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 *I-g*, *I-I*, *s-I* 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



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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



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Two phase flow (I-I) with resolved interphases



Interphase capturing realized by the Level Set method

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

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



Fictitious Boundary Method

- Surface integral is replaced by volume integralUse of monitor function (liquid/solid)
- Normal to particle surface vector is non-zero only at the surface of particles $n_p = \nabla lpha_p$

$$F_{p} = -\int_{\Gamma_{p}} \sigma \cdot n_{p} d\Gamma_{p} = -\int_{\Omega_{T}} \sigma \cdot \nabla \alpha_{p} d\Omega_{T}$$

$$T_{p} = -\int_{\Gamma_{p}} (X - X_{p}) \times (\sigma \cdot n_{p}) d\Gamma_{p} = -\int_{\Omega_{T}} (X - X_{p}) \times (\sigma \cdot \nabla \alpha_{p}) d\Omega_{T}$$

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

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
 - Brute force \rightarrow Finer mesh resolution
 - High resolution interpolation functions
 - Grid deformation (+ monitor function)





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Turbulent (I,g-I) multiphase flow

• Population Balance Equations within the Reynolds Averaged framework

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

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- 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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sauter d -0.539 -0.526 -0.513 mm 0.5



Benchmarking

Flow Simulation for the Flow Around Cylinder problem

Known benchmark problem (DFG) in the CFD community

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- Comparison of CFX 12.0, OpenFoam 1.6 and FeatFlow
- Drag and lift coefficients behave very sensitive to mesh resolution

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- \rightarrow Ideal indicator for computational accuracy
- Five consequently refined meshes L1 (coarse), ..., L5 (fine)
- Same meshes and physical models used in all three codes

Mesh Level	# Elements		
L2	6,144		
L3	49,152		
L4	393,216		
L5	3,145,728		



Benchmarking

Flow Simulation with CFD software available on the market









Benchmarking Flow Simulation with FeatFlow



Less then 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

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Benchmarking 2D Bubble Benchmarks





International Journal for Numerical Methods in Fluids, in press, DOI: 10.1002/fld.1934, 2009







Benchmarking 2D Bubble Benchmarks

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



Hysing, S.; Turek, S.; Kuzmin, D.; Parolini, N.; Burman, E.; Ganesan, S.; Tobiska, L.: Quantitative benchmark computations of two-dimensional bubble dynamics, International Journal for Numerical Methods in Fluids, in press, DOI: 10.1002/fld.1934, 2009







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3D convergence analysis for large density jumps







Benchmarking with experimental results





Validation parameters:

- frequency of droplet generation
- droplet size
- stream length



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Benchmarking with experimental results







Validation based on experimental results

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



Operating conditions

V _D [ml/min]	3,64	4,17	4,70	5,23	5,75
V _C [ml/min]	99,04	113,34	128,34	143,34	156,95



Validation parameters:

- frequency of droplet generation
- droplet size
- stream length





Validation based on experimental results



'Kissing, Drafting, Thumbling' of 2 Particles





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Sedimentation of many Particles







Benchmarking and Validation

Free fall of particles:

- Terminal velocity
- Different physical parameters
- Different geometrical parameters



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

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3D simulations with more complex shapes

Sedimentation of particles in a complex domain

Absorber packing simulations (BASF)

Velocity distribution

Pressure distribution

Absorber packing simulations (BASF)

L4

Twinscrew Flow Simulation with FeatFlow

Geometrical representation of the twinscrews \rightarrow Fictitious Boundary Method

In cooperation with: UNIVERSITÄT PADERBORN Die Universität der Informationsgesellschaft

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 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 CADdescription

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Twinscrew Flow Simulation with FeatFlow

Meshing strategy – Hierarchical mesh refinement

Pre-refined regions in the vicinity of gaps

Vielen Dank!