of the interphase
- Natural treatment of topological changes
- Provides derived geometrical quantities \((\mathbf{n}, \kappa)\)
- Requires reinitializion 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**

\[ M_p \frac{dU_p}{dt} = F_p + F_{ex, col} + (\Delta M_p)g, \]
\[ I_p \frac{d\omega_p}{dt} = T_p - \omega_p \times (I_p \omega_p) \]

**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

\[ n_p = \nabla \alpha_p \]

\[ F_p = -\int_{\Gamma_p} \sigma \cdot n_p d\Gamma_p = -\int_{\Omega_T} \sigma \cdot \nabla \alpha_p d\Omega_T \]
\[ T_p = -\int_{\Gamma_p} (X - X_p) \times (\sigma \cdot n_p) d\Gamma_p = -\int_{\Omega_T} (X - X_p) \times (\sigma \cdot \nabla \alpha_p) d\Omega_T \]
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:
\[ u(X) = U_p + \omega_p \times (X - X_p) \]

For computed
\[ U_{p}^{n+1}, \omega_{p}^{n+1} \]

Position update:
\[ \frac{dX_p}{dt} = U_p, \quad \frac{d\theta_p}{dt} = \omega_p \]

Angle update:
\[ X_{p}^{n+1}, \theta_{p}^{n+1} \]

Brute force \( \rightarrow \) Finer mesh resolution
- High resolution interpolation functions
- Grid deformation (+ monitor function)
**Turbulent (l,g-l) multiphase flow**

- Population Balance Equations within the Reynolds Averaged framework

\[
\frac{\partial f}{\partial t} + \mathbf{u}_g \cdot \nabla f + \nabla \cdot \left( \frac{\nu_T}{\sigma_T} \nabla f \right) = \int_v^\infty r^B(v, \tilde{v}) f(\tilde{v}) \, d\tilde{v} - \frac{f(v)}{v} \int_0^v \tilde{v} r^B(\tilde{v}, v) \, d\tilde{v} \\
+ \frac{1}{2} \int_0^v r^C(\tilde{v}, v - \tilde{v}) f(\tilde{v}) f(v - \tilde{v}) \, d\tilde{v} - f(v) \int_0^\infty r^C(\tilde{v}, v) f(\tilde{v}) \, d\tilde{v}
\]

- Different discretization techniques for PBEs
  - Moment based: Parallel Parent Daughter Classes (PPDC)
  - Class based: Method of Classes (MC)

-Decoupling of the problem to standalone modules

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**Navier-Stokes equation**

- Continuity equation
- Momentum equation

**turbulence model**

- K-ε model

**multiphase model**

- Population balance equation

**Decoupling of the problem to standalone modules**

**ProcessNet 2011**
**Benchmarking**

**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

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

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

<table>
<thead>
<tr>
<th>Mesh Level</th>
<th># Elements</th>
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<tbody>
<tr>
<td>L2</td>
<td>6,144</td>
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<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>
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</table>
Benchmarking

Flow Simulation with CFD software available on the market

<table>
<thead>
<tr>
<th>Case</th>
<th>$L_2$Err</th>
</tr>
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<tbody>
<tr>
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<tr>
<td>cfXL5</td>
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</table>

<table>
<thead>
<tr>
<th>Case</th>
<th>$L_2$Err</th>
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</thead>
<tbody>
<tr>
<td></td>
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<tr>
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<tr>
<td>OFL5</td>
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</table>
Benchmarking

Flow Simulation with FeatFlow

FeatFlow

<table>
<thead>
<tr>
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<th>$L_2$Err</th>
<th>$c_D$</th>
<th>$c_L$</th>
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</tr>
<tr>
<td>Q2P1L4</td>
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<td>0.0015</td>
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Comparison

<table>
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<tr>
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<th>$c_L$</th>
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<tr>
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<td>0.0224</td>
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Less than 2 hours sim. time on 3+1 processors

→ Same order of accuracy with FeatFlow on L3 as L5 with CFX and OpenFOAM on L5!
→ High order Q2/P1 FEM + (parallel) Multigrid Solver
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
\[ \phi = \frac{P_a}{P_b} = \frac{\pi d_a}{P_b} \]


Benchmark quantities

Center of mass
$$x_c = \frac{\int x \, dx}{\int 1 \, dx}$$

Mean rise velocity
$$\mathbf{U}_c = \frac{\int \mathbf{u} \, dx}{\int 1 \, dx}$$

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

Level 2  Level 3  Level 4
**Continuous phase:**

**Glucose-Water mixture**
- \( \mu_D = 500 \text{ mPa} \text{s} \)
- \( \rho_D = 972 \text{ kg m}^{-3} \)
- \( V_D = 3,64 \text{ ml min}^{-1} \)

\[ \sigma_{CD} = 0,034 \text{ N m}^{-1} \]

**Silicon oil**
- \( \mu_C = 500 \text{ mPa} \text{s} \)
- \( \rho_C = 1340 \text{ kg m}^{-3} \)
- \( V_C = 99,04 \text{ ml min}^{-1} \)

**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><strong>Exp</strong></td>
<td>0.58</td>
<td>0.062</td>
<td>0.122</td>
</tr>
<tr>
<td><strong>Sim</strong></td>
<td>0.6</td>
<td>0.058</td>
<td>0.102</td>
</tr>
</tbody>
</table>
Validation based on experimental results

Jetting mode

Experimental setup/results Group of Prof. Walzel (BCI/Dortmund)

Continuous phase:

Glucose-Water mixture

\[ \mu_D = 500 \text{ mPa s} \]

\[ \rho_D = 972 \text{ kg m}^{-3} \]

\[ \sigma_{CD} = 0.034 \text{ N m}^{-1} \]

Silicon oil

\[ \mu_C = 500 \text{ mPa s} \]

\[ \rho_C = 1340 \text{ kg m}^{-3} \]

Dispersed phase:

Operating conditions

<table>
<thead>
<tr>
<th>( V_D ) [ml/min]</th>
<th>3.64</th>
<th>4.17</th>
<th>4.70</th>
<th>5.23</th>
<th>5.75</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_C ) [ml/min]</td>
<td>99.04</td>
<td>113.34</td>
<td>128.34</td>
<td>143.34</td>
<td>156.95</td>
</tr>
</tbody>
</table>

Validation parameters:
- frequency of droplet generation
- droplet size
- stream length
Validation based on experimental results

- Volumetric flow rate [ml/min]: 3.64, 4.17, 4.70, 5.23, 5.75
- Frequency [Hz]: 0, 0.4, 0.8, 1.2, 1.6
- Stream length [dm]: sim, exp

Graphs show the comparison between simulated (f_sim) and experimental (f_exp) results for different flow rates.
'Kissing, Drafting, Thumbling' of 2 Particles
Sedimentation of many Particles
Free fall of particles:
- Terminal velocity
- Different physical parameters
- Different geometrical parameters

$Münster, R.; Mierka, O.; Turek, S.: \text{Finite Element fictitious boundary methods (FEM-FBM) for 3D particulate flow, IJNMF, 2010, accepted}$

<table>
<thead>
<tr>
<th>$d_s = 0.3$</th>
<th>$\rho_s = 1.14$</th>
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<tbody>
<tr>
<td>$\nu$</td>
<td>$U_{\text{feat flow}}$</td>
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<tr>
<td>0.02</td>
<td>5.885</td>
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<td>0.05</td>
<td>4.133</td>
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<tr>
<td>0.1</td>
<td>2.588</td>
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<tr>
<td>0.2</td>
<td>1.492</td>
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<table>
<thead>
<tr>
<th>$d_s = 0.2$</th>
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<tbody>
<tr>
<td>$\nu$</td>
<td>$U_{\text{feat flow}}$</td>
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<tr>
<td>0.02</td>
<td>4.370</td>
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<tr>
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<td>1.649</td>
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<tr>
<td>0.2</td>
<td>0.946</td>
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<tr>
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<td>0.218</td>
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<td>0.4917</td>
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<tr>
<td>0.1</td>
<td>0.2637</td>
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<tr>
<td>0.2</td>
<td>0.1335</td>
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</tbody>
</table>
3D simulations with more complex shapes

‘Kissing, Drafting, Thumbling’

Sedimentation of particles in a complex domain
Velocity distribution

Pressure distribution

\begin{align*}
v_{\text{mean}} &= (1 \mid 0.1 \mid 0.01) \text{ms}^{-1} \\
\rho &= 1.25 \text{g cm}^{-3} \\
\mu &= 17.57 \times 10^{-6} \text{Pa s}
\end{align*}
### Absorber packing simulations (BASF)

<table>
<thead>
<tr>
<th>Level</th>
<th>Mesh points</th>
<th>Velocity DOFs</th>
<th>Pressure DOFs</th>
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</thead>
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<td>$n_{yz}$</td>
<td>$n_{xyz}$</td>
</tr>
<tr>
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<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>
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<tr>
<td>4</td>
<td>617</td>
<td>1,585</td>
<td>977,945</td>
</tr>
</tbody>
</table>

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**Technische Universität Dortmund**

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Twinscrew Flow Simulation with FeatFlow

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:
Twinscrew Flow Simulation with FeatFlow

Meshing strategy – Hierarchical mesh refinement

level 1  level 2  level 3

Pre-refined regions in the vicinity of gaps

2D mesh extrusion into 3D
Twinscrew Flow Simulation with FeatFlow

In cooperation with:

ProcessNet 2011
Vielen Dank!