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On the numerical simulation of population balance systems

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Outline of the talk

1. Modeling of a bulk precipitation by a population balance system
2. Finite element methods for convection–dominated equations
3. Incompressible turbulent flows
4. A finite–element projection–based VMS method
5. Calcium carbonate precipitation in 2d/3d
6. Calcium carbonate precipitation in 3d/4d
7. Summary and outlook

1 Modeling of a bulk precipitation by a population balance system

- calcium carbonate precipitation
- chemical reaction in a flow

$$CaCl_2 + Na_2CO_3 \rightarrow CaCO_3 \downarrow + 2NaCl$$

- main feature: precipitation starts if local concentration of $CaCO_3$ exceeds saturation concentration
- chemical mechanisms:
  - nucleation of particles
  - growth of particles
- reactive flows with particles
- particle size distribution (PSD) is of interest, not the behavior of individual particles
- modeling with population balance systems

1 Momentum balance of the continuous phase

- momentum balance of the Navier–Stokes equations

$$\partial_t(\varrho\, v_m) + \partial_{r_k}\left(\varrho\, v_k v_m + \pi_{mk}\right) = \int_{\Omega_x} J^v_{im}(\phi, v) f_i dV_{\tilde{x}} + \varrho\, g_m$$

  - ϱ – density, v – velocity, π – stress tensor
  - accumulation
  - convection, diffusion
  - exchange with the disperse phase
  - body forces

- in applications: flows very often turbulent

1 Mass and energy balances of the continuous phase

- system of convection–diffusion–reaction equations

$$\partial_t(\varrho\,\phi_l) + \partial_{r_k}\left(\varrho\, v_k \phi_l + j^{\phi}_{lk}\right) = \int_{\Omega_x} J^{\phi}_{il}(\phi, v) f_i dV_{\tilde{x}} + \sigma_l(\phi)$$

  - ϕ_l – concentrations
  - accumulation
  - convection, diffusion
  - exchange with disperse phase
  - chemical reactions
- convection–dominant
- reaction–dominant

1 Population balances of the disperse phase

- disperse – distribute more or less evenly throughout a medium
- system of convection–diffusion equations

$$\partial_t f_i + \partial_{x_j}\left(G_{ij}(\phi, v) f_i\right) + \partial_{r_k}\left(v_k f_i + j_{ik}^f\right) = \int_{\Omega_x} h_{i,br}(f,\phi,v)\,dV_{\tilde{x}} + \int_{\Omega_x} h_{i,agg}(f,\phi,v)\,dV_{\tilde{x}}$$

  - accumulation
  - growth
  - convection, diffusion
  - breakage
  - agglomeration

- PSDs depend on time, space and properties of the particles (internal coordinates)

  equations are defined in a higher dimensional domain than the other equations

- convection–dominant, often even no diffusion
- global integral kernels on right hand side

1 Challenges

- simulation of reaction– and convection–dominated equations with the goal to obtain solutions with sharp layers and without spurious oscillations
- simulation of turbulent flows
- coupling of equations defined in domains with different dimension

2 Finite element methods for convection–dominated equations

- comparison of $\approx$ 20 stabilized finite element methods, J., Schmeyer (2008, 2009)
- talk by its own
- FEM–FCT schemes (Kuzmin (2005,2009)) clearly the best methods
- linear FEM–FCT scheme (Kuzmin (2009)) has good ratio of accuracy and costs

$\Longrightarrow$ method for population balance systems

3 Incompressible turbulent flows

- Navier–Stokes equations: fundamental equations of fluid dynamics
- Claude Louis Marie Henri Navier (1785 – 1836), George Gabriel Stokes (1819 – 1903)

3 The incompressible Navier–Stokes equations

- conservation laws
  - conservation of linear momentum
  - conservation of mass

$$
\begin{array}{rcll}
\mathbf{u}_t - 2Re^{-1}\nabla\cdot\mathbb{D}(\mathbf{u}) + \nabla\cdot(\mathbf{u}\mathbf{u}^T) + \nabla p & = & \mathbf{f} & \text{in } (0,T]\times\Omega \\
\nabla\cdot\mathbf{u} & = & 0 & \text{in } [0,T]\times\Omega \\
\mathbf{u}(0,\mathbf{x}) & = & \mathbf{u}_0 & \text{in } \Omega \\
\text{+ boundary conditions} & & &
\end{array}
$$

- given:
  - $\Omega \subset \mathbb{R}^d, d \in \{2,3\}$: domain
  - T: final time
  - $\mathbf{u}_0$: initial velocity
  - boundary conditions
- to compute:
  - velocity $\mathbf{u}$, where

    $$\mathbb{D}(\mathbf{u}) = \frac{\nabla\mathbf{u} + \nabla\mathbf{u}^T}{2},$$

    is the velocity deformation tensor
  - pressure p
- parameter: Reynolds number Re

3 The incompressible Navier–Stokes equations

- Reynolds number

$$Re = \frac{LU}{\nu}$$

  - L $[m]$ – characteristic length scale (diameter of a channel, diameter of a body in the flow)
  - U $[ms^{-1}]$ – characteristic velocity scale (inflow velocity)
  - ν $[m^2s^{-1}]$ – kinematic viscosity (water: $\nu = 10^{-6}\ m^2s^{-1}$)

- rough classification of flows:

  - Re small: steady–state flow field (if data do not depend on time)
  - Re larger: laminar time–dependent flow field
  - Re very large: turbulent flows

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- rough classification of flows:

  - Re small: steady–state flow field (if data do not depend on time)
  - Re larger: laminar time–dependent flow field
  - Re very large: turbulent flows

- There is no exact definition of what is a turbulent flow !

3 Characteristics of turbulent flows

- posses flow structures of very different size
  - hurricane Katrina (2005)

  - some large eddies (scales), many very small eddies (scales)

3 Characteristics of turbulent flows

- Richardson energy cascade: energy is transported in the mean from large to smaller eddies

  - start of cascade: kinetic energy introduced into flow by productive mechanisms at largest scale
  - inner cascade: transmitting energy to smaller and smaller scales by processes not depending on molecular viscosity
  - end of cascade: molecular viscosity enforcing dissipation of kinetic energy at smallest scales

- smallest scales important for physics of the flow

3 Characteristics of turbulent flows

- Kolmogorov (1941): energy is dissipated from eddies of size (Kolmogorov scale)

$$\lambda \sim Re^{-3/4}$$

Kolmogorov during a visit at the Akademie der Wissenschaften der DDR, mid of 1950-ies

3 Impact on numerical simulations

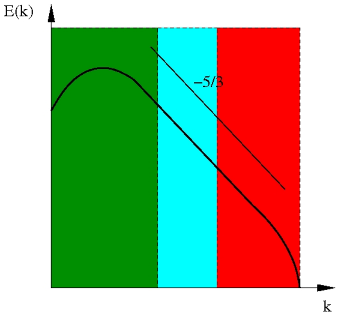
- Galerkin method aims to simulate all persisting eddies, Direct Numerical Simulation (DNS)
- number of degrees of freedom $\sim Re^{9/4}$
  - $\Omega = (0,1)^3 \implies L = 1$
  - approx 10^7 cubic mesh cells ($\approx 215^3$)
  - low order method (mesh width $\approx$ resolution of discretization)
  - $\implies \lambda \approx 1/215$
  - $\implies Re \approx 1290$
- applications: Reynolds numbers larger by orders of magnitude

Direct Numerical Simulation not feasible !

- only resolved scales can be simulated

3 The Kolmogorov energy spectrum

- energy of scales in wave number space (Fourier space)



- logarithmic axes
- resolved scales
  - large scales
  - resolved small scales
- unresolved scales, subgrid scales

- k – wave number
- $E(k)$ – turbulent kinetic energy of modes with wave number k
- $k^{-5/3}$ – law of energy spectrum: $E(k) \sim \epsilon^{2/3} k^{-5/3}$

3 Summary

- DNS impossible
- (very) small scales important, have to be taken into account
- 3d simulations necessary
- literature
  - P.A. Davidson, *Turbulence*, Oxford University Press, 2004
  - U. Frisch, *Turbulence*, Cambridge University Press, 1995
  - S.B. Pope, *Turbulent Flows*, Cambridge University Press, 2000

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Impact on numerical simulations

- only large scales of a turbulent flows possible to simulate, two approaches
  - Large Eddy Simulation (LES)
  - Variational Multiscale (VMS) methods
- impact of the small scales has to be modeled

4 A finite–element projection–based VMS method

- What is large ?
- (traditional) Large Eddy Simulation (LES): large flow structures defined by an average in space
  - two scale decomposition of scales:
    - large, resolved scales
    - small, unresolved, subgrid scales
  - based on strong formulation of equation
  - commutation errors
  - boundary conditions for large scales
  - references: Sagaut (2006), Berselli, Iliescu, Layton (2006), J. (2004)

4 A finite–element projection–based VMS method

- Variational Multiscale (VMS) methods: large flow structures defined by projections
  - based on ideas of Hughes (1995), Guermond (1999)
  - often three scale decomposition of scales:
    - resolved large scales
    - resolved small scales
    - small, unresolved, subgrid scales
  - based on variational formulation of equation
  - variety of realizations can be found in the literature

4 A finite–element projection–based VMS method

- J., Kaya (2005), based on ideas from Layton (2002)
- (V^h, Q^h) – conform velocity–pressure finite element spaces fulfilling the inf–sup condition for all resolved scales
- L^H – finite dimensional space of symmetric tensor–valued functions in $L^2(\Omega)^{d\times d}$ (large scale space)

4 A finite–element projection–based VMS method

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- (V^h, Q^h) – conform velocity–pressure finite element spaces fulfilling the inf–sup condition for all resolved scales
- L^H – finite dimensional space of symmetric tensor–valued functions in $L^2(\Omega)^{d\times d}$ (large scale space)
- find $\mathbf{u}^h : [0,T] \to V^h$, $p^h : (0,T] \to Q^h$, $\mathbb{G}^H : [0,T] \to L^H$:

$$
\begin{array}{rcll}
(\mathbf{u}_t^h, \mathbf{v}^h) + (2Re^{-1}\mathbb{D}(\mathbf{u}^h), \mathbb{D}(\mathbf{v}^h)) + ((\mathbf{u}^h \cdot \nabla)\mathbf{u}^h, \mathbf{v}^h) & & & \\
-(p^h, \nabla \cdot \mathbf{v}^h) + (\nu_T(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H), \mathbb{D}(\mathbf{v}^h)) & = & (\mathbf{f}, \mathbf{v}^h) & \forall\, \mathbf{v}^h \in V^h \\
(q^h, \nabla \cdot \mathbf{u}^h) & = & 0 & \forall\, q^h \in Q^h \\
(\mathbb{D}(\mathbf{u}^h) - \mathbb{G}^H, \mathbb{L}^H) & = & 0 & \forall\, \mathbb{L}^H \in L^H
\end{array}
$$

  $\nu_T(t, \mathbf{x}) \ge 0$ – turbulent viscosity, turbulence model
  $\mathbb{G}^H = P_{L^H}\mathbb{D}(\mathbf{u}^h)$ – L^2–projection
- nonlinear (in the viscosity) version of local projection stabilization (LPS) schemes for stabilizing convection–dominated equations

4 Properties

- three scale decomposition:
  - (resolved) large scales
  - resolved small scales
  - unresolved small scales
- turbulence model acts directly only on the resolved small scales modeling the influence of unresolved small scales
- indirect influence onto large scales by coupling of resolved small and large scales
- parameters of the VMS method
  - L^H
  - ν_T (Smagorinsky–type models)

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- parameters of the VMS method
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- finite element error analysis: J., Kaya (2008); J., Kaya, Kindl (2008)
- similar approach with finite volume methods by Gravemeier (2006)

4 How to choose the large scale space L^H ?

- standard bases for velocity–pressure finite element spaces
- here: L^H defined on the same grid:

$$
\begin{aligned}
L^H \quad = \quad \text{span} \Bigg\{ & \begin{pmatrix} l_j^H & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 0 & l_j^H & 0 \\ l_j^H & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 0 & 0 & l_j^H \\ 0 & 0 & 0 \\ l_j^H & 0 & 0 \end{pmatrix}, \\
& \begin{pmatrix} 0 & 0 & 0 \\ 0 & l_j^H & 0 \\ 0 & 0 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & l_j^H \\ 0 & l_j^H & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & l_j^H \end{pmatrix} \Bigg\}
\end{aligned}
$$

$j = 1, \ldots, n_L$

- two–level method (for convection–diffusion equations), J., Kaya, Layton (2006)

4 How to choose the large scale space L^H ?

- coupled system

$$
\begin{pmatrix}
A_{11} & A_{12} & A_{13} & B_1^T & \tilde{G}_{11} & \tilde{G}_{12} & \tilde{G}_{13} & 0 & 0 & 0 \\
A_{21} & A_{22} & A_{23} & B_2^T & 0 & \tilde{G}_{22} & 0 & \tilde{G}_{24} & \tilde{G}_{25} & 0 \\
A_{31} & A_{32} & A_{33} & B_3^T & 0 & 0 & \tilde{G}_{33} & 0 & \tilde{G}_{35} & \tilde{G}_{36} \\
B_1 & B_2 & B_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
G_{11} & 0 & 0 & 0 & M & 0 & 0 & 0 & 0 & 0 \\
G_{21} & G_{22} & 0 & 0 & 0 & \frac{M}{2} & 0 & 0 & 0 & 0 \\
G_{31} & 0 & G_{33} & 0 & 0 & 0 & \frac{M}{2} & 0 & 0 & 0 \\
0 & G_{42} & 0 & 0 & 0 & 0 & 0 & M & 0 & 0 \\
0 & G_{52} & G_{53} & 0 & 0 & 0 & 0 & 0 & \frac{M}{2} & 0 \\
0 & 0 & G_{63} & 0 & 0 & 0 & 0 & 0 & 0 & M
\end{pmatrix}
\begin{pmatrix}
u_1^h \\ u_2^h \\ u_3^h \\ p^h \\ g_{11}^H \\ g_{12}^H \\ g_{13}^H \\ g_{22}^H \\ g_{23}^H \\ g_{33}^H
\end{pmatrix}
=
\begin{pmatrix}
f_1^h \\ f_2^h \\ f_3^h \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{pmatrix}
$$

- 7 additional matrices

4 How to choose the large scale space L^H ?

- condensation

$$\begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13} & B_1^T \\ \tilde{A}_{21} & \tilde{A}_{22} & \tilde{A}_{23} & B_2^T \\ \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33} & B_3^T \\ B_1 & B_2 & B_3 & 0 \end{pmatrix} \begin{pmatrix} u_1^h \\ u_2^h \\ u_3^h \\ p^h \end{pmatrix} = \begin{pmatrix} f_1^h \\ f_2^h \\ f_3^h \\ 0 \end{pmatrix}$$

$$\begin{aligned} \tilde{A}_{11} &= A_{11} - \tilde{G}_{11} M^{-1} G_{11} - \frac{1}{2} \tilde{G}_{24} M^{-1} G_{42} - \frac{1}{2} \tilde{G}_{36} M^{-1} G_{63} \\ &\vdots \\ \tilde{A}_{33} &= A_{33} - \tilde{G}_{36} M^{-1} G_{63} - \frac{1}{2} \tilde{G}_{11} M^{-1} G_{11} - \frac{1}{2} \tilde{G}_{24} M^{-1} G_{42} \end{aligned}$$

- goal: sparsity pattern of $\tilde{A}_{\alpha\beta}$ same like $A_{\alpha\beta}$

4 How to choose the large scale space L^H ?

- conditions on L^H:
  - support of each basis function of L^H only one mesh cell
  - basis of L^H is L^2–orthogonal

  $\Longrightarrow$ discontinuous finite element spaces with bases of piecewise Legendre polynomials

- simulations found in the literature: J., Kaya (2005), J., Roland (2007), J., Kindl (2008)
  - $L^H(K) = P_0(K)$ for all mesh cells K
  - $L^H(K) = P_1^{\text{disc}}(K)$ for all mesh cells K

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  - $L^H(K) = P_1^{\mathrm{disc}}(K)$ for all mesh cells K

- 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

4 Adaptive large scale space

- 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
- compute the deformation tensor of the large scales G^H
    - computation is not necessary for static L^H
    - additional matrices to assemble in comparison to static L^H

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- compute the deformation tensor of the large scales G^H
  - computation is not necessary for static L^H
  - additional matrices to assemble in comparison to static L^H
- 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

4 Adaptive large scale space

- compare η_K to some reference value
  - similar to a posteriori error estimation and mesh refinement
- reference values
  - mean value at current time $\quad \overline{\eta} := \dfrac{1}{\text{no. of cells}} \displaystyle\sum_{K \in \mathcal{T}^h} \eta_K$
  - time average of mean values $\quad \overline{\eta}^t := \dfrac{1}{\text{no. of time steps}} \displaystyle\sum_{\text{time steps}} \overline{\eta}$
  - linear combination $\quad \overline{\eta}^{t/2} := \dfrac{\overline{\eta} + \overline{\eta}^t}{2}$

4 Adaptive large scale space

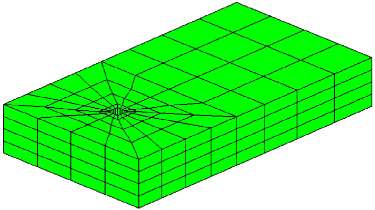
- local spaces ($V^h = Q_2$ or $V^h = P_2^{\text{bubble}}$)
  - $\mathbb{L}^H(K) = 0 = P_{00}(K)$ turbulence model influences locally all resolved scales
  - $\mathbb{L}^H(K) = P_0(K)$
  - $\mathbb{L}^H(K) = P_1(K)$
  - $\mathbb{L}^H(K) = P_2(K)$ set $\nu_T(K) = 0$, locally no turbulence model

4 Adaptive large scale space: procedure

- procedure:
  - choose three values
$$0 \le C_1 \le C_2 \le C_3$$
  - choose a mean value η
  - choose a frequency of updating the large scale space
$$n_{\text{update}}$$
  - in every n_{update}–th step:
    compute η_K and determine the local large scale space
$$\begin{array}{ll} L^H(K) = P_2^{\text{disc}}(K),\ \nu_T(K) = 0 & \text{if } \eta_K \le C_1\eta \\ L^H(K) = P_1^{\text{disc}}(K) & \text{if } C_1\eta < \eta_K \le C_2\eta \\ L^H(K) = P_0(K) & \text{if } C_2\eta < \eta_K \le C_3\eta \\ L^H(K) = P_{00}(K) & \text{if } C_3\eta < \eta_K \end{array}$$
- first VMS method with adaptive large scale space

4 Turbulent flow around a cylinder at $Re = 22000$

- domain and coarse grid



- vortex street (iso–surfaces of the velocity)
- statistically periodic flow
- $Re = 22000$ (mean inflow, diameter of cylinder, viscosity)

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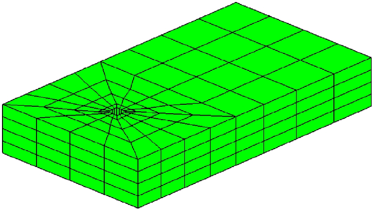

- vortex street (iso–surfaces of the velocity)
- statistically periodic flow
- $Re = 22000$ (mean inflow, diameter of cylinder, viscosity)
- Q_2/P_1^{disc}, no. of d.o.f.: 522 720 velocity, 81 920 pressure
- Crank–Nicolson scheme with $\Delta t = 0.005$
- static Smagorinsky model with van Driest damping for ν_T

$$\nu_T = 0.01(2h_{K,\min})^2 \|\mathbb{D}(\mathbf{u}^h)\|_F, \quad h_{K,\min} \text{ – shortest edge of } K$$

4 Turbulent flow around a cylinder at $Re = 22000$

- characteristic values of the flow
  - lift coefficient c_l, $\bar{c}_l$ – temporal mean, $c_{l,\mathrm{rms}}$ – root mean squared
  - drag coefficient c_d
  - Strouhal number St

4 Turbulent flow around a cylinder at $Re = 22000$

- characteristic values of the flow
  - lift coefficient c_l, $\bar{c}_l$ – temporal mean, $c_{l,\text{rms}}$ – root mean squared
  - drag coefficient c_d
  - Strouhal number St
- time–averaged values and rms values (30 periods)

C_1	C_2	C_3	mean	n_{update}	$\bar{c}_l$	$c_{l,\text{rms}}$	$\bar{c}_d$	$c_{d,\text{rms}}$	St
static large scale space									
VMS with $L^H = P_0$					-0.002	0.96	2.48	0.15	0.139
VMS with $L^H = P_1^{\text{disc}}$					-0.015	0.97	2.42	0.17	0.137
large–space–adaptive method: results not much different									
0.3	0.75	2	$\overline{\eta}$	1	-0.016	1.28	2.55	0.14	0.139
0.2	0.75	2	$\overline{\eta}$	10	-0.002	1.26	2.52	0.16	0.138
0.3	0.75	3	$\overline{\eta}$	1	-0.002	1.11	2.49	0.14	0.136
0.2	0.75	2	$\overline{\eta}^{t/2}$	1	-0.019	1.20	2.53	0.13	0.141
experimental results									
						0.7–1.4	1.9–2.1	0.1–0.2	0.132

4 Turbulent flow around a cylinder at $Re = 22000$

- over-prediction of $\bar{c}_d$ in all simulations
- all other values in reference intervals or close to reference value
- notable difference in $\bar{c}_l$ between static and adaptive large scale space
- good parameter choices similar to other flow problems
- large scale space (pictures for every 100-th time steps)

4 Summary and outlook for large scale adaptive VMS method

- more details: J., Kindl (2010)
- first VMS method with adaptive large scale space
- size of the resolved small scales is used to determine large scale space
- large–space–adaptive VMS method is able to adapt large scale space to local intensity of the turbulence
- method can be extended to tetrahedral meshes and $P_2^{\text{bubble}}/P_1^{\text{disc}}$ finite element (J., Kindl, Suciu (2009), in press)

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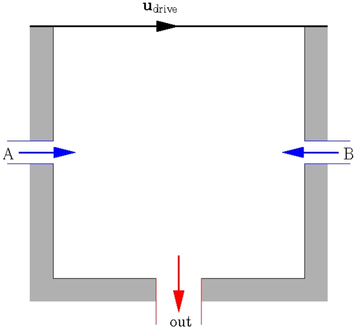
- method can be extended to tetrahedral meshes and $P_2^{\text{bubble}}/P_1^{\text{disc}}$ finite element (J., Kindl, Suciu (2009), in press)
- often results with respect to time–averaged references similar to method with fixed large scale space
- further studies of parameters of the method $(C_1, C_2, C_3, n_{\text{update}})$ necessary
- mathematical analysis for adaptive method not yet available

5 Calcium carbonate precipitation in 2d/3d

- J., Mitkova, Roland, Sundmacher, Tobiska, Voigt (2009); J., Roland (2010, in press)
- flow: 2d, incompressible, laminar
- chemical reaction: $CaCl_2 + Na_2CO_3 \rightarrow CaCO_3 \downarrow + 2NaCl$
- PSD: one internal coordinate (diameter of particles) $\Longrightarrow$ 3d



- chemical processes:
  - nucleation of particles
  - growth of particles
- no back coupling of PSD and concentrations to flow

5 Calcium carbonate precipitation in 2d/3d

- dimensionless population balance system

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} - \frac{1}{Re}\Delta \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{0} \quad \text{in } (0,T]\times\Omega \\
\nabla\cdot\mathbf{u} &= 0 \quad \text{in } [0,T]\times\Omega \\
\frac{\partial c_A}{\partial t} - \frac{D_A}{u_\infty l_\infty}\Delta c_A + \mathbf{u}\cdot\nabla c_A + k_R\frac{l_\infty c_\infty}{u_\infty} c_A c_B &= 0 \quad \text{in } (0,T]\times\Omega \\
\frac{\partial c_B}{\partial t} - \frac{D_B}{u_\infty l_\infty}\Delta c_B + \mathbf{u}\cdot\nabla c_B + k_R\frac{l_\infty c_\infty}{u_\infty} c_A c_B &= 0 \quad \text{in } (0,T]\times\Omega \\
\frac{\partial c_C}{\partial t} - \frac{D_C}{u_\infty l_\infty}\Delta c_C + \mathbf{u}\cdot\nabla c_C - \Lambda_{\text{chem}} c_A c_B & \\
+\Lambda_{\text{nuc}} \max\left\{0, (c_C - 1)^5\right\} & \\
+\left(c_C - \frac{c_{C,\infty}^{\text{sat}}}{c_{C,\infty}}\right)\int_{d_{\text{p,min}}}^1 d_p^2 f \, d(d_p) &= 0 \quad \text{in } (0,T]\times\Omega
\end{aligned}
$$

$$
\frac{\partial f}{\partial t} + \mathbf{u}\cdot\nabla f + k_G c_{C,\infty}\left(c_C - \frac{c_{C,\infty}^{\text{sat}}}{c_{C,\infty}}\right)\frac{l_\infty}{u_\infty d_{p,\infty}}\frac{\partial f}{\partial d_p} = 0 \quad \text{in } (0,T]\times\Omega\times(d_{\text{p,min}},1)
$$

A – $CaCl_2$
B – Na_2CO_3
C – $CaCO_3$

5 Calcium carbonate precipitation in 2d/3d

- discretization of Navier–Stokes equations
  - Crank–Nicolson scheme (fully implicit)
  - Galerkin FEM
  - Q_2/P_1^{disc} finite element, inf–sup stable
- discretization of convection–diffusion–reaction equations
  - Crank–Nicolson scheme
  - linear FEM–FCT
  - Q_1 finite element
  - explicit treatment of coupling terms with PSD

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  - explicit treatment of coupling terms with PSD
- solution of PSD equation expensive because of higher dimension

What happens if cheap methods are used?

- studied methods:
  - explicit Euler method with finite difference upwind stabilization
  - implicit Euler method with finite difference upwind stabilization
  - implicit linear FEM–FCT method

5 Coupling strategy

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- 3. solve equation for c_{CaCO_3}
  - use velocity field (step 1) and c_{CaCl_2}, $c_{Na_2CO_3}$ (step 2)
  - use PSD and c_{CaCO_3} from t_{k-1} in nucleation and in coupling term $\Longrightarrow$ linear equation

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  - use PSD and c_{CaCO_3} from t_{k-1} in nucleation and in coupling term $\Longrightarrow$ linear equation
- 4. solve equation for PSD f
  - use velocity field (step 1) and c_{CaCO_3} (step 3)

5 Calcium carbonate precipitation in 2d/3d

- volume fraction

$$q_3(t,\widetilde{d}_p) := \frac{\widetilde{d}_p^3 \widetilde{f}(t,\widetilde{d}_p)}{\int_{\widetilde{d}_{\mathrm{p},0}}^{\widetilde{d}_{\mathrm{p,max}}} \widetilde{d}_p^3 \widetilde{f}(t,\widetilde{d}_p)\; d(\widetilde{d}_p)}$$

$\widetilde{d}_p$ $[m]$ – diameter of particles,
$\widetilde{f}(t,\widetilde{d}_p)$ $[1/m^4]$ – PSD

- cumulative volume fraction

$$Q_3(t,\widetilde{d}_p) := \int_{\widetilde{d}_{\mathrm{p},0}}^{\widetilde{d}_{\mathrm{p}}} q_3(t,\widetilde{d}_p)\; d(\widetilde{d}_p)$$

- median of volume fraction

$$\widetilde{d}_{\mathrm{p},50}(t) := \{\widetilde{d}_p \;:\; Q_3(t,\widetilde{d}_p) = 0.5\}$$

5 Calcium carbonate precipitation in 2d/3d

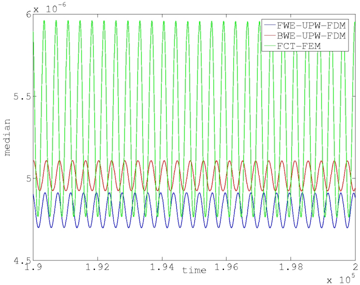
velocity	concentration $CaCl_2$
concentration Na_2CO_3	concentration $CaCO_3$

5 Calcium carbonate precipitation in 2d/3d

- structured flow field

5 Calcium carbonate precipitation in 2d/3d

- structured flow field
- median of the volume fraction at the center of the outlet



- temporal mean values (64 intervals for internal coordinate)

	$\Delta t = 0.005$	$\Delta t = 0.0025$	$\Delta t = 0.00125$
FWE–UPW–FDM	3.055e-6	5.235e-6	4.809e-6
BWE–UPW–FDM	4.030e-6	5.487e-6	5.020e-6
FEM–FCT	4.246e-6	4.672e-6	5.196e-6

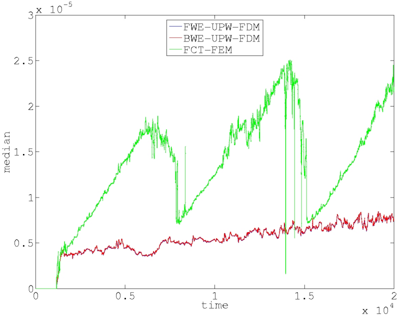
- iso surfaces of PSD (100, 1000, 10000, 10000 particles)

5 Calcium carbonate precipitation in 2d/3d

- unstructured flow field

5 Calcium carbonate precipitation in 2d/3d

- unstructured flow field
- median of volume fraction at center of outlet



- temporal mean values (64 intervals for internal coordinate)

	$\Delta t = 0.0025$	$\Delta t = 0.00125$	$\Delta t = 0.000625$
FWE–UPW–FDM	1.125e-5	6.227e-6	6.591e-6
BWE–UPW–FDM	1.207e-5	6.281e-6	6.621e-6
FEM–FCT	1.947e-5	1.358e-5	1.643e-5

5 Calcium carbonate precipitation in 2d/3d

- academic test example at coupled 2d/3d problem: FEM–FCT scheme more accurate than the other schemes
- conclusion:
  - accurate method for PSD equation necessary for turbulent flows, e.g. linear FEM–FCT scheme

5 Calcium carbonate precipitation in 2d/3d

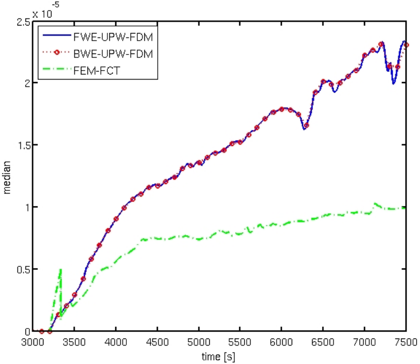
- academic test example at coupled 2d/3d problem: FEM–FCT scheme more accurate than the other schemes
- conclusion:
  - accurate method for PSD equation necessary for turbulent flows, e.g. linear FEM–FCT scheme
- drawback: computing time (per time step, in seconds), unstructured flow field

	$\Delta t = 0.0025$	$\Delta t = 0.00125$	$\Delta t = 0.000625$
FWE–UPW–FDM	3.68	1.64	2.20
BWE–UPW–FDM	5.11	3.11	3.37
FEM–FCT	8.19	6.21	6.39

  - bottle neck: matrix assembling
  - possible remedy: Group–FEM method, Fletcher (1983)

6 Calcium carbonate precipitation in 3d/4d

- setup simular to 2d/3d problem
- 3d/4d simulation, $Re = 10000$, turbulent flow
  - turbulence model: finite element variational multiscale (VMS) method
  - median of the volume fraction at the center of the outlet



- similar observations as in 2d/3d example with unstructured flow field

7 Summary and outlook

- accurate and non–oscillatory schemes necessary for discretizing all equations
  - FEM: alternatives to FEM–FCT? Discontinuous Galerkin methods?
  - developing good schemes for simulating turbulent flow fields
- increasing the efficiency of the simulations
  - parallelization of the code
  - adaptive time stepping schemes
- current topics in the numerical simulation of population balance systems:
  - precipitations in 3d/4d
  - simulation of turbulent flows with droplets (clouds), E. Schmeyer
  - simulation of the synthesis of urea, C. Suciu

http://www.wias-berlin.de/people/john/