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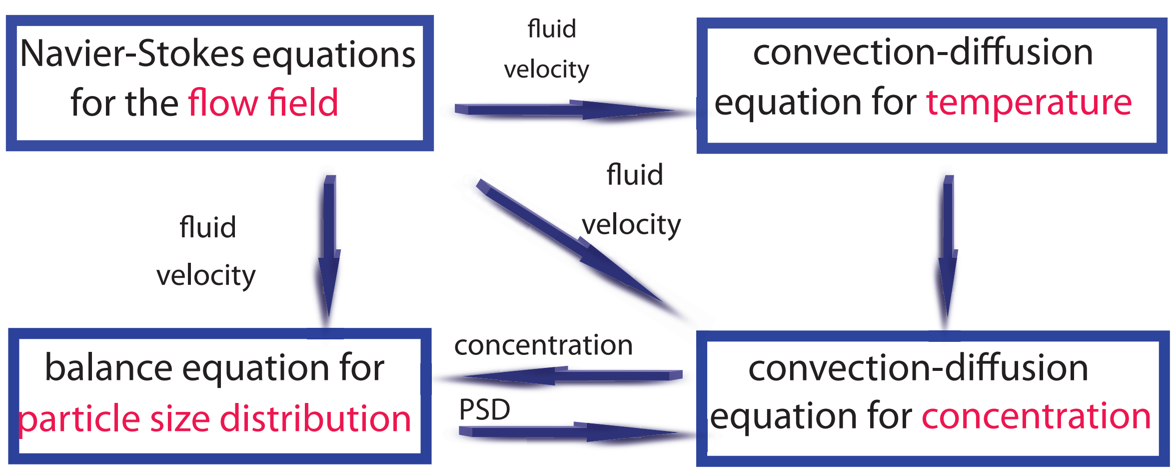
Volker John and Carina Suciu

Saarland University, Saarbrücken

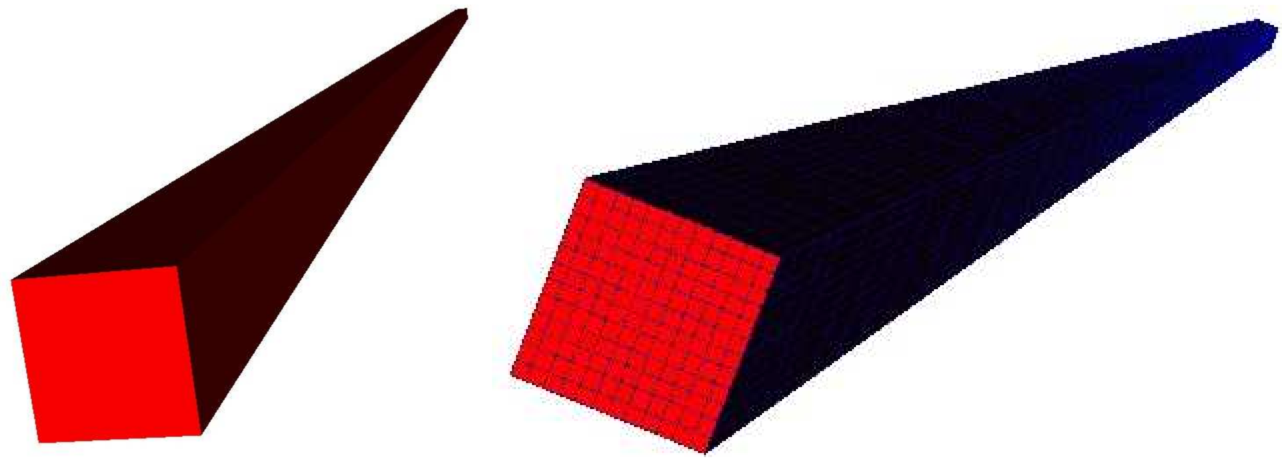
The population balance system

- coupled system of
  - Navier–Stokes equations (flow field)
  - energy balance (temperature)
  - mass balance (concentration)
  - population (particle size distribution)



Domain and grid

- domain Ω
  - length $2.10\ m$
  - width $0.01\ m$
  - height $0.01\ m$



- anisotropic grid in streamwise direction
- inlet:

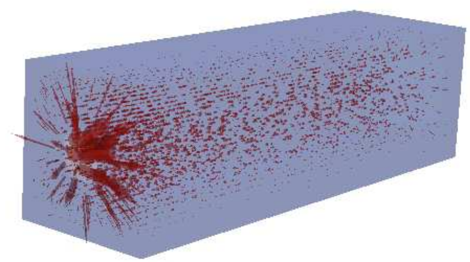
$$I = 0 \times \left[\frac{1}{3}, \frac{2}{3}\right] \times \left[\frac{1}{3}, \frac{2}{3}\right]$$

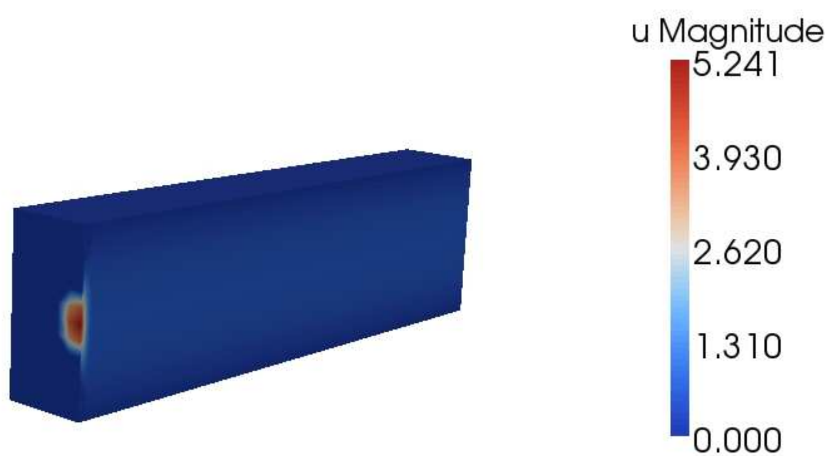
Flow field

- Navier–Stokes equations
- flow is steady state
- Reynolds number

$$Re = \frac{l_\infty u_\infty}{\nu} \approx 73.475386$$

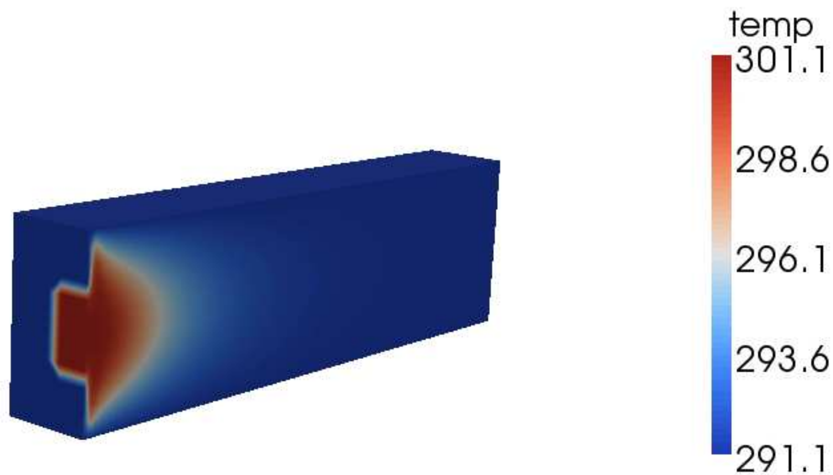
- Galerkin FEM with about 573 000 degrees of freedom (Q_2/P_1^{disc})





Energy balance (temperature)

- convection–dominated convection–diffusion equation
- temperature only necessary for computing the growth rate of the particles
- Crank–Nicolson linear Finite–Element–Method Flux–Corrected–Transport (FEM–FCT) scheme to reach steady state
- about 22 500 d.o.f. (Q_1)
- temperature distribution



- discontinuous Dirichlet boundary condition

Mass balance for solute (concentration)

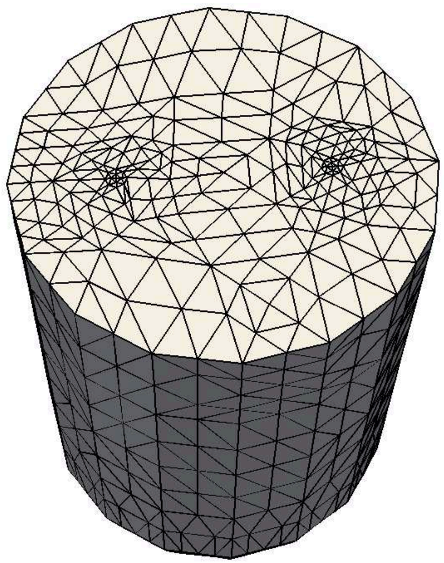
- convection–dominated convection–diffusion equation
- Crank–Nicolson linear FEM–FCT scheme
- about 22 500 d.o.f. (Q_1)
- not steady state
- concentration distribution

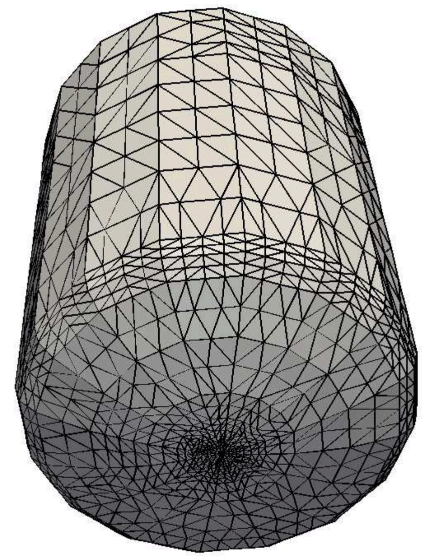
Population (particle size distribution)

- transport equation in 4D
- implemented schemes (test phase)
  - forward Euler upwind finite difference scheme
  - backward Euler upwind finite difference scheme
  - Crank–Nicolson linear FEM–FCT scheme
- discretization of internal coordinate: 17 nodes
- about 382 000 d.o.f.
- interface to computation of aggregation and breakage developed

A variational multiscale (VMS) method for turbulent flow simulations on tetrahedral meshes

- V.J., A. Kindl, C.S., J. Comp. Appl. Math., in press
- motivation
  - complicated geometry used in chemical engineering
  - no access to hexahedral grid generator
  - reactor with a torispherical head





  - grid with Tetgen

A VMS method for turbulent flow simulations on tetrahedral meshes

- properties of the VMS method
  - based on variational form of Navier–Stokes equations
  - separation of scale groups through projections into appropriate spaces
  - three scale separations
    - resolved large scales
    - resolved small scales
    - unresolved small scales – only influence on the resolved small scales modeled with a turbulence modell

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- realization of the VMS method
  - standard pair of conforming finite element spaces for all resolved scales $V^h \times Q^h$ fulfilling inf–sup stability condition
  - choose an additional space for the large scales L^H-finite dimensional space of symmetric tensor-valued functions in $L^2(\Omega)$
  - define the large scales as a projection into this space

A VMS method for turbulent flow simulations on tetrahedral meshes

- find $\mathbf{u}^h : [0, T] \to V^h$, $p^h : (0, T] \to Q^h$, and $\mathbb{G}^H : [0, T] \to L^H$ such that

$$
\begin{aligned}
(\mathbf{u}_t^h, \mathbf{v}^h) + (2\nu\mathbb{D}(\mathbf{u}^h), \mathbb{D}(\mathbf{v}^h)) + ((\mathbf{u}^h \cdot \nabla)\mathbf{u}^h, \mathbf{v}^h) & & \\
-(p^h, \nabla \cdot \mathbf{v}^h) + (\nu_T(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H), \mathbb{D}(\mathbf{v}^h)) &= (\mathbf{f}, \mathbf{v}^h), \ \forall \mathbf{v}^h \in V^h, \\
(q^h, \nabla \cdot \mathbf{u}^h) &= 0, \qquad \forall q^h \in Q^h, \\
(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H, \mathbb{L}^H) &= 0, \qquad \forall \mathbb{L}^H \in L^H.
\end{aligned}
$$

  - $\nu_T((\mathbf{u}^h, p^h), h) \geq 0$ – turbulent viscosity
  - $\mathbb{G}^H$ represents the large scales
  - $\nu_T(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H), \mathbb{D}(\mathbf{v}^h))$: viscous term acting directly only on the resolved small scales
  - $\mathbb{D}(\mathbf{v}) = (\nabla v + \nabla v^T)/2$
  - parameters: ν_T, L^H

A VMS method for turbulent flow simulations on tetrahedral meshes

- adaptive choice of the large scale space L^H
  - following V.J., Adela Kindl (2008, preprint)
  - different polynomial degrees on different mesh cells
  - a posteriori choice
- goal: method should determine local coarse space $L^H(K)$ a posteriori such that
  - $L^H(K)$ is a small space where flow is strongly turbulent
    $\Longleftrightarrow$ turbulence model has large influence
  - $L^H(K)$ is a large space where flow is less turbulent
    $\Longleftrightarrow$ turbulence model has little influence

A VMS method for turbulent flow simulations on tetrahedral meshes

- assumption: local turbulence intensity reflected by size of local resolved small scales
  - size of resolved small scales large $\Longrightarrow$ many unresolved scales can be expected
  - size of resolved small scales small $\Longrightarrow$ little unresolved scales can be expected

A VMS method for turbulent flow simulations on tetrahedral meshes

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  - size of resolved small scales large $\Longrightarrow$ many unresolved scales can be expected
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- define indicator of the size of the resolved small scales in mesh cell K

$$\eta_K = \frac{\|\mathbb{G}^H - \mathbb{D}(\mathbf{u}^h)\|_{L^2(K)}}{\|1\|_{L^2(K)}} = \frac{\|\mathbb{G}^H - \mathbb{D}(\mathbf{u}^h)\|_{L^2(K)}}{|K|^{1/2}}, \quad K \in \mathcal{T}^h$$

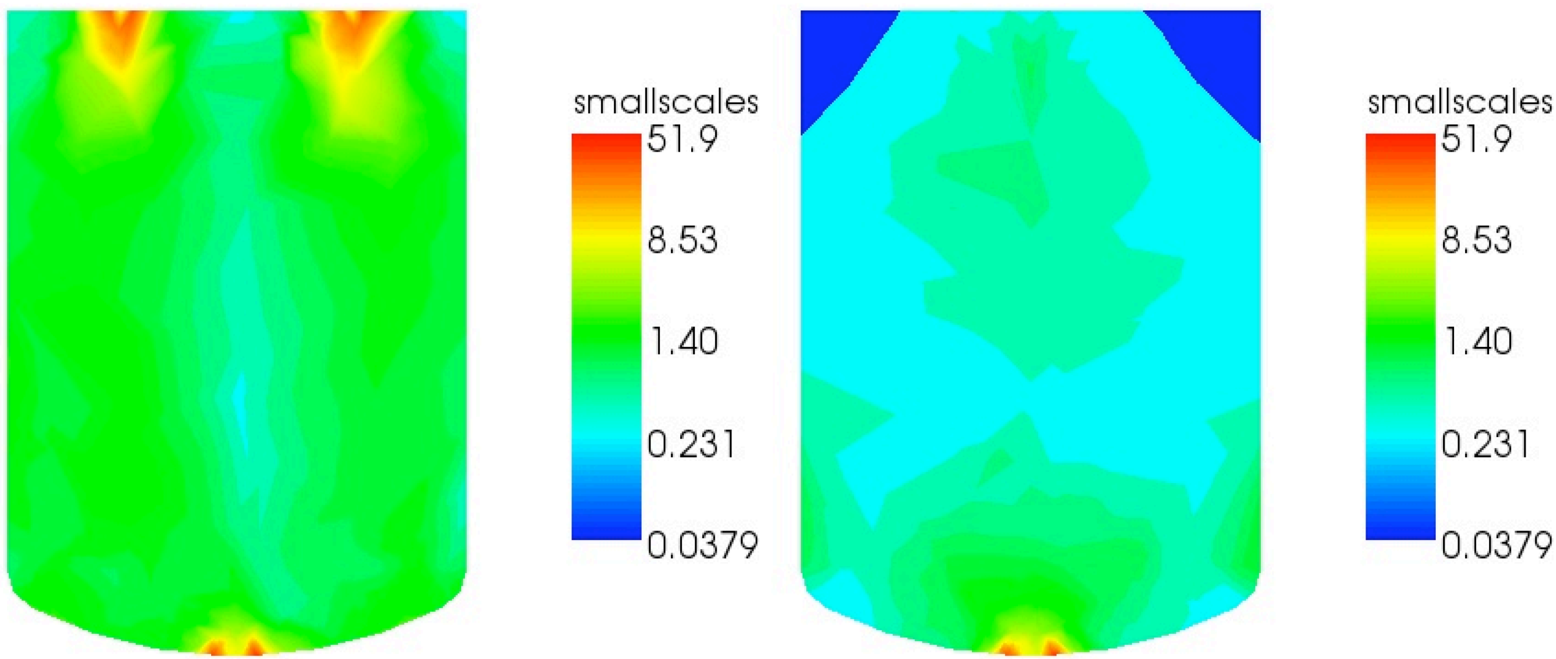
  - size of the resolved small scales does not depend on size of mesh cell
  - size of the mesh cell scales out
- compare η_K to some reference value
  - similar to a posteriori error estimation and mesh refinement

A VMS method for turbulent flow simulations on tetrahedral meshes

- numerical study
- Smagorinsky model

$$\nu_T = C_S \delta^2 \left\| \mathbb{D}\left(\mathbf{u}^h\right) \right\|_F$$

- indicator for local turbulence intensity
- cut along with inlets (left) and without inlets (right)



- most turbulence at inlets and outlet

Future goals and connection to other groups

- test methods for PSD equations
- further investigations of VMS method
- include aggregation and breakage of particles (AG Hackbusch)
- parallelization of the code (AG Tobiska)
- improved methods for convection–dominated problems, improved boundary conditions (AG Tobiska)
- compare with experimental results (AG Sundmacher)
- correct and extend the model and its parameters (AG Sundmacher)
- use results (flow fields) for POD and control problems (AG Kienle)