



Upscaling of Porous Media Flow with DuMu^x and dune-multidomaingrid

Bernd Flemisch, Markus Wolff

Dune User Meeting, 6.-8.10.10, Stuttgart



Outline

- DuMu^x
- Tensorial Permeabilities
- Upscaling Concept
- Implementation Concept
- Summary



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DuMu^x

Duⁿe for Mu^lti-{phase, component, scale, physics, ...} Flow in Porous Media

Used / developed by:

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- Melanie Darcis
- Karin Erbertseder
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- Andreas Lauser
- Klaus Mosthaf
- Philipp Nuske
- Sergey Oladyshkin
- Nicolas Schwenck
- Alex Tatomir
- Lena Walter
- Markus Wolff

- Yufei Cao
- Marc Schlienger

- Leopold Stadler



dumux.org

- **1/2007**: started
- **~4300**: svn revision
- **~50,000** lines (stable)
- **1.7.09**: release 1.0
- soon: next release



Coupled Fully Implicit Models

- **Implicit** Euler time discretization
- Vertex centered FV (**box**) space discretization
- **Newton** method
- **Models:**
 - One phase: 1p, 1p2c
 - Two phases: 2p, 2pni, 2p2c, 2p2cni, (2p3c, 2pia, 2p2cia)
 - (MpNc)
 - (Double continuum, MINC, DFN)
 - (Richards equation)



Decoupled Semi-implicit Models

- **Standard** and **phase pressure** fractional flow formulation
- Twophase(-**twocomponent-nonisothermal**), (3p3c in progress)
- (**Multiscale** approaches for pressure and transport equations)
- (**Multiphysics** approaches like 2p2c – 1p2c coupling)
- **Transport** equation:
 - Cell centered FV, implicit and explicit
 - Vertex centered FV, implicit
 - (Characteristic method)
 - (Operator splitting framework)
- **Pressure** equation:
 - Cell centered FV (with MPFA (2D))
 - Mimetic FD (2D)
 - (P1 FE with post-processed conservative fluxes)



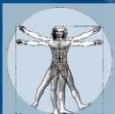
(Other Models and Capabilities)

- Parker-Lenhard type **hysteresis**
- **Brinkman** equation: coupling (single-phase) free flow with porous media flow
- **Coupling of free flow and porous media flow:**
 - Use of dune-multidomain
 - 2c free flow and 2p2c porous media flow
- **Matrix deformation:**
 - linear elasticity model implemented
 - Coupling to flow via dune-multidomain
- **Fractured media:**
 - Nonmatching (d-1) and d-dimensional grids
 - X-FEM approach using dune-multidomain

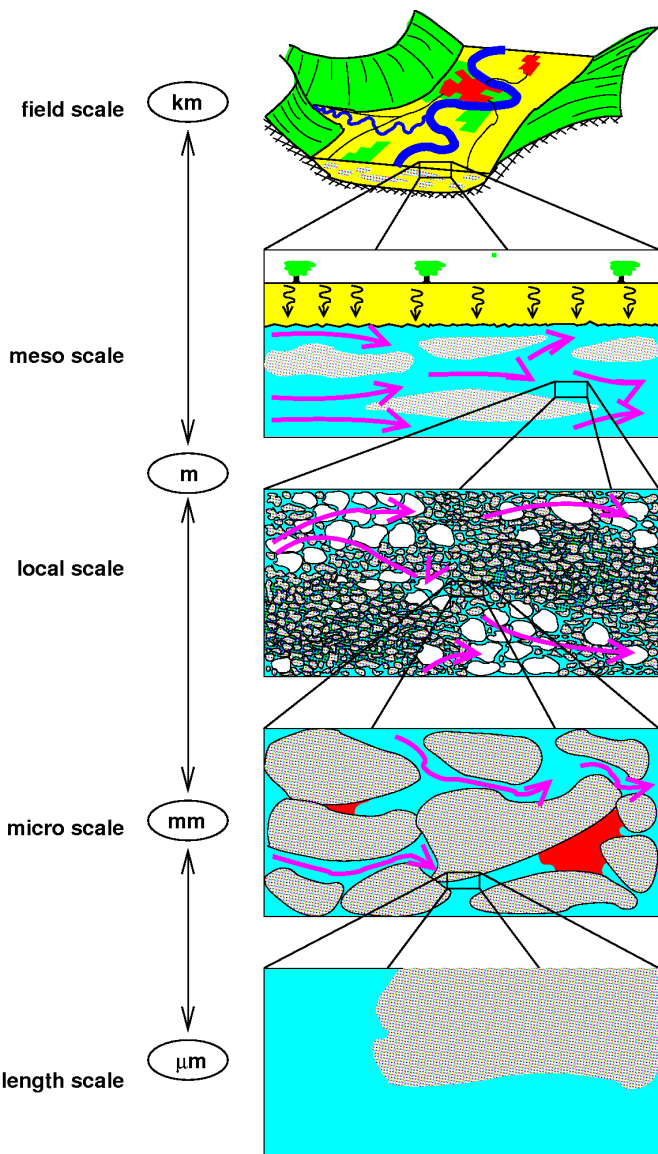


Outline

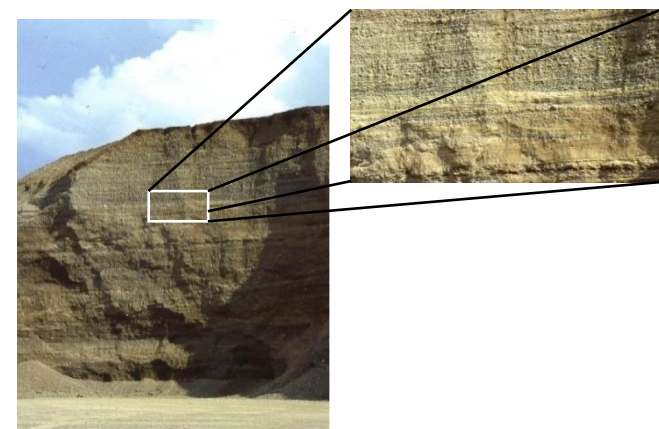
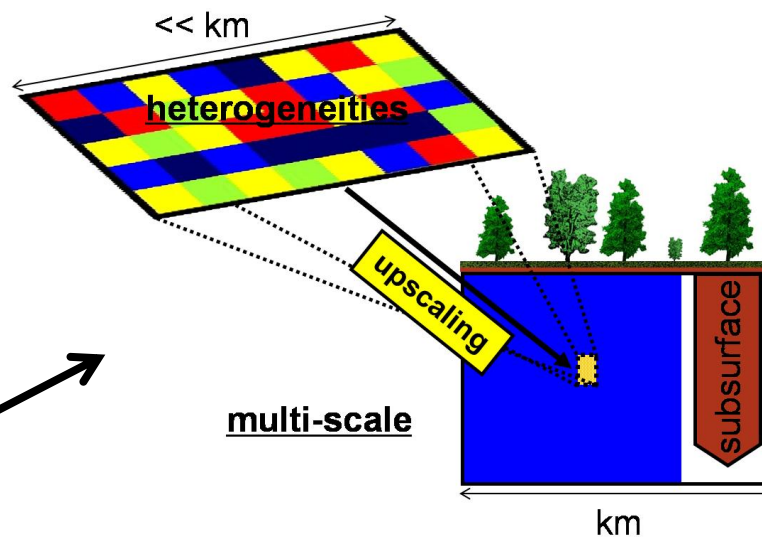
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Scales



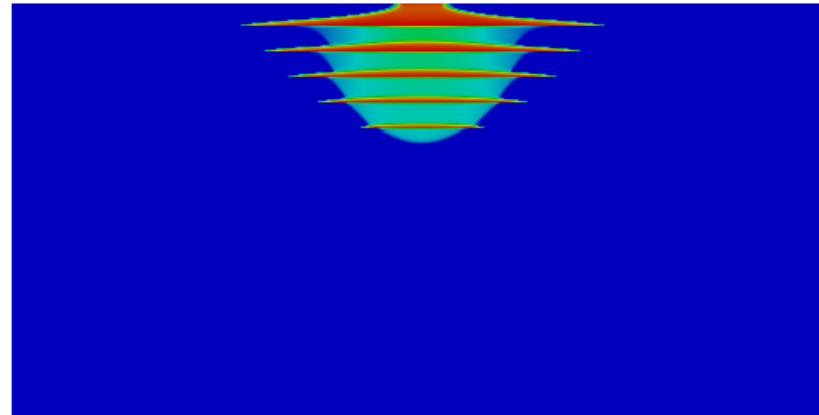
(Helmig)



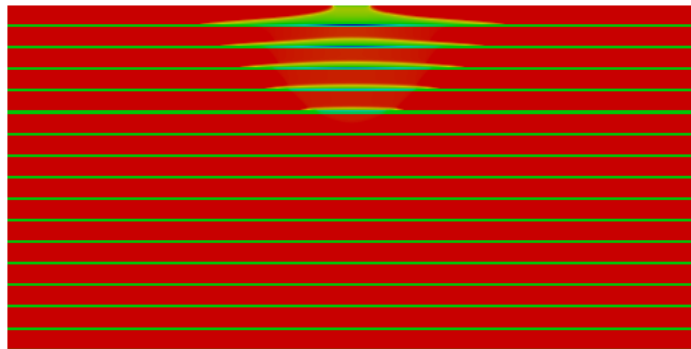
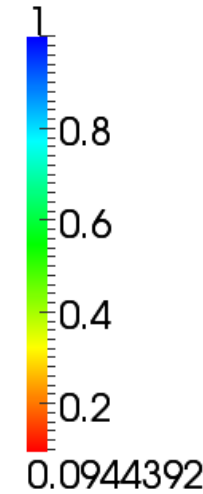


Necessity of coarse-scale full tensor coefficients

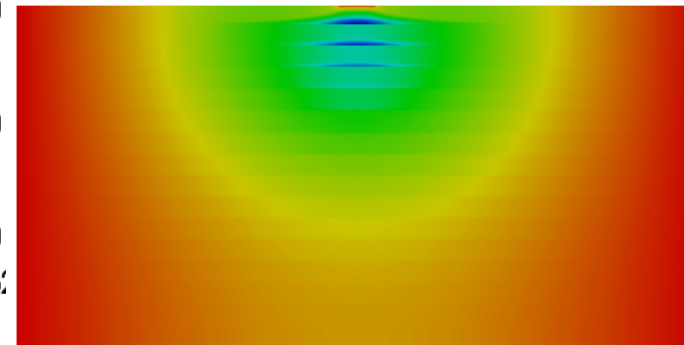
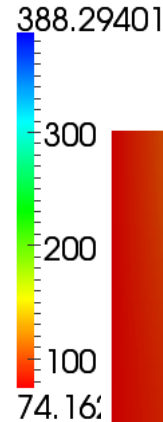
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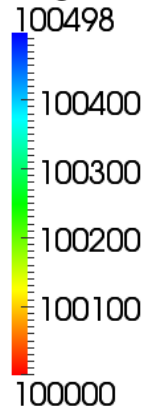
wetting saturation



capillary pressure



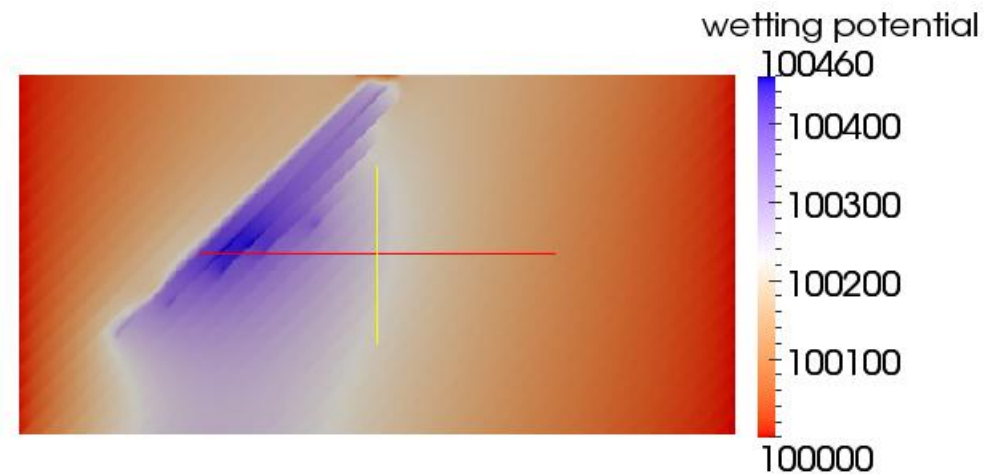
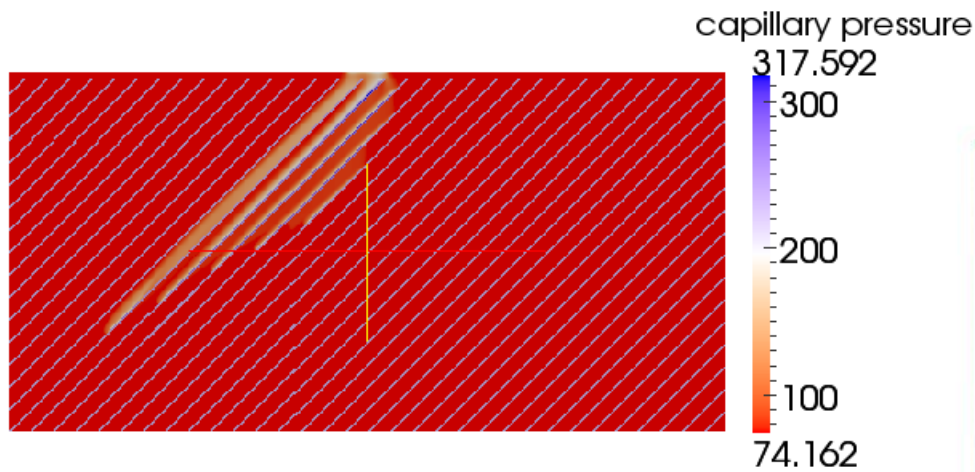
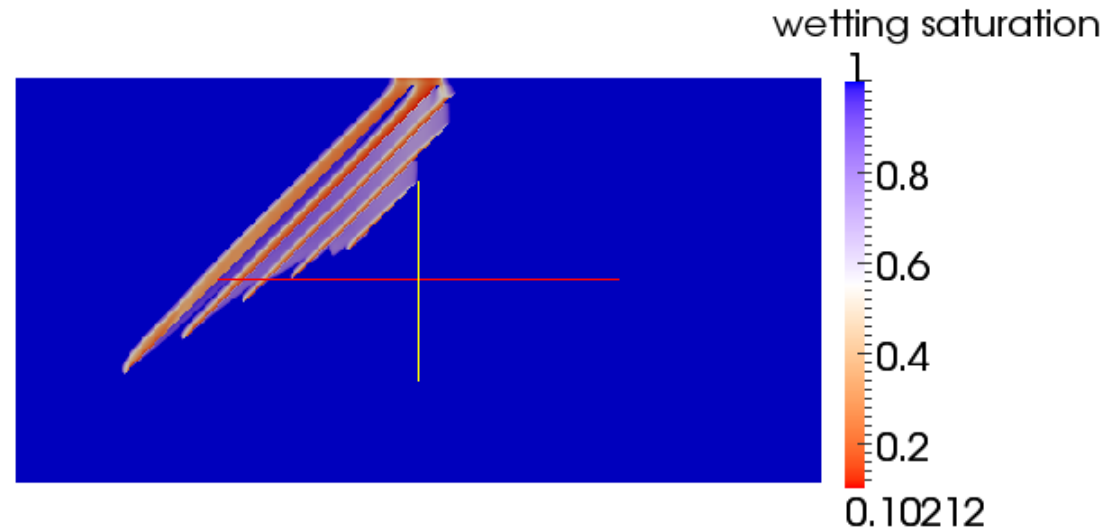
wetting potential





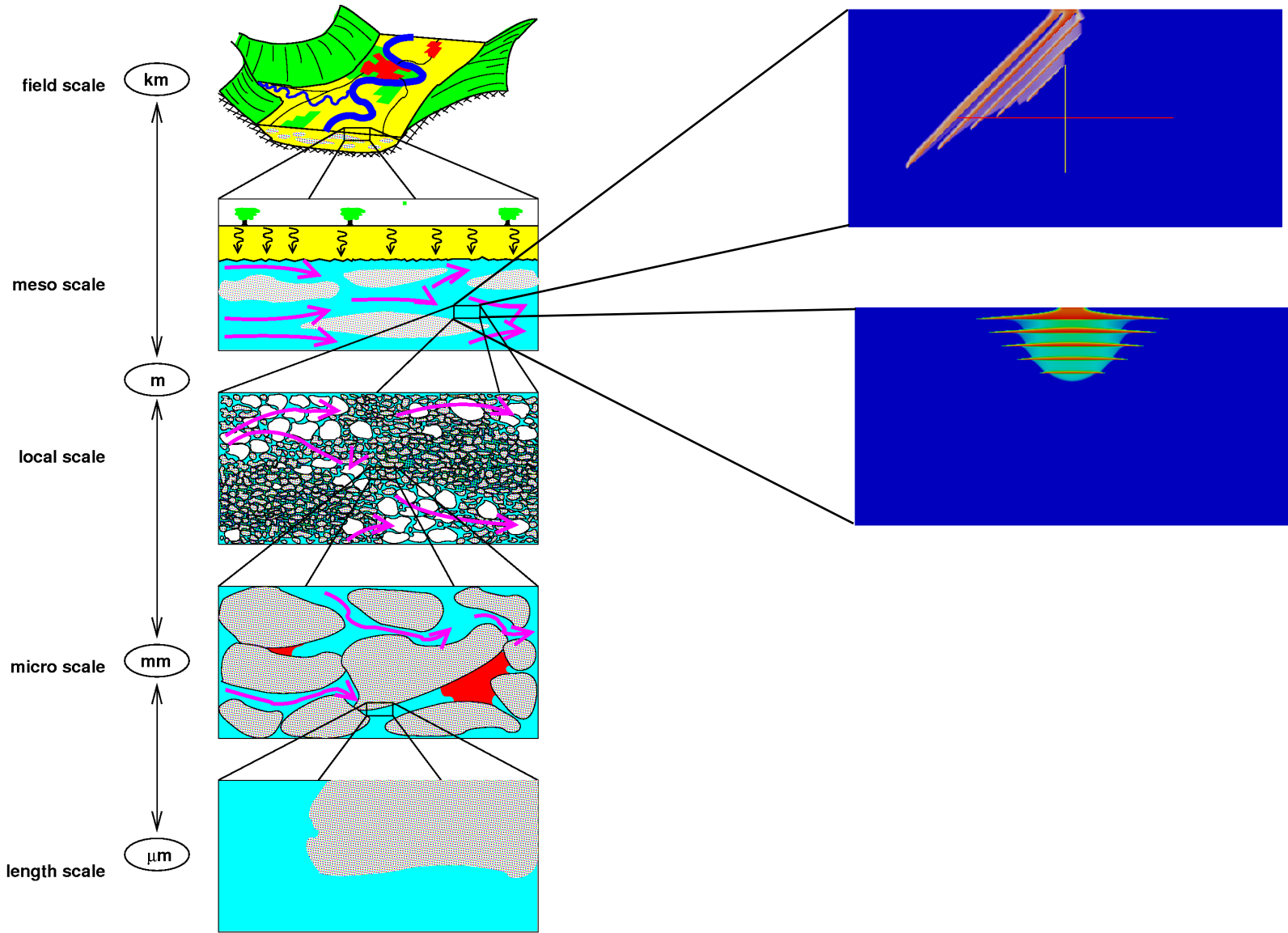
Necessity of coarse-scale full tensor coefficients

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Necessity of coarse-scale full tensor coefficients



(Helmig)



Upscaled Equations

■ Averaged equations

$$\frac{\partial(\phi^* S_w^*)}{\partial t} + \nabla \cdot \langle \mathbf{v}_w \rangle = 0$$

$$\langle \mathbf{v}_w \rangle = -\frac{\mathbf{K}^* \mathbf{K}_{r_w}^*}{\mu_w} \cdot [\nabla \langle p_w \rangle_w - \rho_w g \nabla z]$$

$$\frac{\partial(\phi^* S_n^*)}{\partial t} + \nabla \cdot \langle \mathbf{v}_n \rangle = 0$$

$$\langle \mathbf{v}_n \rangle = -\frac{\mathbf{K}^* \mathbf{K}_{r_n}^*}{\mu_n} \cdot [\nabla \langle p_n \rangle_n - \rho_n g \nabla z]$$

$$S_n^* = \frac{V_{n_{\text{mobile}}}}{V_{\text{pores}} - V_{\text{immobile}}}$$

$$S_w^* = \frac{V_{w_{\text{mobile}}}}{V_{\text{pores}} - V_{\text{immobile}}}$$

$$p_c^* = \langle p_n \rangle_n - \langle p_w \rangle_w$$

$$S_w^* + S_n^* = 1$$

$$\langle \Psi_\alpha \rangle_\alpha = \frac{1}{V_\alpha} \int_{V_\alpha} \Psi_\alpha dV$$



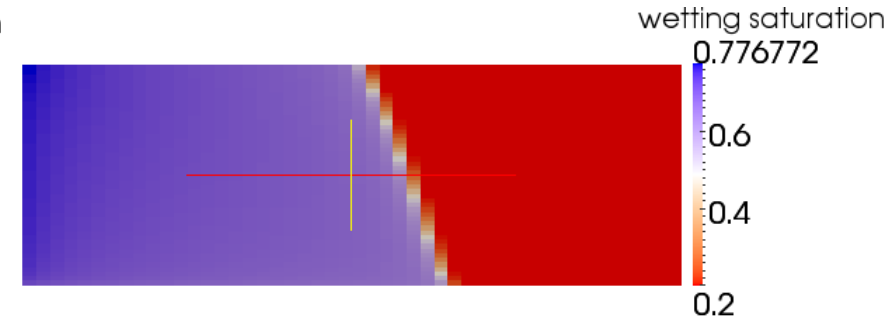
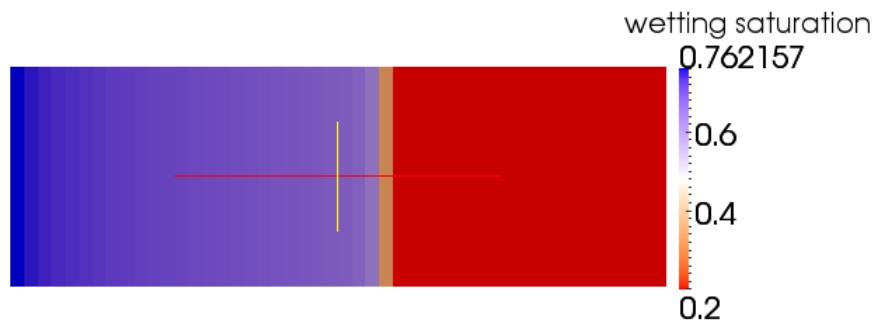
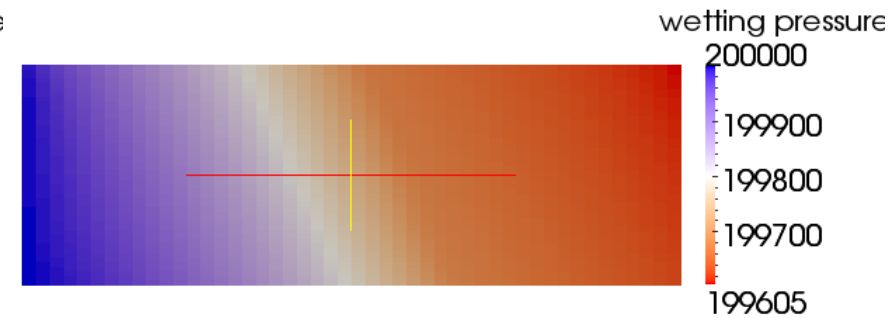
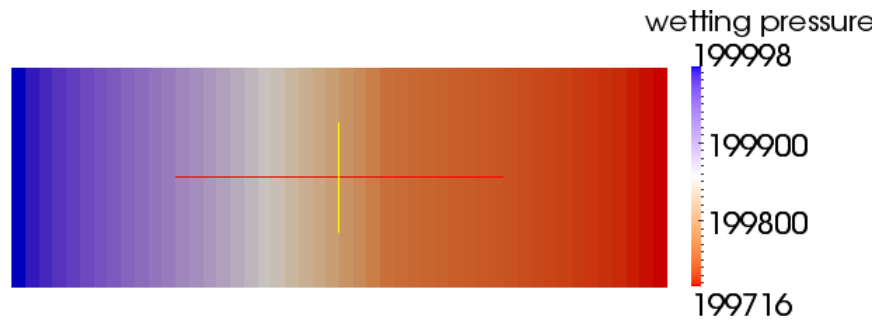
Choice of Discretization

- Discretization must be able to treat the tensor coefficients!



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Choice of Discretization

- Discretization must be able to treat the tensor coefficients!
 - Two-Point Flux Approximation (TPFA) NOT sufficient!



Choice of Discretization

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 - Two-Point Flux Approximation (TPFA) NOT sufficient!
 - ➔ Standard finite volume methods cannot be used



Choice of Discretization

- Discretization must be able to treat the tensor coefficients!
 - Two-Point Flux Approximation (TPFA) NOT sufficient!
 - ➔ Standard finite volume methods cannot be used
 - Alternatives:
 - Mixed finite elements
 - Mimetic finite differences
 - **Multi-Point-Flux-Approximation (MPFA)**

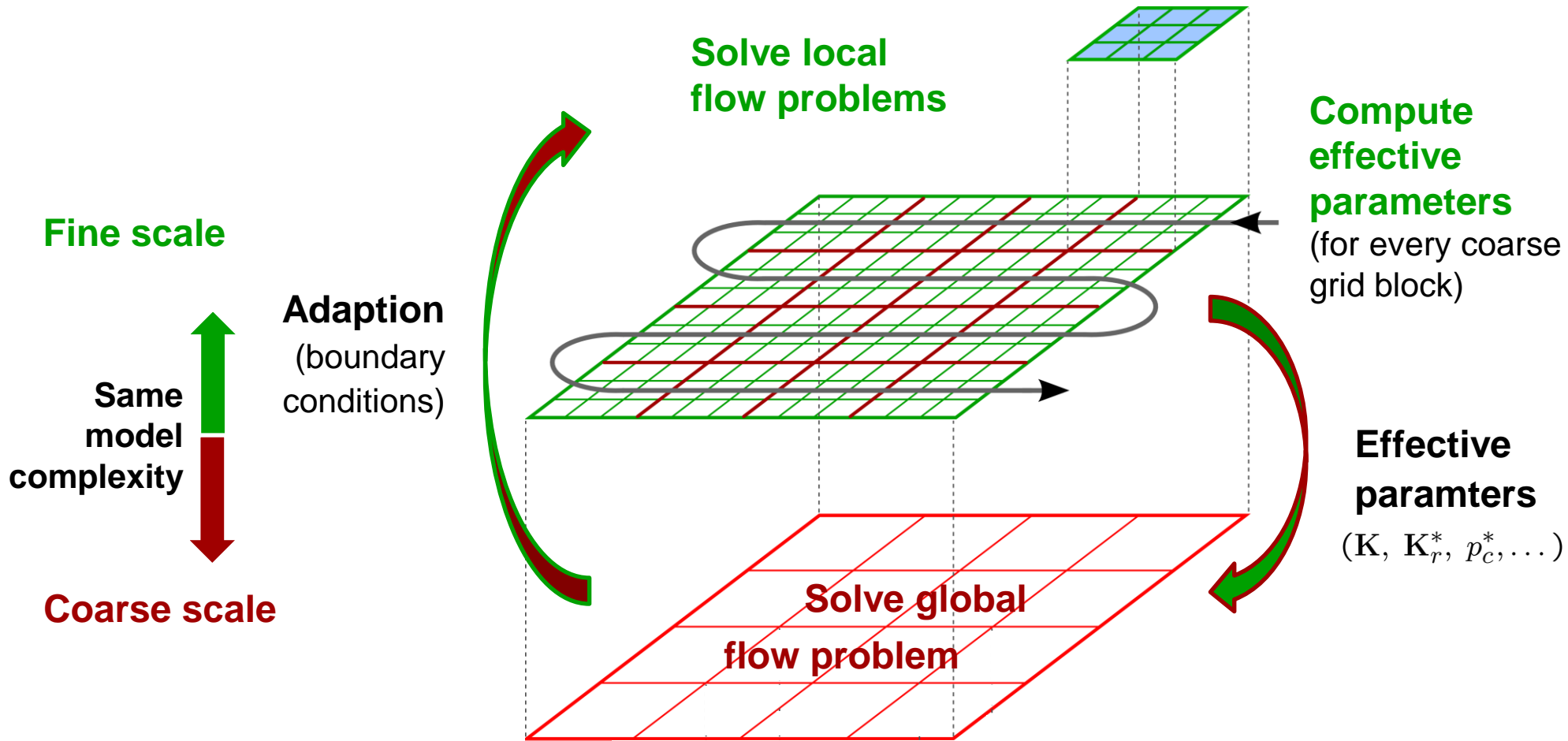


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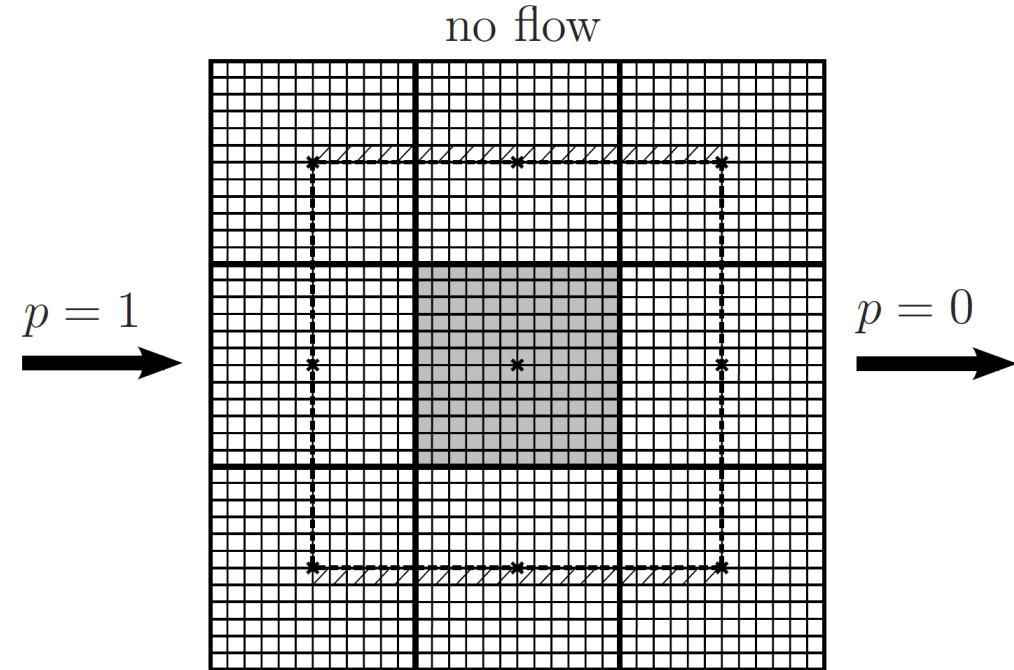
Upscaling Concept





Intrinsic permeability upscaling

- X. H. Wen, L. J. Durlofsky, 2003



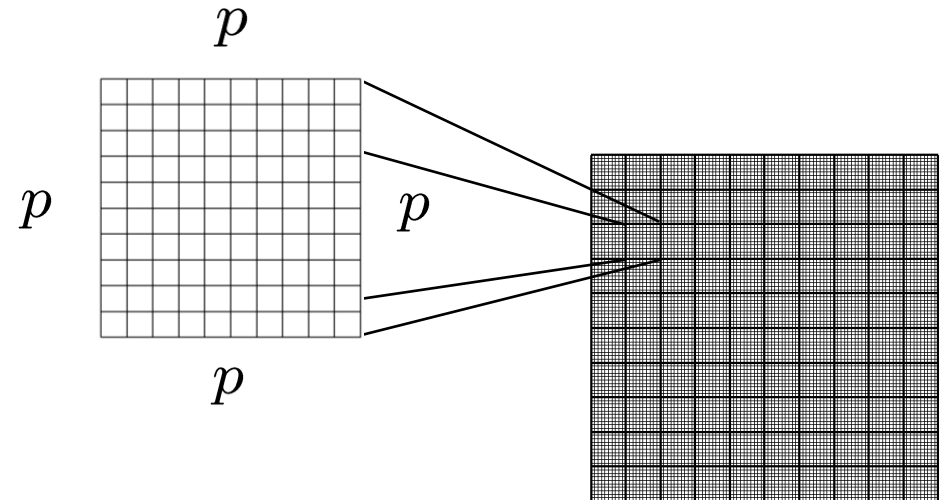
$$\begin{pmatrix} \left\langle \frac{\partial p}{\partial x} \right\rangle^x & \left\langle \frac{\partial p}{\partial y} \right\rangle^x & 0 & 0 \\ 0 & 0 & \left\langle \frac{\partial p}{\partial x} \right\rangle^x & \left\langle \frac{\partial p}{\partial y} \right\rangle^x \\ \left\langle \frac{\partial p}{\partial x} \right\rangle^y & \left\langle \frac{\partial p}{\partial y} \right\rangle^y & 0 & 0 \\ 0 & 0 & \left\langle \frac{\partial p}{\partial x} \right\rangle^y & \left\langle \frac{\partial p}{\partial y} \right\rangle^y \end{pmatrix} \begin{pmatrix} K_{xx}^* \\ K_{xy}^* \\ K_{yx}^* \\ K_{yy}^* \end{pmatrix} = - \begin{pmatrix} \langle v_x \rangle^x \\ \langle v_y \rangle^x \\ \langle v_x \rangle^y \\ \langle v_y \rangle^y \end{pmatrix}$$

$$K_{xy}^* = K_{yx}^* = (K_{xy}^* + K_{yx}^*)/2$$



Relative permeability upscaling

- Use pressure field of global calculations for boundary conditions
- Calculate velocity field and solve system of eq.



$$\begin{pmatrix} \Psi_{\alpha,x}^x & \Psi_{\alpha,y}^x & 0 & 0 \\ 0 & 0 & \Psi_{\alpha,x}^x & \Psi_{\alpha,y}^x \\ \Psi_{\alpha,x}^y & \Psi_{\alpha,y}^y & 0 & 0 \\ 0 & 0 & \Psi_{\alpha,x}^y & \Psi_{\alpha,y}^y \end{pmatrix} \begin{pmatrix} K_{\text{tot}xx\alpha}^* \\ K_{\text{tot}xy\alpha}^* \\ K_{\text{tot}yx\alpha}^* \\ K_{\text{tot}yy\alpha}^* \end{pmatrix} = - \begin{pmatrix} \langle v_{\alpha x} \rangle_{\alpha}^x \\ \langle v_{\alpha y} \rangle_{\alpha}^y \\ \langle v_{\alpha x} \rangle_{\alpha}^y \\ \langle v_{\alpha y} \rangle_{\alpha}^x \end{pmatrix}$$



Relative permeability upscaling

$$\begin{pmatrix} \Psi_{\alpha,x}^x & \Psi_{\alpha,y}^x & 0 & 0 \\ 0 & 0 & \Psi_{\alpha,x}^x & \Psi_{\alpha,y}^x \\ \Psi_{\alpha,x}^y & \Psi_{\alpha,y}^y & 0 & 0 \\ 0 & 0 & \Psi_{\alpha,x}^y & \Psi_{\alpha,y}^y \end{pmatrix} \begin{pmatrix} K_{\text{tot}xx\alpha}^* \\ K_{\text{tot}xy\alpha}^* \\ K_{\text{tot}yx\alpha}^* \\ K_{\text{tot}yy\alpha}^* \end{pmatrix} = - \begin{pmatrix} \langle v_{\alpha x} \rangle_{\alpha}^x \\ \langle v_{\alpha y} \rangle_{\alpha}^y \\ \langle v_{\alpha x} \rangle_{\alpha}^y \\ \langle v_{\alpha y} \rangle_{\alpha}^x \end{pmatrix}$$

$$\Psi_{\alpha,x}^x = \frac{1}{\mu_{\alpha}} \left\langle \frac{\partial p_{\alpha}}{\partial x} \right\rangle_{\alpha}^x + \rho_{\alpha} g \nabla z$$

$$\Psi_{\alpha,y}^x = \frac{1}{\mu_{\alpha}} \left\langle \frac{\partial p_{\alpha}}{\partial y} \right\rangle_{\alpha}^x + \rho_{\alpha} g \nabla z$$

$$\Psi_{\alpha,x}^y = \frac{1}{\mu_{\alpha}} \left\langle \frac{\partial p_{\alpha}}{\partial x} \right\rangle_{\alpha}^y + \rho_{\alpha} g \nabla z$$

$$\Psi_{\alpha,y}^y = \frac{1}{\mu_{\alpha}} \left\langle \frac{\partial p_{\alpha}}{\partial y} \right\rangle_{\alpha}^y + \rho_{\alpha} g \nabla z$$

$$\mathbf{K}_r^* = \mathbf{K}_{\text{tot}}^* \mathbf{K}^{*-1}$$



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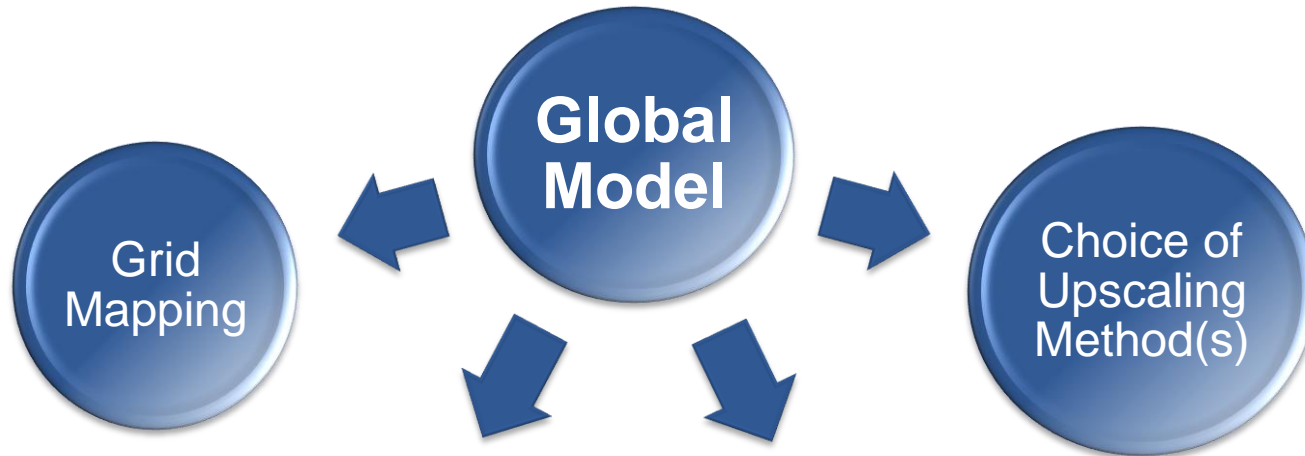


Implementation in DuMu^x

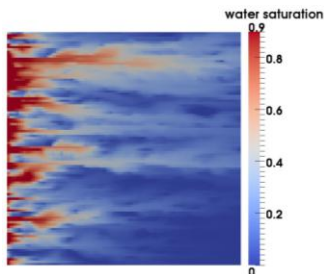
- **Aim: General framework** for use/combination of different local(-global) methods implemented in DuMu^x.



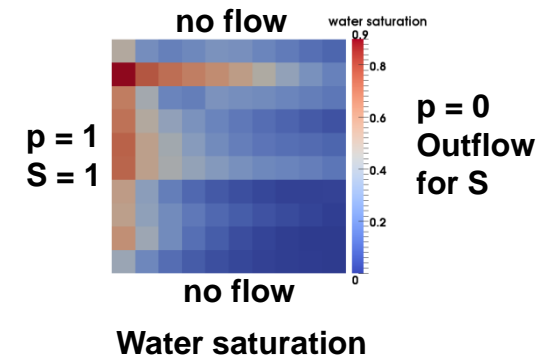
Control Structure



Reference solution



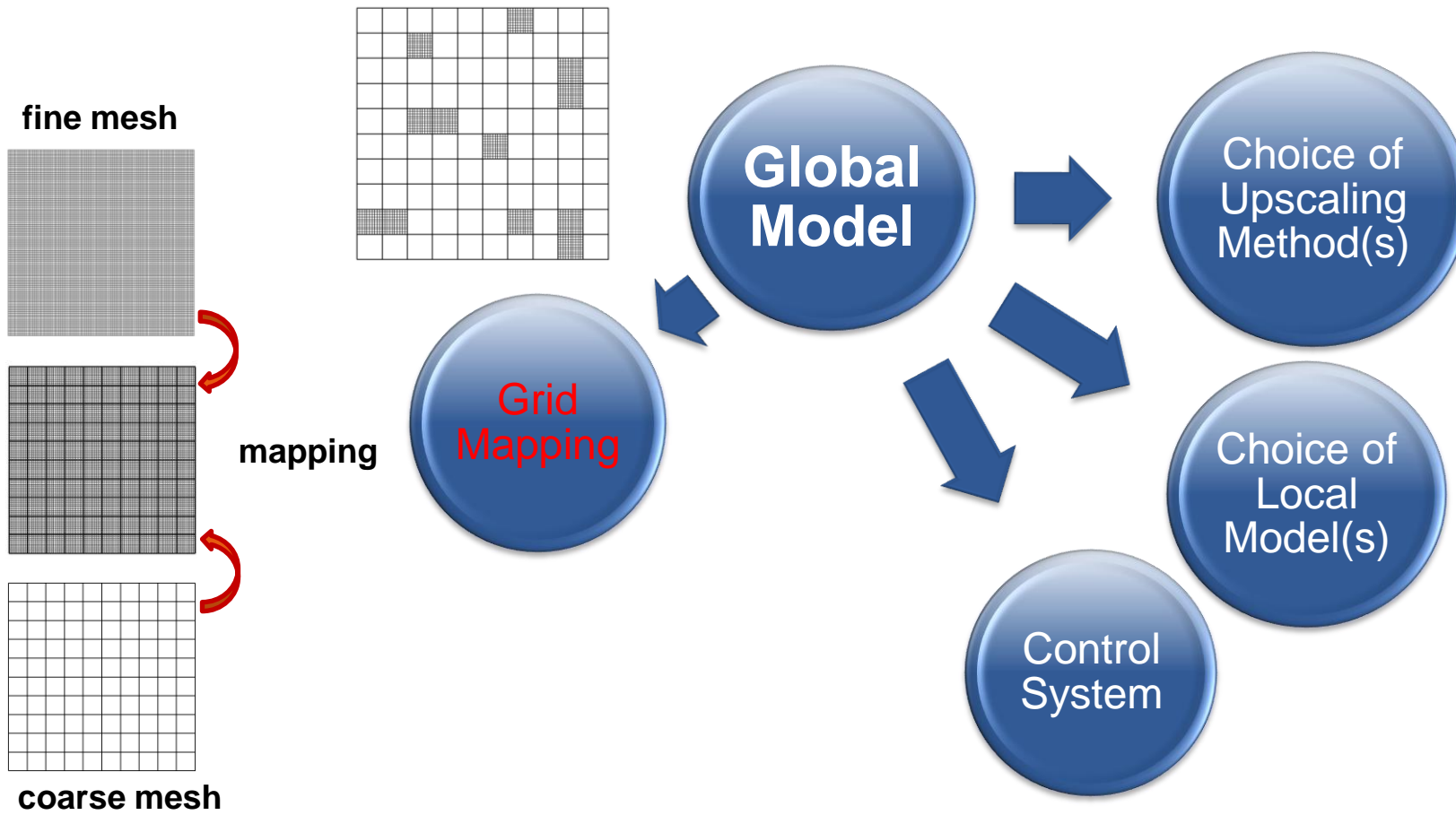
Water saturation





Grid Mapping

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➤ dune-multidomaingrid



Grid Mapping Ingredient: SubdomainGenerator

```

template<class TypeTag>
void SubdomainGenerator<TypeTag>::createSubgridsOneCell(Scalar radius)
{
  gridMultiScale_.startSubDomainMarking();

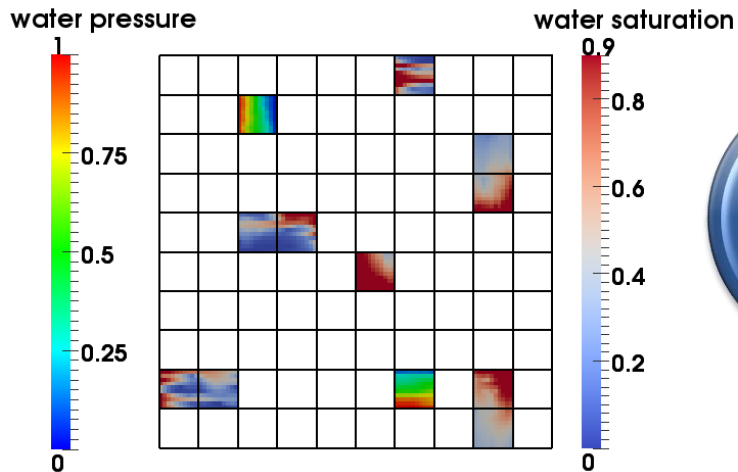
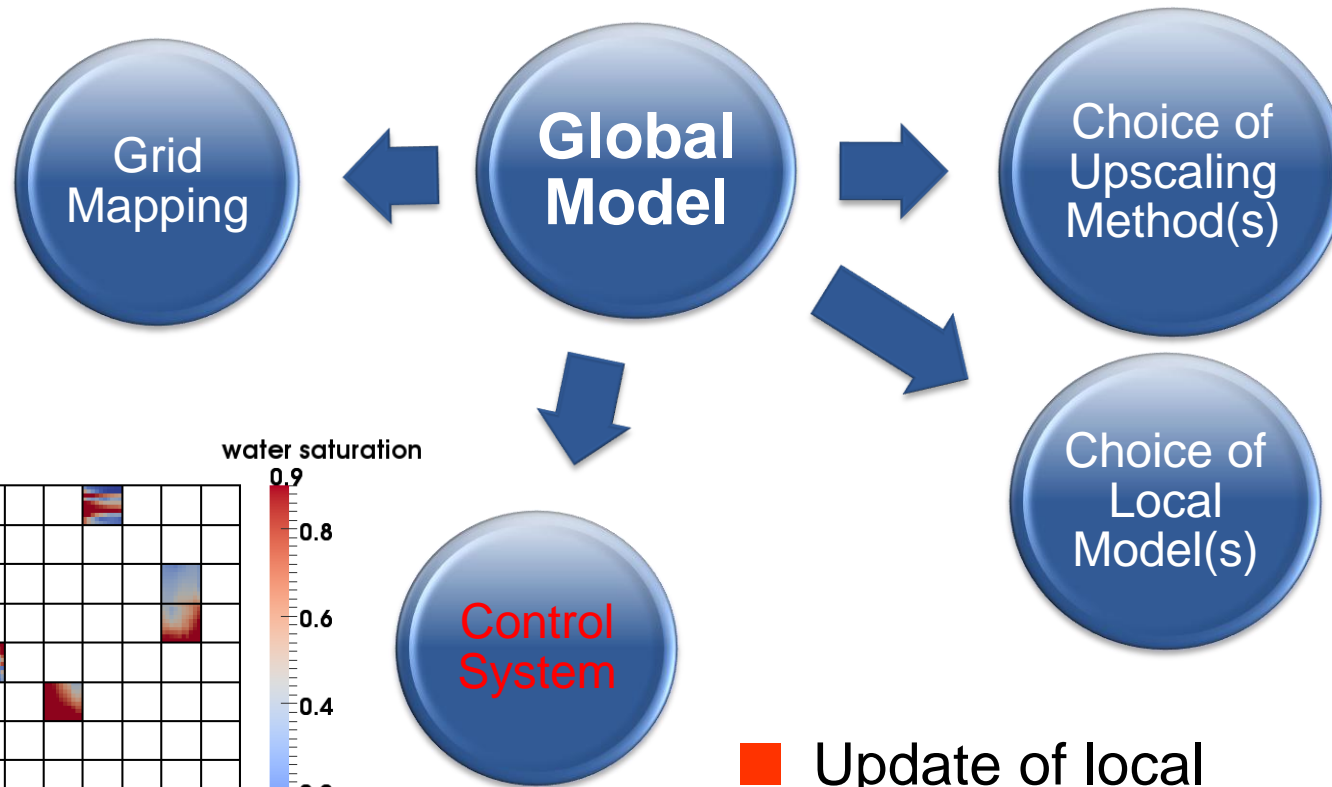
  for (ElementIteratorFine eItFine = gridViewFine_.template begin<0>()
      {
        int subdomainIndex = ...;

        gridMultiScale_.addToSubDomain(subDomainIndex, *eItFine);
      }

  gridMultiScale_.preUpdateSubDomains();
  gridMultiScale_.updateSubDomains();
  gridMultiScale_.postUpdateSubDomains();
}
  
```



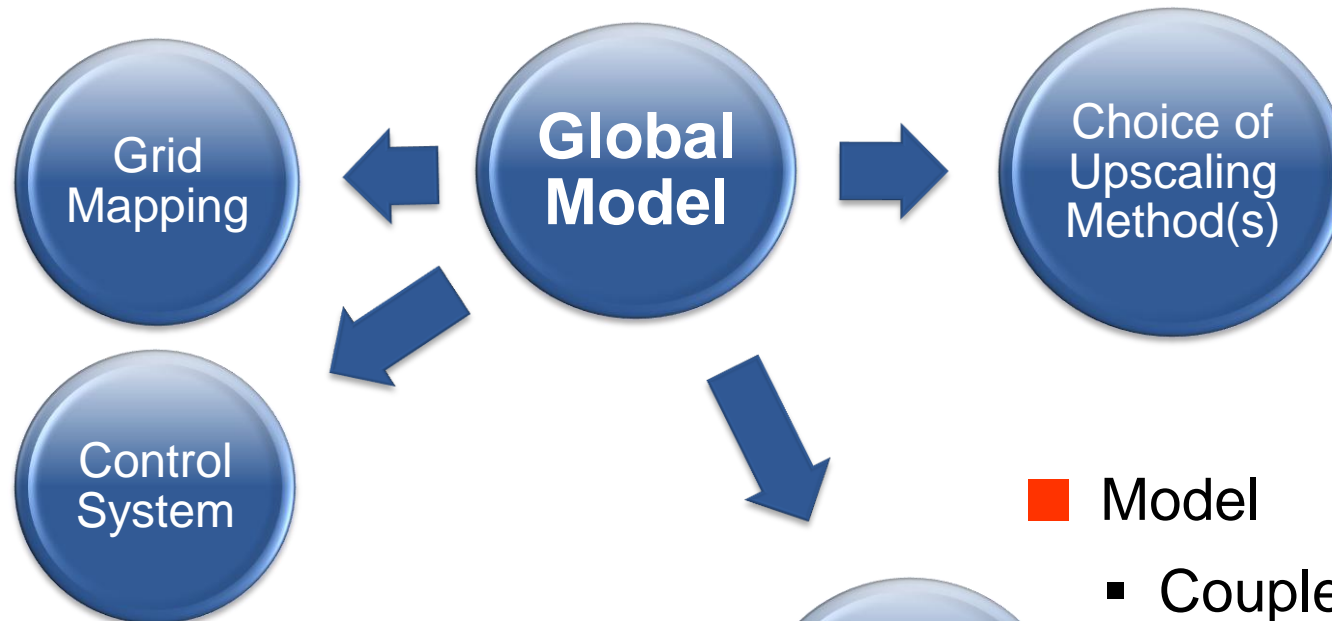
Control System



- Update of local calculations
 - Preprocessing
 - Adaptive



Choice of Local Model(s)



- Discretization
 - FV
 - Box-method
 - Mimetic FD
 - ...

- Model
 - Coupled
 - Decoupled
 - Fractional flow
 - Phase pressure formulation
 - ...



Ingredient: Property System

- Definition of default local problem type:

```
SET_TYPE_PROP (MultiScale,
               LocalMultiScaleBaseProblem,
               Diffusion1P<TypeTag>) ;
```

- Can be overwritten at any higher level:

```
SET_TYPE_PROP (MyProblem,
               LocalMultiScaleBaseProblem,
               IMPET<TypeTag>) ;
```

- Easy typedef extraction:

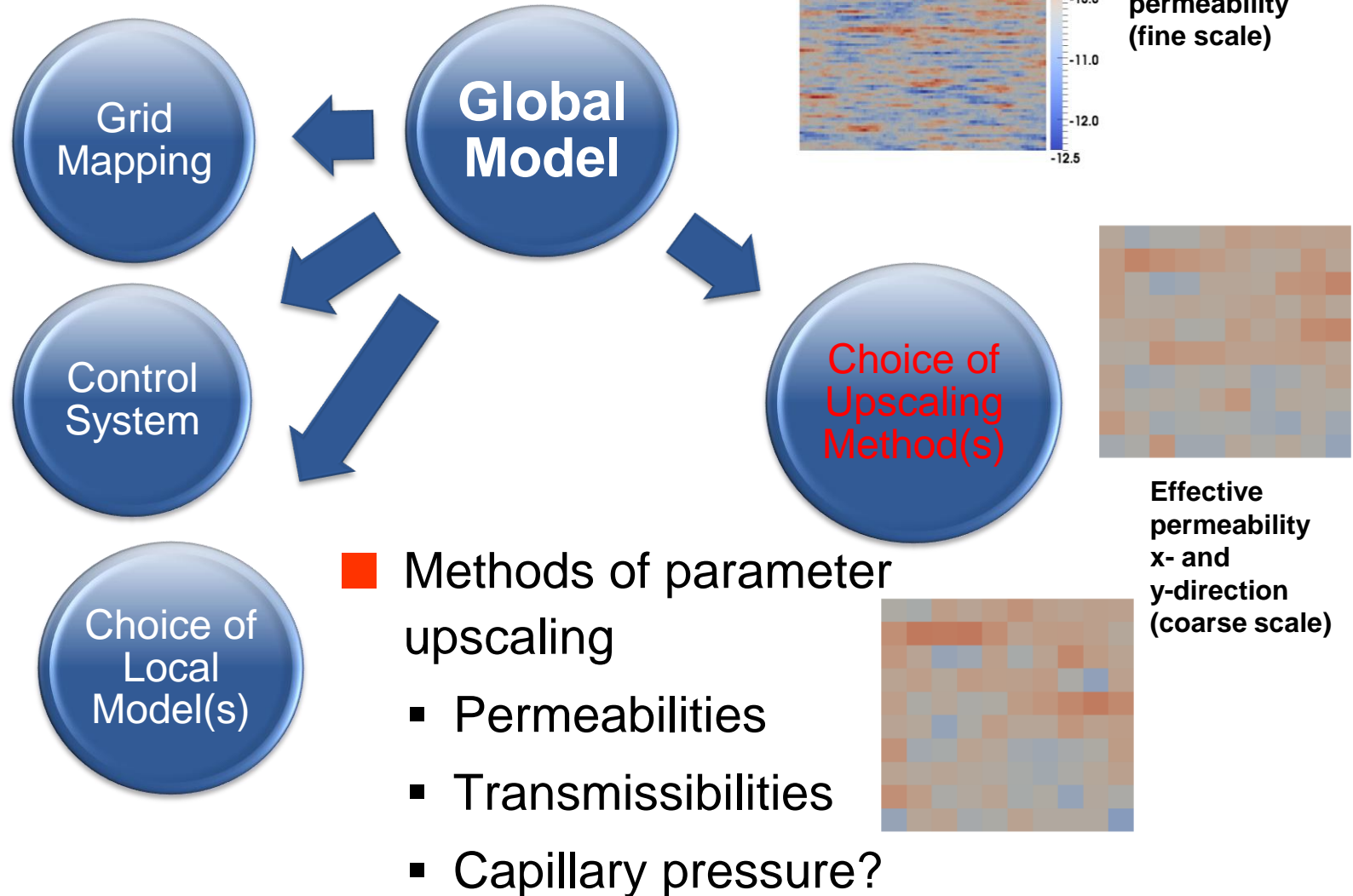
```
template<class TypeTag>
```

...

```
typedef typename GET_PROP_TYPE (TypeTag,
                               PTAG (LocalMultiScaleBaseProblem)) MyType ;
```



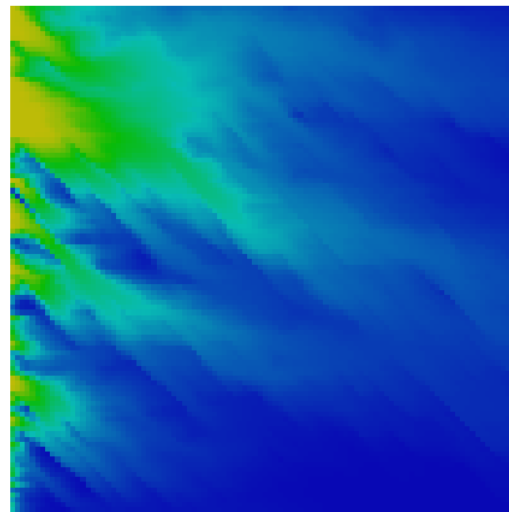

Choice of Upscaling Method(s)



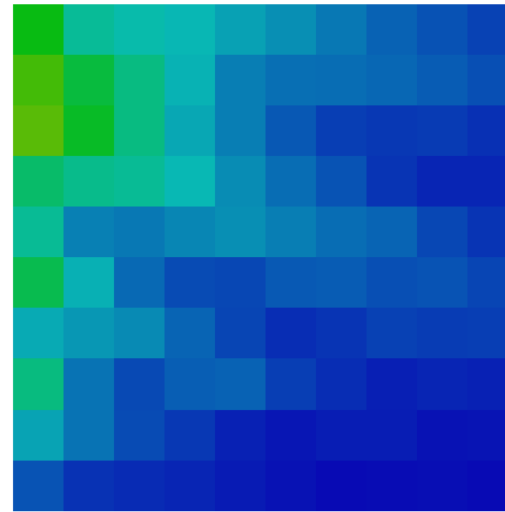


First results: 2-phase flow without p_c and gravity

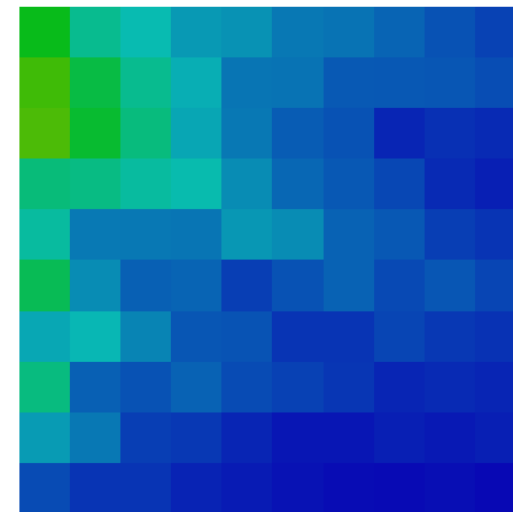
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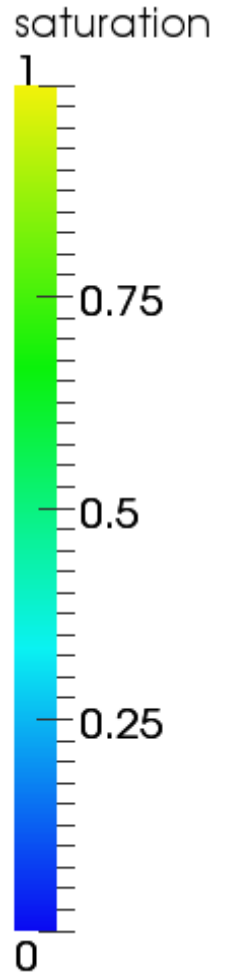
Fine scale reference



Full tensor \mathbf{K}^*



Full tensor \mathbf{K}^* and \mathbf{K}_r^*





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Summary

- Especially for upscaling, tensorial permeabilities are important.
- Discretizations have to be able to treat tensorial permeabilities.
- Upscaling concept based on calculation of effective parameters.
- Intrinsic permeability upscaling is well understood.
- Relative permeability and capillary pressure upscaling not at all.
- Implementation based on dune-multidomaingrid.
- Flexible choice of local and global model and upscaling method.
- Parallelized preprocessing.

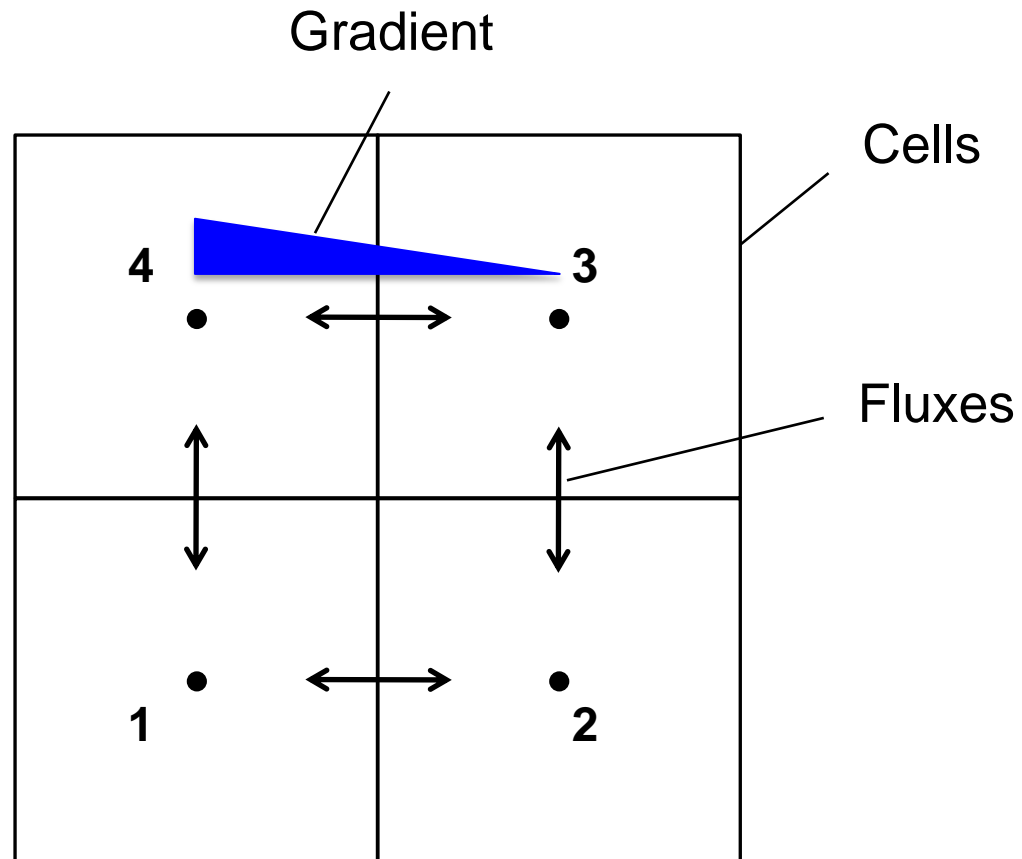


Thank you!



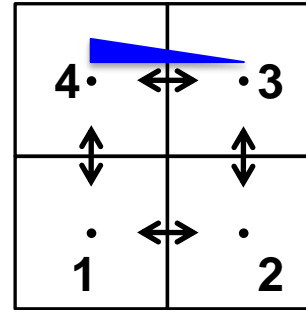
TPFA vs. MPFA

■ TPFA:





TPFA vs. MPFA



TPFA:

▪ Gradient: $(grad \Phi)_{34} = \frac{\Phi_3 - \Phi_4}{\Delta x} \mathbf{n}_{34} = \begin{pmatrix} \frac{\Phi_3 - \Phi_4}{\Delta x} \\ 0 \end{pmatrix}$

▪ Permeability:
$$\mathbf{K}_{34} = \begin{pmatrix} \frac{2 * K_{xx3} * K_{xx4}}{K_{xx3} + K_{xx4}} & 0.5 * (K_{xy3} + K_{xy4}) \\ 0.5 * (K_{yx3} + K_{yx4}) & \frac{2 * K_{yy3} * K_{yy4}}{K_{yy3} + K_{yy4}} \end{pmatrix}$$

▪ Mobility: $\Lambda_{34} = \frac{\mathbf{K}_{r34}}{\mu_{34}} = \Lambda_{34}^{(upw)}$

▪ Flux:
$$F_{34} = (\Lambda_{34} \mathbf{K}_{34} grad \Phi_{34}) \mathbf{n}_{34} A_{34}$$

$$= (\Lambda_{xx34} K_{xx34} + \Lambda_{xy34} K_{yx34}) \Delta \Phi_{34} A_{34}$$



TPFA vs. MPFA

- Potential in a cell is assumed to be linear:

$$\Phi_j(\mathbf{x}) = \nabla \Phi_j \cdot (\mathbf{x} - \mathbf{x}_{j,0}) + \Phi_{j,0}$$

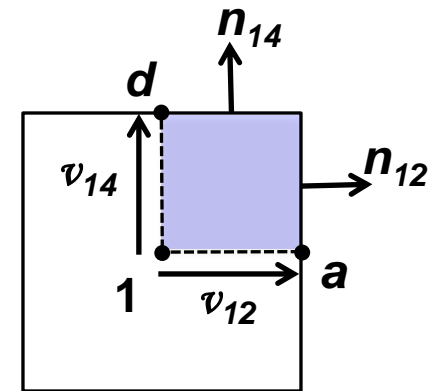
- Use this approximation and the continuity points (a , d) (2-d):

$$\underbrace{\begin{pmatrix} (\mathbf{x}_{1,a} - \mathbf{x}_{1,0})^T \\ (\mathbf{x}_{1,d} - \mathbf{x}_{1,0})^T \end{pmatrix}}_{\mathbf{X}} \nabla \Phi_1 = \begin{pmatrix} \Phi_{1,a} - \Phi_{1,0} \\ \Phi_{1,d} - \Phi_{1,0} \end{pmatrix}$$

- After some reformulation the gradient can be approximated as:

$$\nabla \Phi_1 = \frac{1}{V_t} (\nu_{12}(\Phi_{1,a} - \Phi_{1,0}) + \nu_{14}(\Phi_{1,d} - \Phi_{1,0}))$$

$$\mathbf{X}^{-1} = \frac{1}{V_t} [\nu_{12}, \nu_{14}]$$

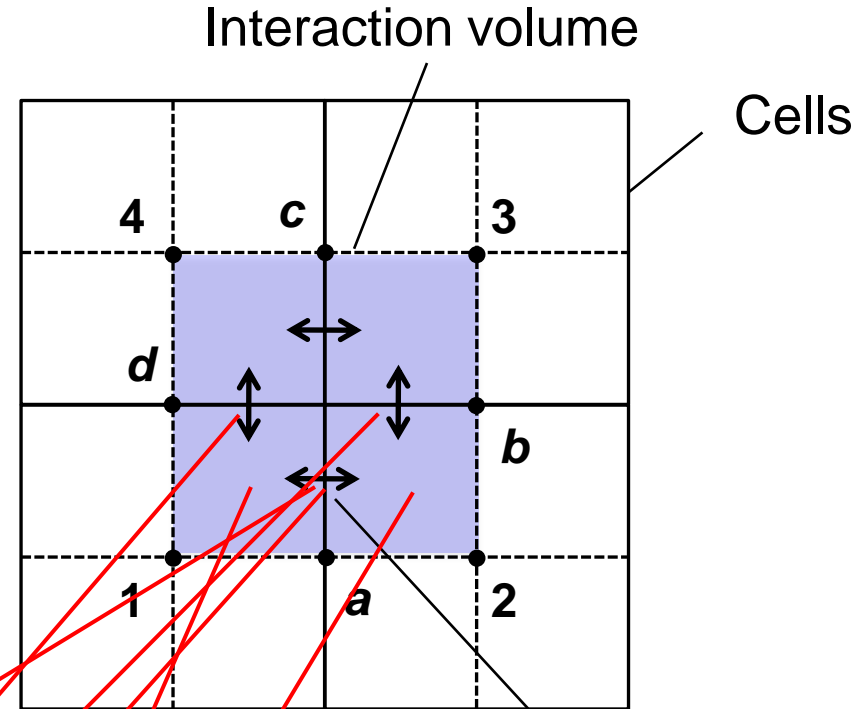




TPFA vs. MPFA

MPFA-O:

- Introduce pressures/potentials at face centers (a, b, c, d)
- Formulate fluxes over half cell edges for every quarter of the interaction



volume:

$$\begin{pmatrix} f_{12} \\ f_{14} \end{pmatrix} = -\mathbf{G}_1 \begin{pmatrix} \Phi_a - \Phi_1 \\ \Phi_d - \Phi_1 \end{pmatrix}$$

$$\begin{pmatrix} f_{23} \\ f_{21} \end{pmatrix} = -\mathbf{G}_2 \begin{pmatrix} \Phi_b - \Phi_2 \\ \Phi_2 - \Phi_a \end{pmatrix}$$

...

Fluxes over half edges

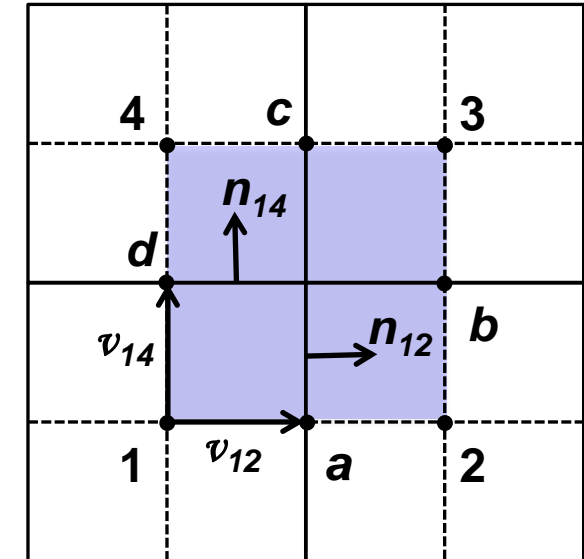


TPFA vs. MPFA

■ MPFA-O:

- G_1 includes \mathbf{K} , Λ and geometric information

$$\nu_{12} = \frac{(\mathbf{x}_a - \mathbf{x}_1)}{|(\mathbf{x}_a - \mathbf{x}_1)|} A_{14}$$



$$G_1 = \frac{1}{V_t} \begin{pmatrix} A_{12} \mathbf{n}_{12}^T \Lambda_1 \mathbf{K}_1 \nu_{12} & A_{12} \mathbf{n}_{12}^T \Lambda_1 \mathbf{K}_1 \nu_{14} \\ A_{14} \mathbf{n}_{14}^T \Lambda_2 \mathbf{K}_2 \nu_{12} & A_{14} \mathbf{n}_{14}^T \Lambda_2 \mathbf{K}_2 \nu_{14} \end{pmatrix}$$

- Structured grid

$$G_1 = \frac{1}{V_t} \begin{pmatrix} A_{12} \mathbf{n}_{12}^T \Lambda_1 \mathbf{K}_1 A_{14} \mathbf{n}_{12} & A_{12} \mathbf{n}_{12}^T \Lambda_1 \mathbf{K}_1 A_{12} \mathbf{n}_{14} \\ A_{14} \mathbf{n}_{14}^T \Lambda_2 \mathbf{K}_2 A_{14} \mathbf{n}_{12} & A_{14} \mathbf{n}_{14}^T \Lambda_2 \mathbf{K}_2 A_{12} \mathbf{n}_{14} \end{pmatrix}$$



TPFA vs. MPFA

■ MPFA-O:

- Fluxes:
$$f_{12} = -\frac{1}{V_t} A_{12} A_{14} (\Lambda_{xx} K_{xx} + \Lambda_{xy} K_{yx}) (\Phi_a - \Phi_1) - \frac{1}{V_t} A_{12} A_{12} (\Lambda_{xx} K_{xy} + \Lambda_{xy} K_{yy}) (\Phi_d - \Phi_1)$$

- Solve the system of equations arising from a flux balance to get the Transmissibility matrix **T**:

$$\begin{pmatrix} f_{12} \\ f_{23} \\ f_{34} \\ f_{41} \end{pmatrix} = \mathbf{T} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \end{pmatrix}$$

$$f_{12} = f_{21}$$

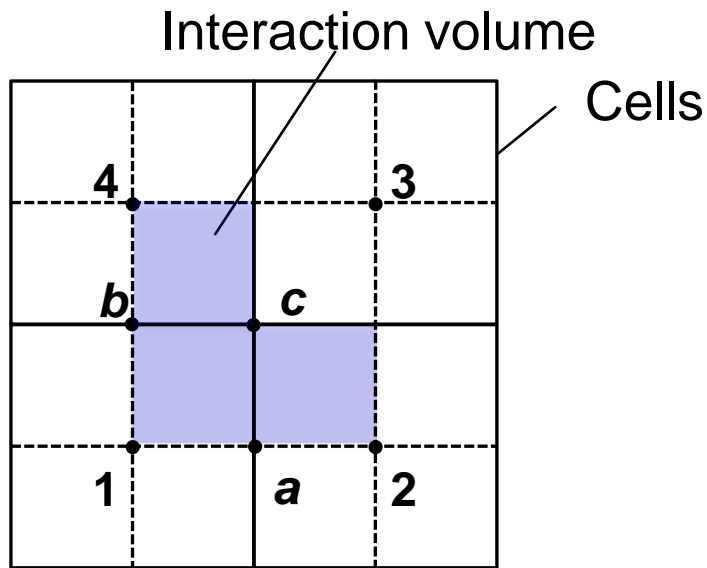
$$f_{23} = f_{32}$$

$$f_{34} = f_{43}$$

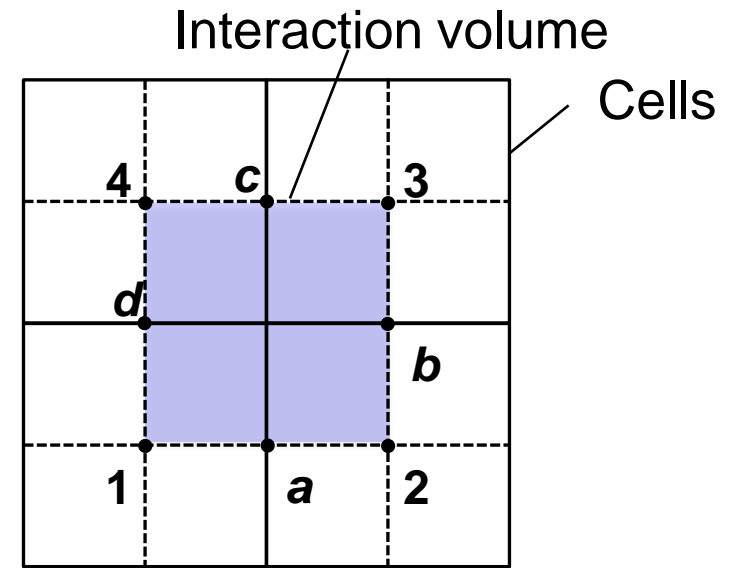
$$f_{41} = f_{14}$$



TPFA vs. MPFA



L-Method



O-Method



TPFA vs. MPFA

■ TPFA

- only for structured grids (CCFV)

■ MPFA-O

- Accurate for unstructured grids (CCFV)



TPFA vs. MPFA

■ TPFA

- only for structured grids (CCFV)
- Face flux with information of the 2 neighbor cells

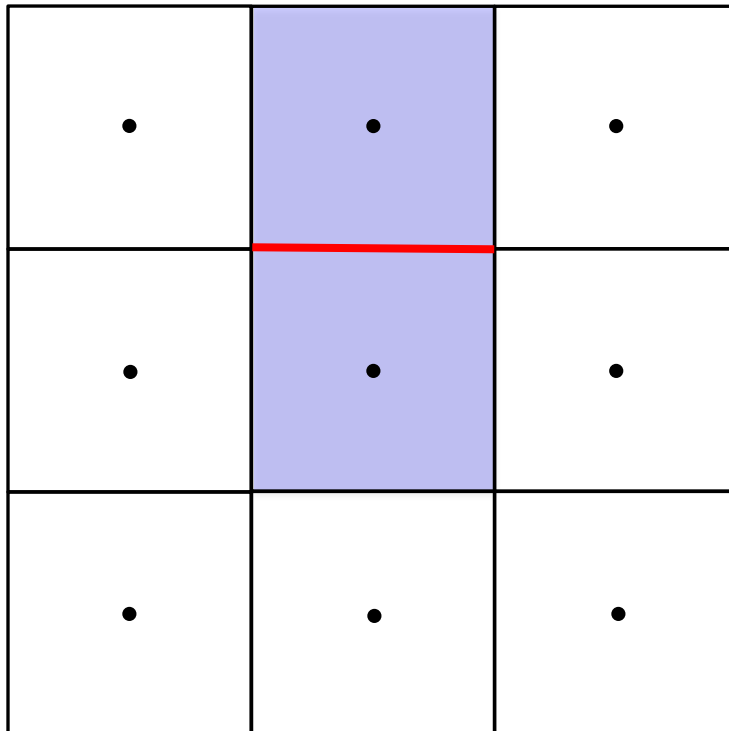
■ MPFA-O

- Accurate for unstructured grids (CCFV)
- Face flux with information of 6 (2-D) surrounding cells

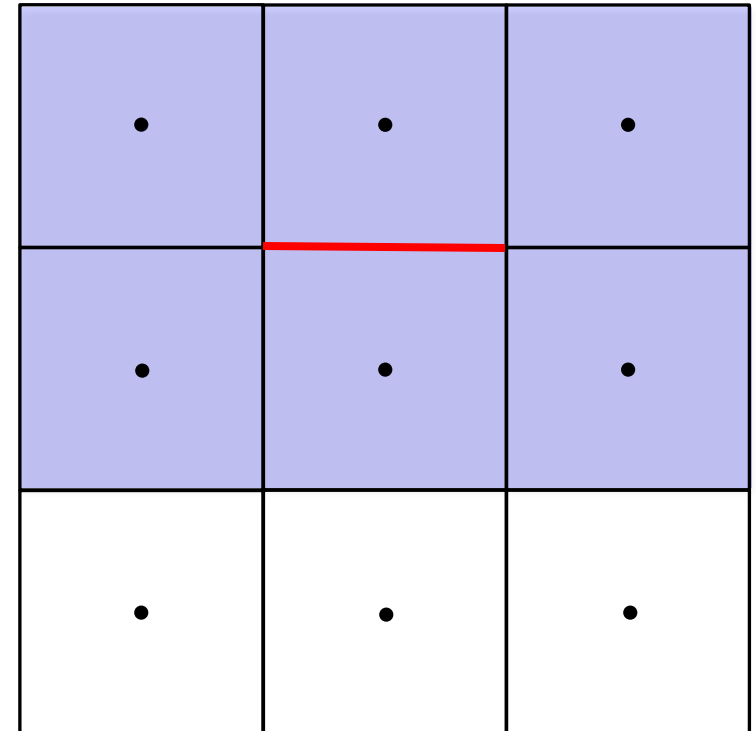


TPFA vs. MPFA

■ TPFA



■ MPFA-O





TPFA vs. MPFA

■ TPFA

- only for structured grids (CCFV)
- Face flux with information of the 2 neighbor cells
- 5-point stencil → problem if flux is not aligned with the principal grid axes

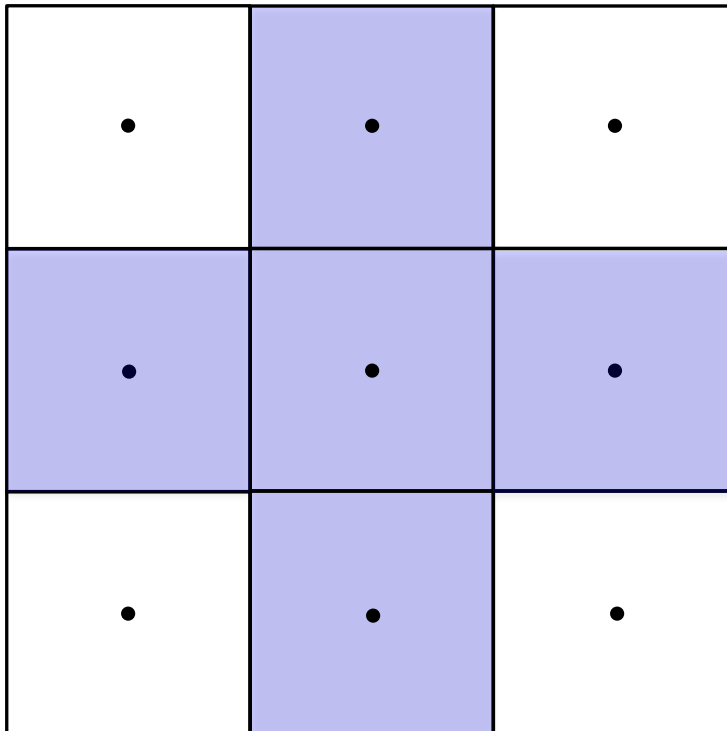
■ MPFA-O

- Accurate for unstructured grids (CCFV)
- Face flux with information of 6 (2-D) surrounding cells
- 9-point stencil → diagonal effects accounted for

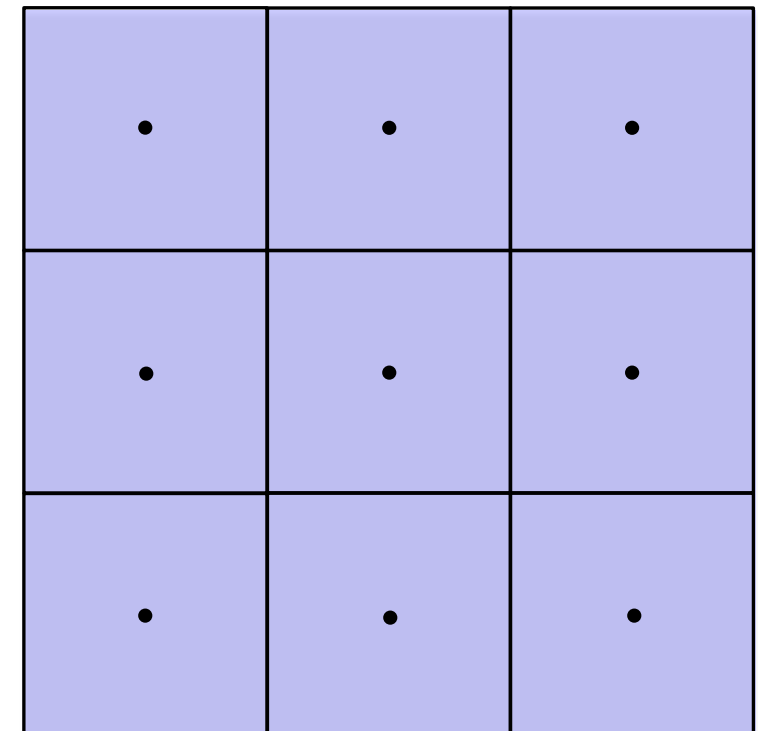


TPFA vs. MPFA

■ TPFA



■ MPFA-O





TPFA vs. MPFA

■ TPFA

- only for structured grids (CCFV)
- Face flux with information of the 2 neighbor cells
- 5-point stencil → problem if flux is not aligned with the principal grid axes
- Not able to account properly for the full tensor effects

■ MPFA-O

- Accurate for unstructured grids (CCFV)
- Face flux with information of 6 (2-D) surrounding cells
- 9-point stencil → diagonal effects accounted for
- Accounts for full tensor effects



Small Summary

- It can be necessary to use full tensor coefficients
- A MPFA-O method is able to treat them

 We need a MPFA method for two-phase flow with capillary pressure and gravity!



Treatment of tensor coefficients with MPFA-O

■ Two-phase flow formulation (*Hotetiti & Firoozabadi*):

- Definition of potentials:

$$\Phi_w = p_w + \rho_w g z$$

$$\Phi_n = p_n + \rho_n g z$$

$$\Phi_c = \Phi_n - \Phi_w = p_c + (\rho_n - \rho_w) g z$$

- Total velocity:

$$\mathbf{v}_t = \mathbf{v}_w + \mathbf{v}_n$$

$$\Lambda_t = \Lambda_w - \Lambda_n$$

$$\mathbf{v}_t = \underbrace{-\Lambda_t \mathbf{K} \nabla \Phi_w}_{\mathbf{v}_{(adv)}} + \underbrace{\Lambda_t^{-1} \Lambda_n \Lambda_t \nabla \Phi_c}_{\mathbf{v}_{(cap)}}$$

$$\Lambda_\alpha = \frac{1}{\mu_\alpha} \mathbf{K} r_\alpha$$

- Pressure equation:

$$\nabla \cdot \mathbf{v}_t = q_t$$



Treatment of tensor coefficients with MPFA-O

- Discretization of the pressure equation with finite volumes and

MPFA:

$$\int_V \nabla \cdot \mathbf{v}_t \, dV = \sum_i \left(F_{(\text{adv})_i} + F_{(\text{cap})_i} \right) = q_t V$$

- Total transmissibility \mathbf{T}_t as operator for $\Lambda_n \Lambda_t \mathbf{K} \nabla$:

$$\underbrace{\mathbf{F}_{(\text{adv})_w} = \mathbf{T}_t \Phi_w}_{\text{advective flux}}$$

$$\underbrace{\mathbf{F}_{(\text{cap})} = \Lambda_t^{-1} \Lambda_n \mathbf{T}_t \Phi_c}_{\text{capillary flux}}$$



Treatment of tensor coefficients with MPFA-O

- Calculation of phase velocities:

$$\mathbf{v}_{w_i} = \Lambda_{t_i}^{(\text{upw})^{-1}} \Lambda_{w_i}^{(\text{upw})} (\mathbf{T}_t \Phi_w)_i \frac{\mathbf{n}_i}{A_i}$$

$$\mathbf{v}_{n_i} = \left[\Lambda_{t_i}^{(\text{upw})^{-1}} \Lambda_{n_i}^{(\text{upw})} (\mathbf{T}_t \Phi_w)_i + \Lambda_{t_i}^{-1} \Lambda_{n_i} (\mathbf{T}_t \Phi_{(\text{cap})})_i \right] \frac{\mathbf{n}_i}{A_i}$$

- Discretisation of the saturation equation with finite volumes:

$$\varphi \frac{\partial S_w}{\partial t} V + \sum_i (\mathbf{v}_w \cdot \mathbf{n})_i A_i = q_i V$$



How can tensor parameters be determined?

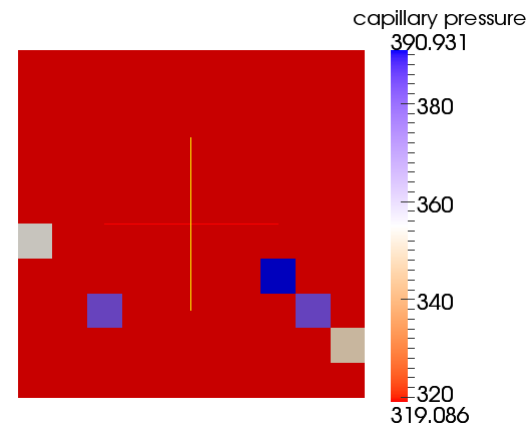
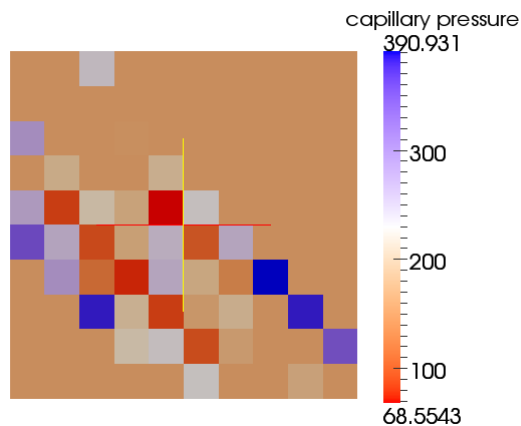
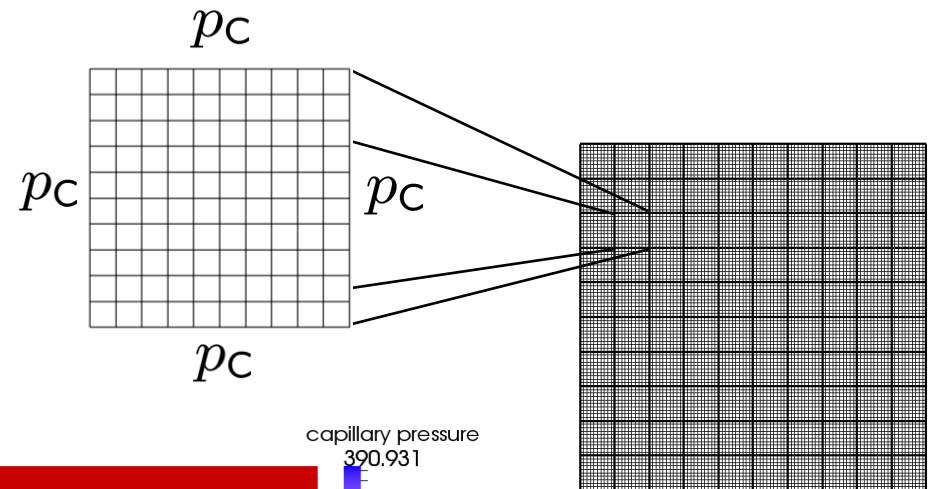
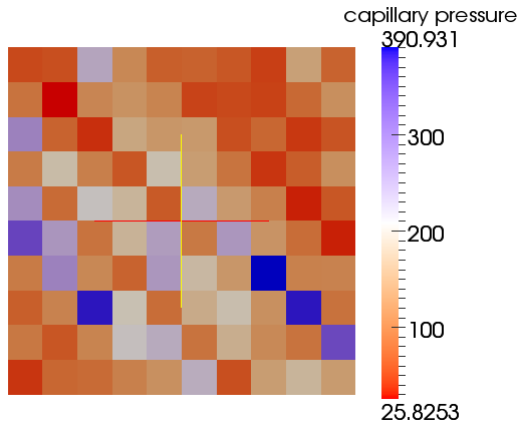
- Can arise from upscaling
 - Analytical methods (only simple structures)
 - Numerical methods
 - ...
- Well tested methods for intrinsic permeability upscaling available
- Tensor relative permeabilities?



Relative permeability upscaling

- Determine initial saturation distribution from capillary

equilibrium





Example of an upscaled relative permeability function

... k_{rn}
— k_{rw}

k_r

