SimParTurS – work report 2009–01–12

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Contents

1. Precipitation process modeled by population balance systems

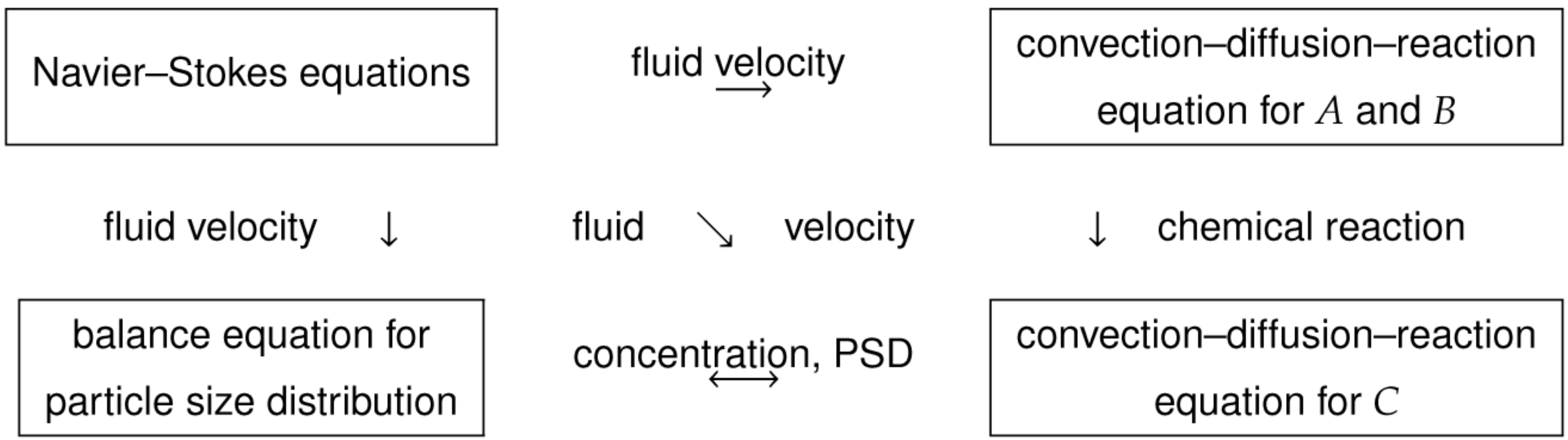
- chemical reaction in a flow

$$A + B \to C \downarrow + D$$

- precipitation starts if local concentration of C exceeds saturation concentration
- chemical mechanisms:
  - nucleation
  - growth of particles
- flows with particles
- particles size distribution (PSD) is of interest, not the behavior of the individual particles

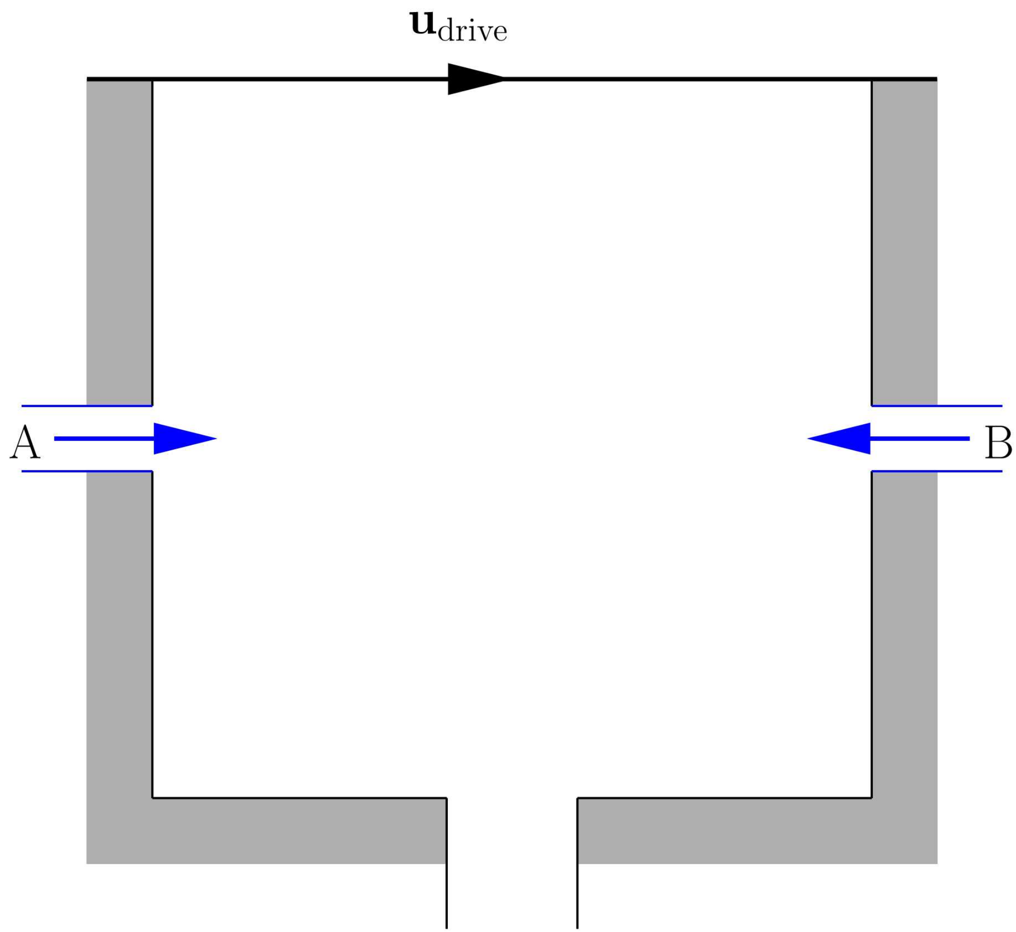
1. Precipitation process modeled by population balance systems

- Population balance system
  - coupled system



2. Further Studies of Bulk Precipitations in 2d/3d

- chemical reaction: $CaCl_2 + Na_2CO_3 \to CaCO_3 \downarrow +2NaCl$
- domain in 2D



2. Further Studies of Bulk Precipitations in 2d/3d

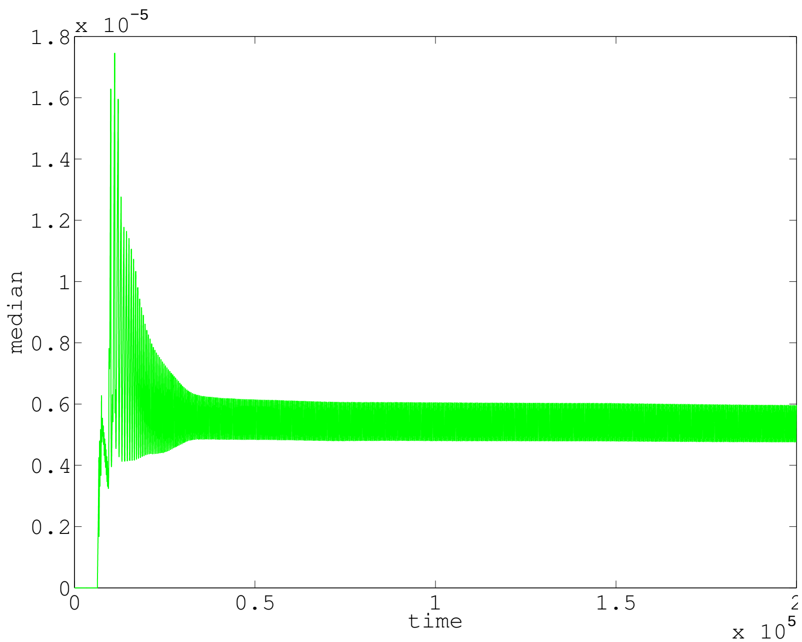
Discretisation and Simulation

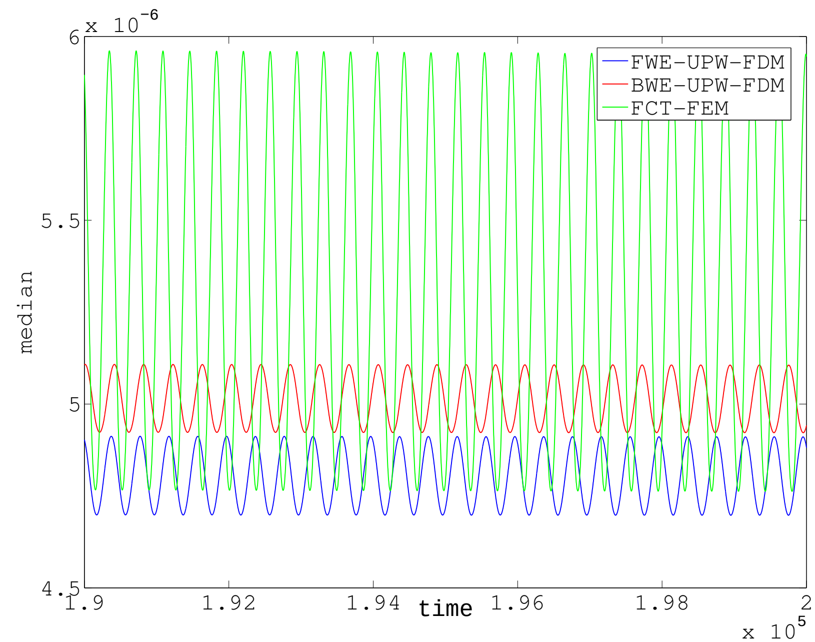
- Navier-Stokes equations
  - Crank-Nicolson scheme
  - Galerkin finite element method (Q_2/P_1^{disc})
- convection-diffusion-reaction equations
  - Crank-Nicolson scheme
  - exchange term with disperse phase is treated explicitly
  - (linear) finite element-method flux corrected transport (FEM-FCT)
  - Kuzmin, Möller, Turek (2004), Kuzmin, Möller (2005), Kuzmin (2008)
- population balance of the disperse phase
  - (linear) FEM-FCT scheme with Q_1 Galerkin finite element method
  - forward Euler/upwind finite difference method
  - backward Euler/upwind finite difference method

2. Further Studies of Bulk Precipitations in 2d/3d

Studies with Re=1000 (structured flow field)

- simulation of precipitation process
- simulation of particle size distribution
- different methods for PSD for $\Delta t = 0.00125$, median of the volume fraction



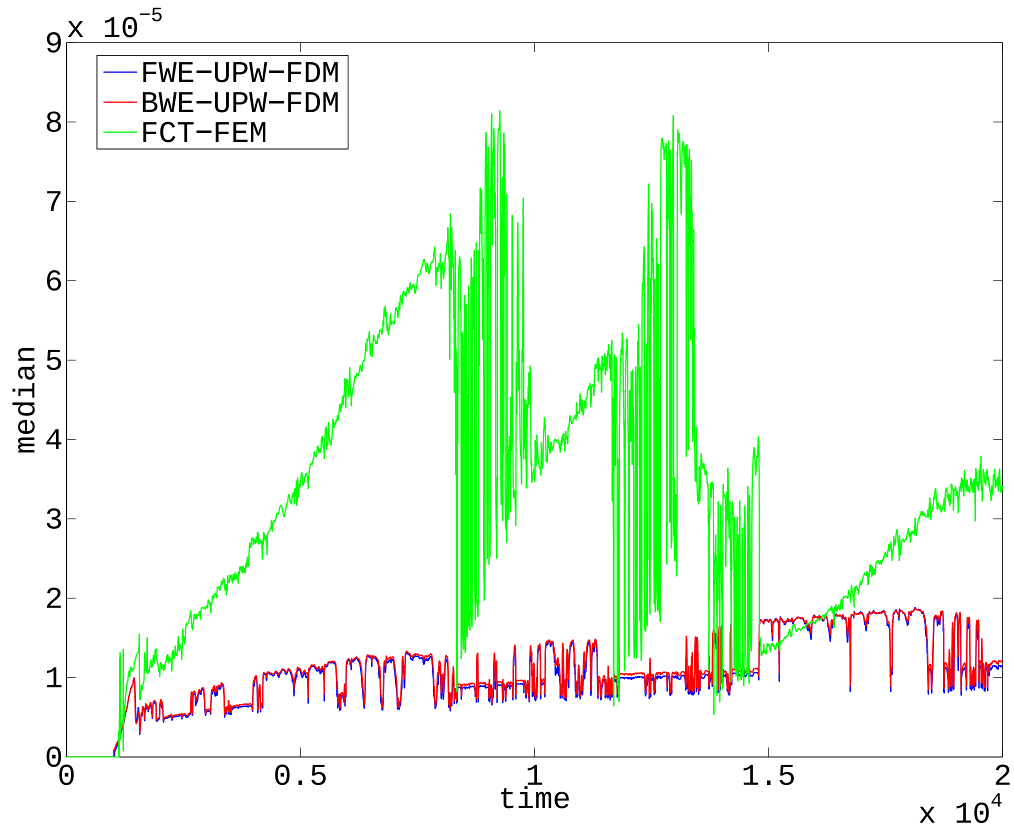


For small changes in time all methods were qualitatively the same.

2. Further Studies of Bulk Precipitations in 2d/3d

Studies with Re=10.000 (highly time–dependent flow field)

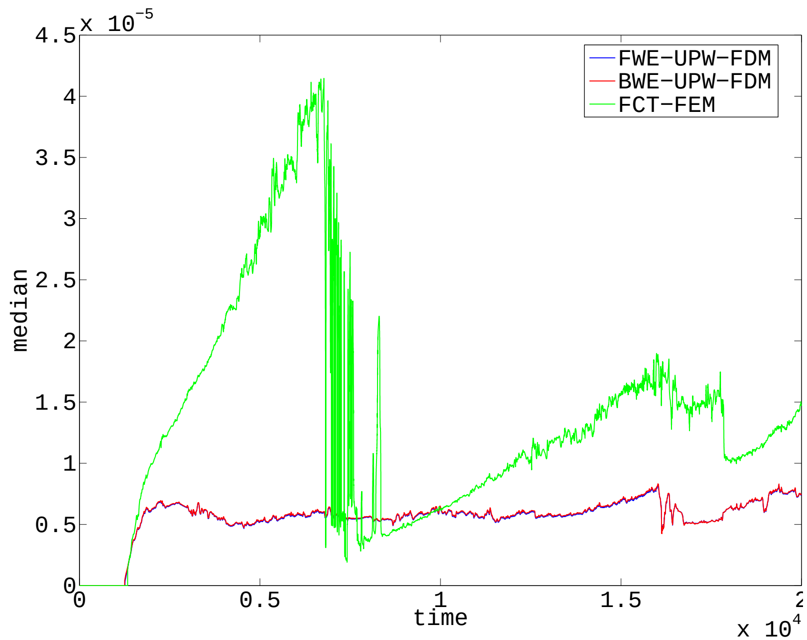
- simulation of precipitation process
- different methods for PSD, median of the volume fraction



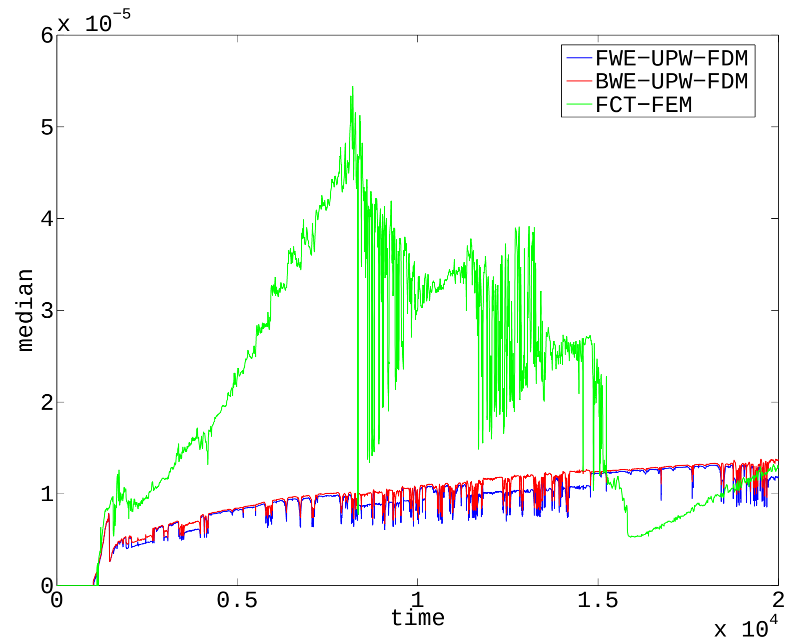
$\Delta t = 0.0025$, number of layers w.r.t. internal coordinate $L = 32$

2. Further Studies of Bulk Precipitations in 2d/3d

Studies with Re=10.000



$\Delta t = 0.0025,\ L = 64$



$\Delta t = 0.000625,\ L = 64$

- both Euler methods are very similar
- the results of the Crank-Nicolson FEM-FCT scheme are qualitatively different to the first order results

2. Further Studies of Bulk Precipitations in 2d/3d

- Crank-Nicolson FEM-FCT scheme known to be accurate for highly convection-dominated problems; John, Schmeyer (2008)

Crank-Nicolson FEM-FCT scheme should be used
for highly time-dependent processes

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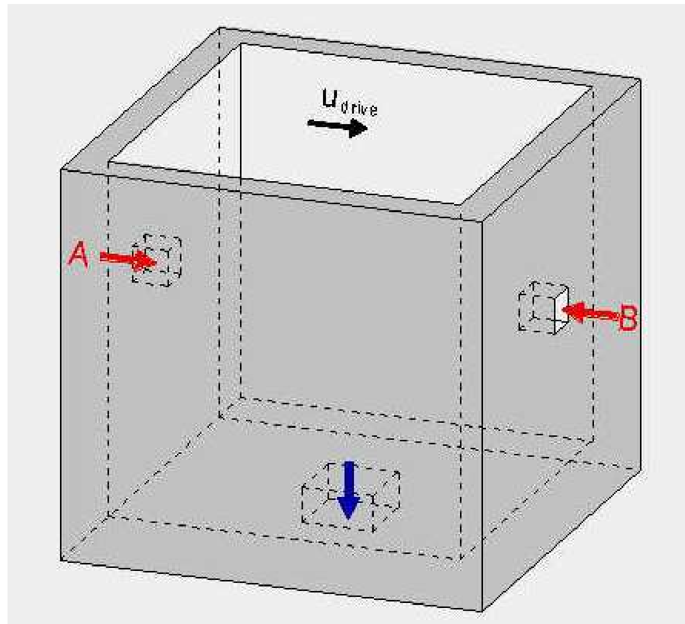
- typical computing times per time step, in seconds ($\Delta t = 0.000625$)

	$L = 32$	$L = 48$	$L = 64$
FWE–UPW–FDM	2.08	2.12	2.20
BWE–UPW–FDM	2.79	3.10	3.37
FEM–FCT	4.35	5.37	6.39

  - FEM–FCT by far the most time-consuming method
  - costs increase with refinement in property space
  - most important bottle neck: matrix assembling
- more details: John, Roland (2008), Preprint

3. First Simulations in 3d/4d

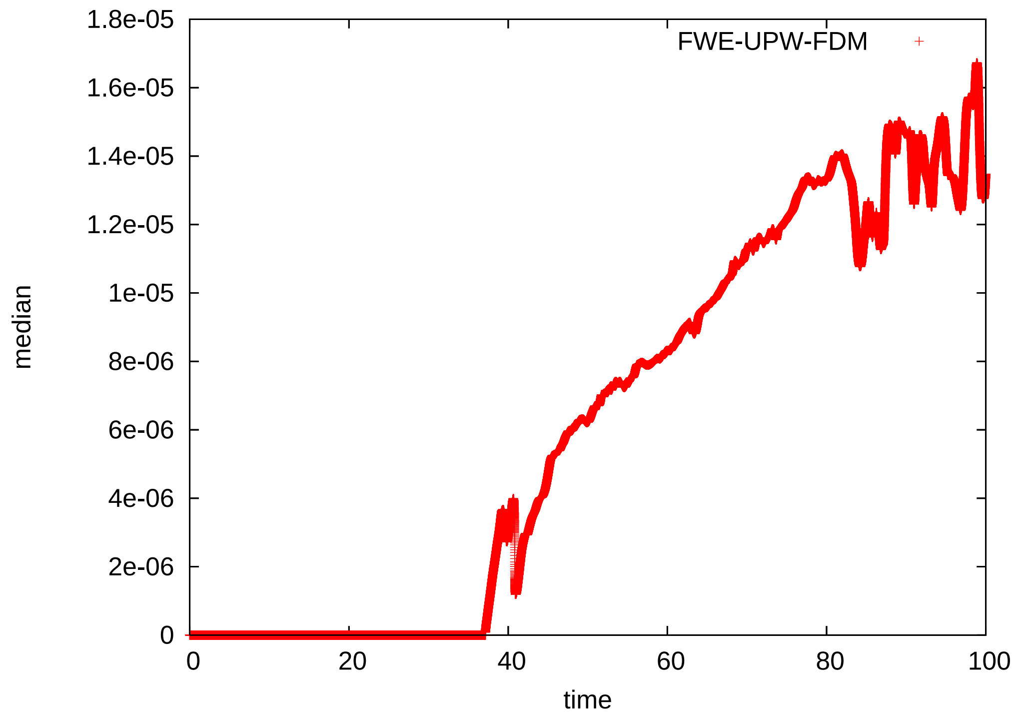
- domain in 3d



- Re=10.000 $\Longrightarrow$ turbulent flow
  - turbulence model: projection–based Variational Multiscale Methods (VMS) with P_0, John, Kaya (2005)

3. First Simulations in 3d/4d

- simulation with FWE–UPW–FDM for population balance equation
  - $\Delta t = 0.001$, $L = 16$
  - simulation of precipitation process ($Re = 10.000$)
  - median of the volume fraction



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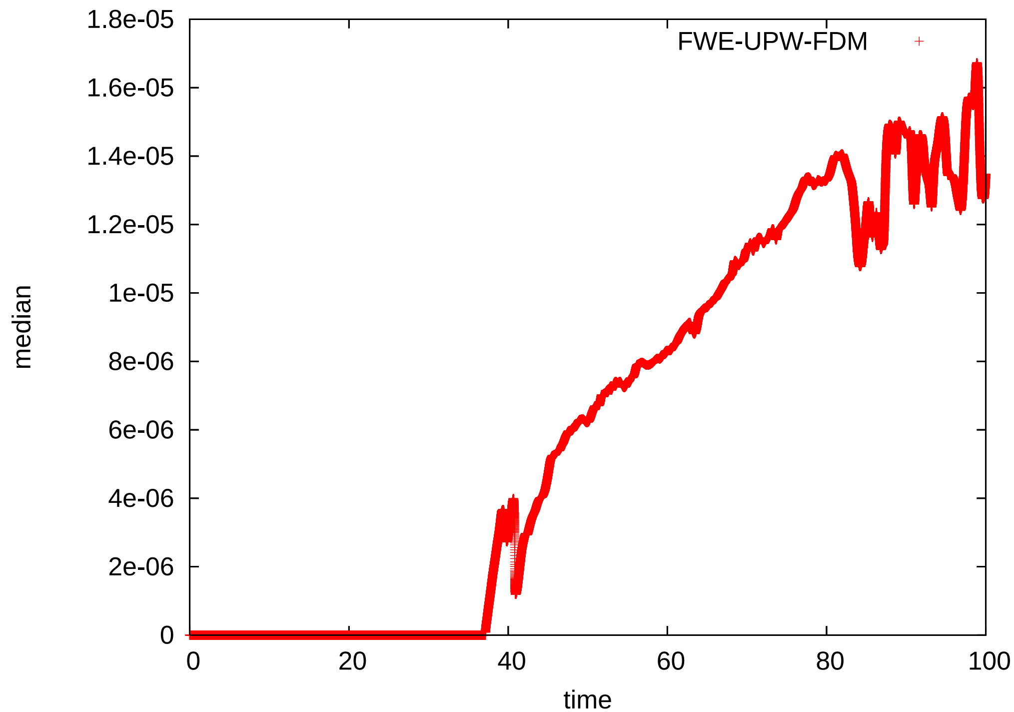


- simulation with FEM–FCT for population balance equation
  - started, simulation time will be of the order of months

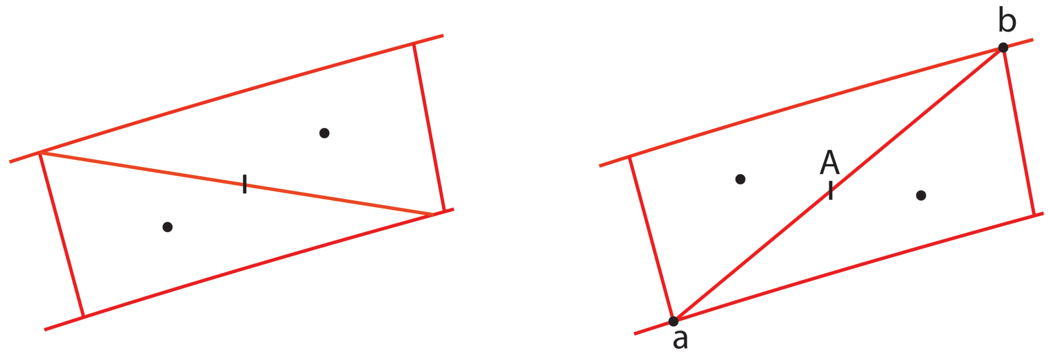
Further studies require parallelization of the code !!!

3. First Simulations in 3d/4d

- next goals for precipitation simulations:
  - implementation of an improved linear FEM-FCT method, Kuzmin (2009)
  - implementation of an approximation in the matrix assembling which reduces the costs, Kuzmin, Möller (2005)
  - interface to software for integral terms, MPI Leipzig

4. Shear Slip Mesh Update Method (SSMUM) in 2d

- principle: switching of edges in the shear slip layer



- difficulty: interpolation of velocity after change of grid

- pressure with linear interpolation (version from October)
  - spurious oscillations clearly visible
- pressure with enforced discretely divergence free interpolation
  - no spurious oscillations

- next (long term) goal: implementation of SSMUM for simplified 3D example (present 2D example with extension in third direction)