SimTech Cluster of Excellence
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Coupling free flow and flow in porous media using mortar elements

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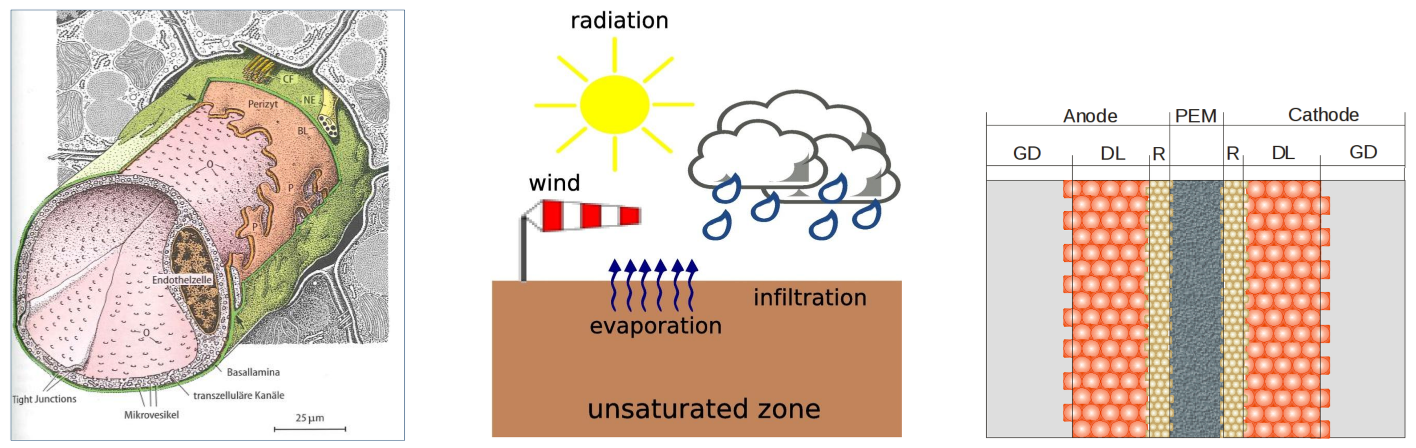
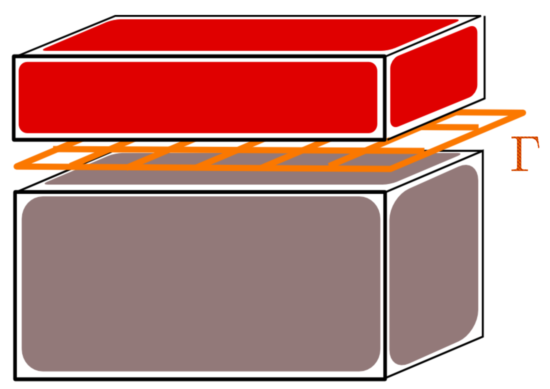
Motivation

Modelling flow and transport processes across complex interfaces separating a free-flow and a porous-medium region
→ focus on interface structure and processes



Applications: transvascular exchange (Junqueira et al. 2002), evaporation influenced by a wind field, water management in fuel cells influenced by the gas-channel/diffusion-layer interface

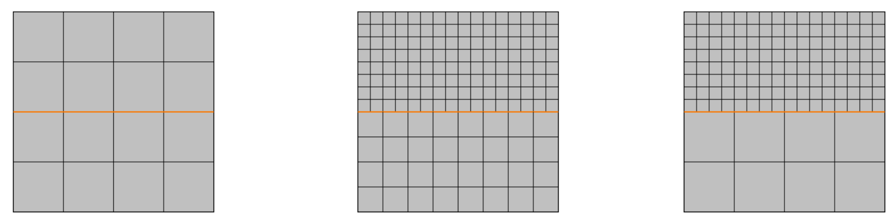
Coupling concept: Mortar Method



Two interacting domains are coupled using the **mortar method**:

- compositional, **one-phase**, non-isothermal Stokes flow
- compositional, **two-phase**, non-isothermal Darcy flow

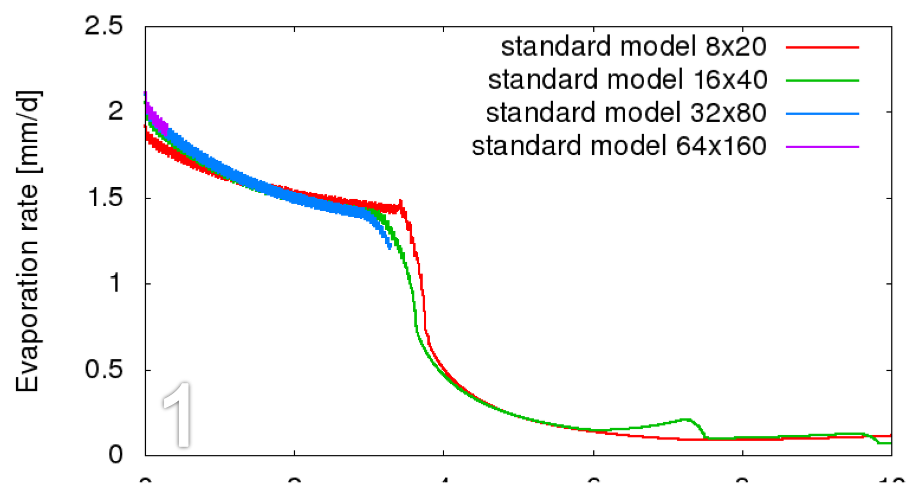
Numerical example: Evaporation from soil

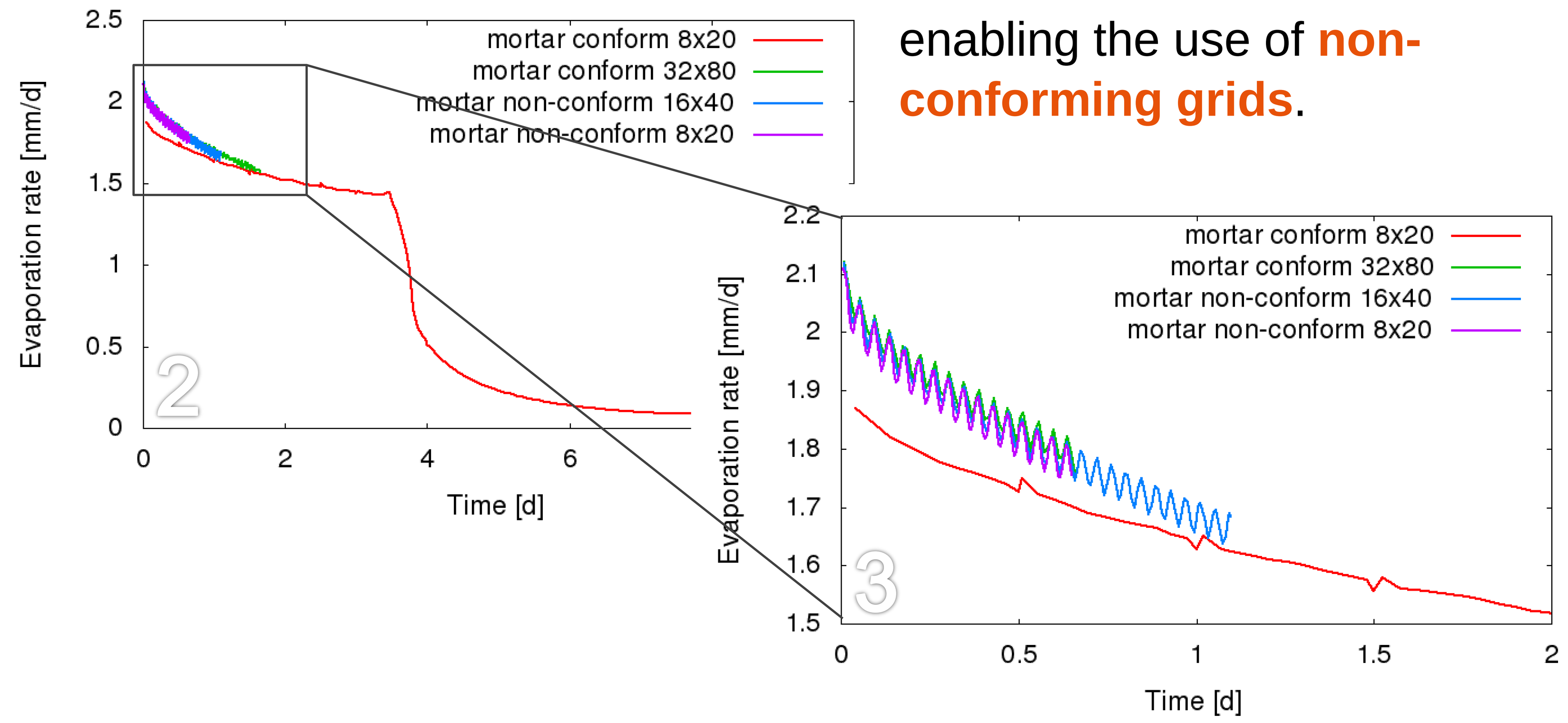


The evaporation rate from porous soil is calculated using the coupled free-flow porous-medium model.[3]

Figure 1 shows the grid convergence for the standard model without the mortar method.[1]

Figures 2 and 3 illustrate the benefit of the mortar method enabling the use of **non-conforming grids**.





Coupling concept based on thermodynamic equilibrium using the mortar method:

Stokes equation (free-flow region):

$$\int_{B_{\mathrm{ff}}} \frac{\partial \varrho \mathbf{v}}{\partial t} \mathrm{d}B_{\mathrm{ff}} + \int_{\partial B_{\mathrm{ff}\,i}} [p\mathbf{I} - \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T)] \cdot \mathbf{n}\, \mathrm{d}s + \int_{\partial B_{\mathrm{ff}\,\Gamma}} \underbrace{([p\mathbf{I} - \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T)] \cdot \mathbf{n})_{\mathbf{n}}}_{\lambda_p} \mathrm{d}s$$

$$+ \int_{\partial B_{\mathrm{ff}\,\Gamma}} \underbrace{([p\mathbf{I} - \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T)] \cdot \mathbf{n})_{\mathbf{t}}}_{\lambda_{v_x}} \mathrm{d}s = \int_{B_{\mathrm{ff}}} \mathbf{f}\, \mathrm{d}B_{\mathrm{ff}}$$

Mass balance (porous medium, $\mathbf{v}_\alpha$ given by Darcy's law):

$$\int_{B_{\mathrm{pm}}} \sum_\alpha \phi \frac{\partial \varrho_\alpha S_\alpha}{\partial t} \mathrm{d}B_{\mathrm{pm}} - \int_{\partial B_{\mathrm{pm}\,i}} \sum_\alpha (\varrho_\alpha \mathbf{v}_\alpha) \cdot \mathbf{n}\, \mathrm{d}s - \int_{\partial B_{\mathrm{pm}\,\Gamma}} \underbrace{\sum_\alpha (\varrho_\alpha \mathbf{v}_\alpha) \cdot \mathbf{n}}_{\lambda_{\mathbf{v}\cdot\mathbf{n}}} \mathrm{d}s = \int_{B_{\mathrm{pm}}} \sum_\alpha \mathbf{q}_\alpha\, \mathrm{d}B_{\mathrm{pm}}$$

Transport equation, Lagrange multiplier enforce continuity of component fluxes:

$$\int_B \sum_\alpha \phi \frac{\partial \varrho_\alpha S_\alpha x_\alpha^\kappa}{\partial t} \mathrm{d}B - \int_{\partial B_i} F^\kappa \cdot \mathbf{n}\, \mathrm{d}s - \int_{\partial B_\Gamma} \underbrace{\sum_\alpha (\varrho_\alpha \mathbf{v}_\alpha x_\alpha^\kappa - D_\alpha^\kappa \varrho_\alpha \nabla x_\alpha^\kappa) \cdot \mathbf{n}}_{\lambda_x} \mathrm{d}s = \int_B \sum_\alpha \mathbf{q}_\alpha^\kappa\, \mathrm{d}B$$

Energy balance, Lagrange multiplier enforce continuity of energy fluxes:

$$\int_B \sum_\alpha \phi \frac{\partial (\varrho_\alpha u_\alpha S_\alpha)}{\partial t} + (1-\phi) \frac{\partial (\varrho_s c_s T)}{\partial t} \mathrm{d}B - \int_{\partial B_i} F^T \cdot \mathbf{n}\, \mathrm{d}s - \int_{\partial B_\Gamma} \underbrace{\sum_\alpha (\varrho_\alpha h_\alpha \mathbf{v}_\alpha - \lambda \nabla T) \cdot \mathbf{n}}_{\lambda_T} \mathrm{d}s = \int_B \mathbf{q}^T\, \mathrm{d}B$$

Local mechanical equilibrium

Continuity of normal forces:

$$\int_\Gamma \lambda_p\, \mathrm{d}s - \int_\Gamma p_g^{\mathrm{pm}}\, \mathrm{d}s = 0$$

Beavers-Joseph-Saffman condition:

$$\int_\Gamma \lambda_{v_x}\, \mathrm{d}s - \int_\Gamma \frac{\sqrt{k_i}}{\alpha_{\mathrm{BJ}} \mu} \boldsymbol{\tau}\, \mathbf{n} \cdot \mathbf{t}\, \mathrm{d}s = 0$$

Continuity of normal fluxes:

$$\int_\Gamma \lambda_{\mathbf{v}\cdot\mathbf{n}}\, \mathrm{d}s - \int_\Gamma [\varrho \mathbf{v} \cdot \mathbf{n}]^{\mathrm{ff}} \mathrm{d}s = 0$$

Local chemical equilibrium:

Continuity of mole fractions:

$$\int_\Gamma [x_g^w]^{\mathrm{ff}}\, \mathrm{d}s - \int_\Gamma [x_g^w]^{\mathrm{pm}} \mathrm{d}s = 0$$

Local thermal equilibrium:

$$\int_\Gamma [T]^{\mathrm{ff}}\, \mathrm{d}s - \int_\Gamma [T]^{\mathrm{pm}} \mathrm{d}s = 0$$

Outlook: Water management in fuel cells

Water management is crucial for the performance of PEM-fuel-cells.[2] The water transport is significantly influenced by the processes at the interface between gas channel (GC) and gas-diffusion layer (GDL):

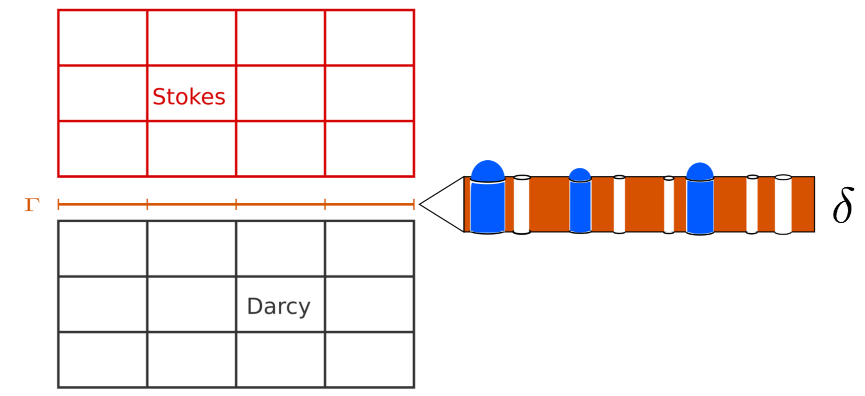
Goals:

- a consistent GC-GDL coupling strategy using the developed coupling concept to account for evaporation and condensation [1,3]
- the prediction of droplet formation on the GDL-surface

Interface Model: Bundle-of-Tubes

One-phase, three-component non-isothermal Stokes flow

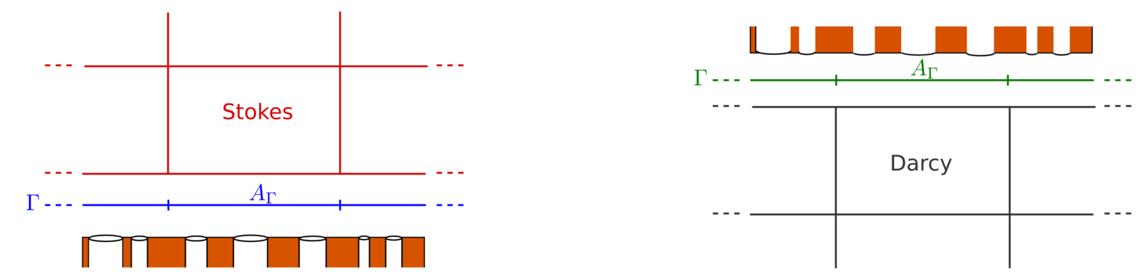
Two-phase, three-component non-isothermal Darcy flow



→ the top layer of the GDL is approximated by a bundle-of-tubes description
→ Poiseuille flow is assumed within the tubes: $v^{\mathrm{tubes}} = -\underbrace{\frac{r^2}{8\mu}}_{K^{\mathrm{tubes}}} \frac{\mathrm{d}p}{\mathrm{d}z}$

→ the Young-Laplace equation is used to determine which tubes are filled with water: $p_c = \frac{2\sigma cos\alpha}{r}$

Coupling concept for the one-phase micro-/macro-model:



$$\int_\Gamma \lambda_p\, \mathrm{d}s - \frac{1}{A^{\mathrm{tubes}}} \sum_i \left(\underbrace{\frac{\int_\Gamma \mathbf{v}^{\mathrm{ff}} \cdot \mathbf{n}}{\sum_i \frac{1}{4}\pi d_i^2}}_{v^{\mathrm{tubess}}} \frac{\delta}{K_i^{\mathrm{tubes}}} + p^{\mathrm{pm}}(x_i) \right) \cdot \underbrace{\frac{1}{4}\pi d_i^2}_{A_i} = 0$$

$$\int_\Gamma \lambda_{\mathbf{v}\cdot\mathbf{n}}\, \mathrm{d}s - \sum_i -K_i^{\mathrm{tubes}}(d_i) \frac{p^{\mathrm{pm}}(x_i) - \frac{\lambda_p \cdot A^{\mathrm{tubes}}}{A_i}}{\delta} \varrho A_i = 0$$

Literature:

[1] Baber, K., Mosthaf, K., Flemisch, B., Helmig, R., Müthing, S. and Wohlmuth, B.: Numerical scheme for coupling two-phase compositional porous-medium flow and one-phase compositional free flow, accepted in IMA Journal of Applied Mathematics, 2011.

[2] Qin, C.: Numerical investigations on two-phase flow in polymer electrolyte fuel cells, Utrecht University, 2012.

[3] Mosthaf, K., Baber, K., Flemisch, B., Helmig, R., Leijnse, A., Rybak, I. and Wohlmuth, B.: A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow, Water Resources Research, 2011.