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Department of Hydromechanics and Modelling of Hydrosystems

Coupling non-isothermal, two-component Darcy and Navier-Stokes flow to investigate evaporation of soil water

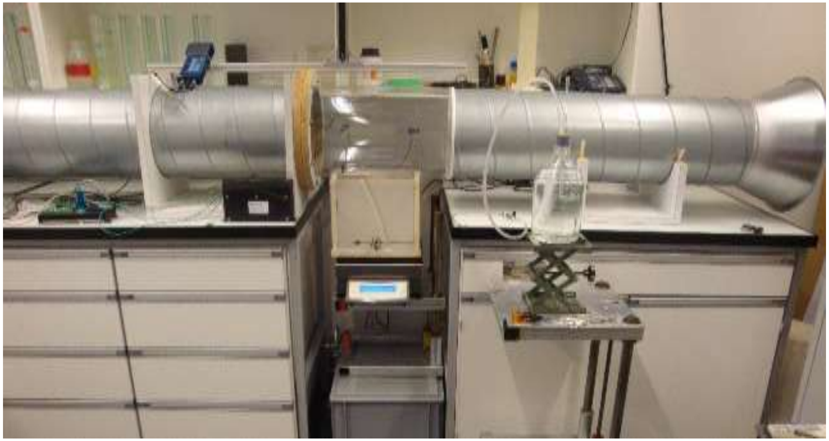
Grüninger, Fetzer, Flemisch, Helmig

CMWR 2016, Toronto

Motivation

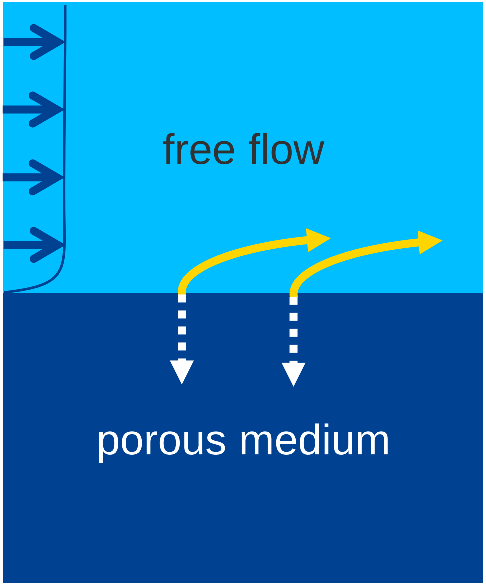
- Evaporation of soil water
- Salt precipitation
- Water management in fuel cells
- Analysis of relevant processes based on comparison studies with lab-scale experiments

www.vaderstad.com/knowhow/let-nature-do-the-work/soil-water-management



In collaboration with Dani Or, ETH Zurich

Simulation setup, physical justification



Free flow with single-phase two-component system

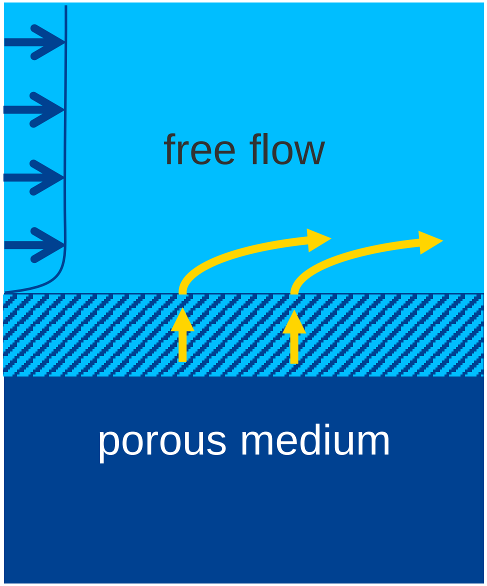
- boundary layer effects

Coupling

- sharp interface
- transfer of mass, momentum, energy

Darcy flow with two phases, two components

Simulation setup, physical justification



Relevant processes

- advection
- vapor diffusion
- convection

Additional processes

- turbulent mixing
- boundary layer effects
- …

Balance equations: free flow

Mass $$\frac{\partial}{\partial t}\varrho_\mathrm{g} + \mathrm{div}\left(\varrho_\mathrm{g} v_\mathrm{g}\right) = 0$$

Momentum $$\frac{\partial}{\partial t}\left(\varrho_\mathrm{g} v_\mathrm{g}\right) + \mathrm{div}\left(\varrho_\mathrm{g} v_\mathrm{g} v_\mathrm{g}^\mathsf{T}\right) - \mathrm{div}\left(\mu_\mathrm{g}\,\mathrm{grad}\, v_\mathrm{g}\right) + \mathrm{grad}\, p_\mathrm{g} = 0$$

Component mass $$\frac{\partial}{\partial t}\left(\varrho_\mathrm{g} X_\mathrm{g}^\mathrm{w}\right) + \mathrm{div}\left(\varrho_\mathrm{g} X_\mathrm{g}^\mathrm{w} v_\mathrm{g}\right) + \mathrm{div}\, j_\mathrm{ff}^\mathrm{w} = 0$$

Energy

$$\frac{\partial}{\partial t}\left(\varrho_\mathrm{g} u_\mathrm{g}\right) + \mathrm{div}\left(\varrho_\mathrm{g} h_\mathrm{g} v_\mathrm{g}\right) + \sum_{\kappa \in \{\mathrm{a},\mathrm{w}\}} \mathrm{div}\left(h_\mathrm{g}^\kappa j_\mathrm{ff}^\kappa\right) - \mathrm{div}\left(\lambda_\mathrm{g}\,\mathrm{grad}\, T\right) = 0$$

Primary variables $p_\mathrm{g}, v_\mathrm{g}, X_\mathrm{g}^\mathrm{w}, T$

Balance equations: porous-medium flow

Mass for $\kappa \in \{\mathrm{a},\, \mathrm{w}\}$:

$$\sum_{\alpha \in \{\mathrm{g},\mathrm{l}\}} \left(\phi \frac{\partial}{\partial t} \left(\varrho_\alpha S_\alpha X_\alpha^\kappa \right) - \operatorname{div} \left(\varrho_\alpha X_\alpha^\kappa \frac{k_{\mathrm{r},\alpha}}{\mu_\alpha} K \left(\operatorname{grad} p_\alpha - \varrho_\alpha g \nabla z \right) \right) + \operatorname{div} j_{\mathrm{pm},\alpha}^\kappa \right) = 0$$

Energy

$$\sum_{\alpha \in \{\mathrm{g},\mathrm{l}\}} \phi \frac{\partial}{\partial t} \left(\varrho_\alpha S_\alpha u_\alpha \right) + (1-\phi) \frac{\partial}{\partial t} \left(\varrho_\mathrm{s} c_\mathrm{s} T \right) + \sum_{\alpha \in \{\mathrm{g},\mathrm{l}\}} \operatorname{div} \left(\varrho_\alpha h_\alpha v_\alpha \right) - \operatorname{div} \left(\lambda_\mathrm{pm} \operatorname{grad} T \right) = 0$$

Primary variables $p_\mathrm{g}, S_\mathrm{l}/X_\alpha^\kappa, T$

Coupling conditions

Momentum transfer:

- Continuity of normal stresses

$$p_{\mathrm{g}}^{\mathrm{ff}} + n^{\intercal} \left(\varrho_{\mathrm{g}} v_{\mathrm{g}} v_{\mathrm{g}}^{\intercal} - \mu_{\mathrm{g}} \operatorname{grad} v_{\mathrm{g}} \right)^{\mathrm{ff}} n = p_{\mathrm{g}}^{\mathrm{pm}}$$

- Beavers-Joseph-Saffman condition

$$\left(\alpha_{\mathrm{BJ}} v_{\mathrm{g}}^{\mathrm{ff}} - \sqrt{k} \operatorname{grad} v_{\mathrm{g}}^{\mathrm{ff}} n \right) \cdot t_i = 0$$

Mass transfer:

- Continuity of vapor mass fluxes

$$X_{\mathrm{g}}^{\mathrm{w,ff}} = X_{\mathrm{g}}^{\mathrm{w,pm}}$$

- Chemical equilibrium:

$$\left(\varrho_{\mathrm{g}} X_{\mathrm{g}}^{\mathrm{w}} v_{\mathrm{g}} + j_{\mathrm{ff}}^{\mathrm{w}} \right)^{\mathrm{ff}} \cdot n = \sum_{\alpha \in \{\mathrm{g,l}\}} \left(\varrho_{\alpha} X_{\alpha}^{\mathrm{w}} v_{\alpha} + j_{\mathrm{pm},\alpha}^{\mathrm{w}} \right)^{\mathrm{pm}} \cdot n$$

Energy transfer:

- Continuity of temperature

$$T^{\mathrm{ff}} = T^{\mathrm{pm}}$$

- Continuity of energy fluxes

$$\left(\varrho_{\mathrm{g}} h_{\mathrm{g}} v_{\mathrm{g}} + h_{\mathrm{g}}^{\mathrm{w}} j_{\mathrm{ff}}^{\mathrm{w}} + h_{\mathrm{g}}^{\mathrm{a}} j_{\mathrm{ff}}^{\mathrm{a}} - \lambda_{\mathrm{g}} \operatorname{grad} T \right)^{\mathrm{ff}} \cdot n = \left(\varrho_{\mathrm{g}} h_{\mathrm{g}} v_{\mathrm{g}} + \varrho_{\mathrm{l}} h_{\mathrm{l}} v_{\mathrm{l}} - \lambda_{\mathrm{pm}} \operatorname{grad} T \right)^{\mathrm{pm}} \cdot n$$

Mosthaf et al. 2011, Fetzer et al. 2016

Discretization I

Free flow

- Navier-Stokes: Marker and cell scheme
- mass and energy transport: cell-centered FVM

Porous-medium flow

- Darcy, mass, energy: cell-centered FVM

- advective fluxes / transported quantities are up-winded
- complex physical laws

$$\underbrace{\varrho_g v_g}_{\text{up-winding}} \; \underbrace{v_g}_{\text{average}}$$

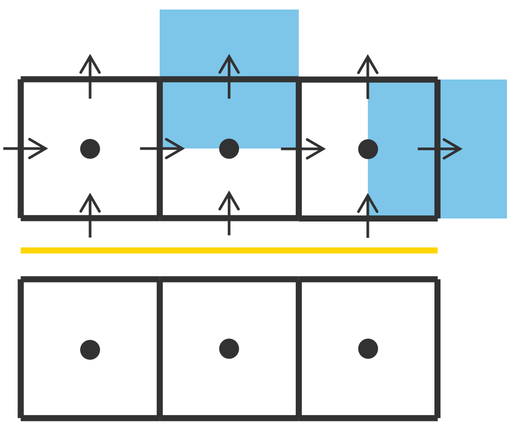
average

up-winding

degrees of freedom:

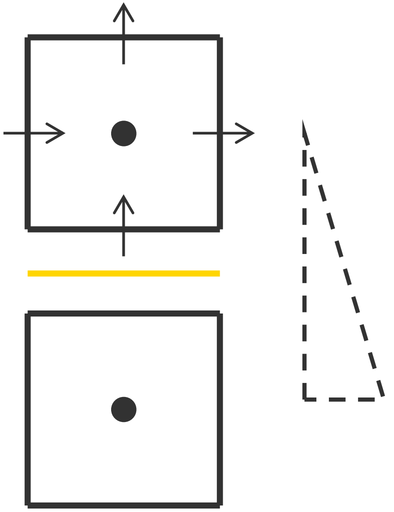
● pressure, component, temperature

→ velocity



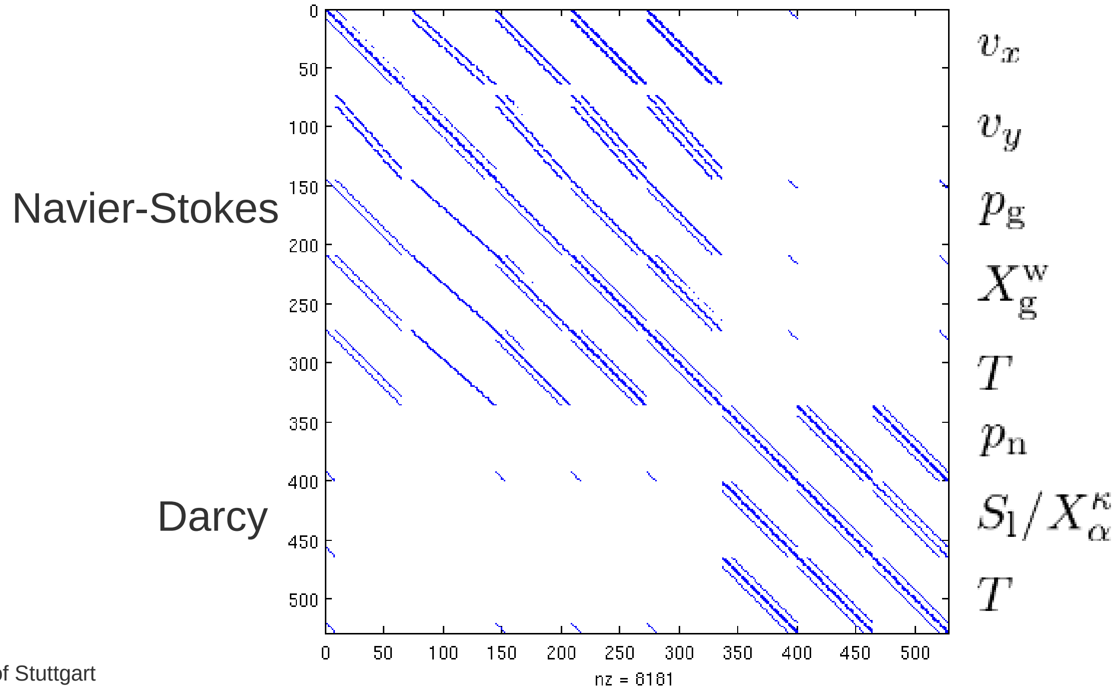
Discretization II: Coupling strategy

- Momentum
  - Dirichlet-Neumann coupling
  - Beavers-Joseph: Robin boundary type
- Mass, energy: finite-volume fluxes
  - fluxes calculated from free-flow side of continuity equations
  - gradient approximated over interface



Jacobian matrix

- linearize coupled system with Newton‘s method
- single large linear system
- contains a saddle point problem
- non-symmetric because of advective terms



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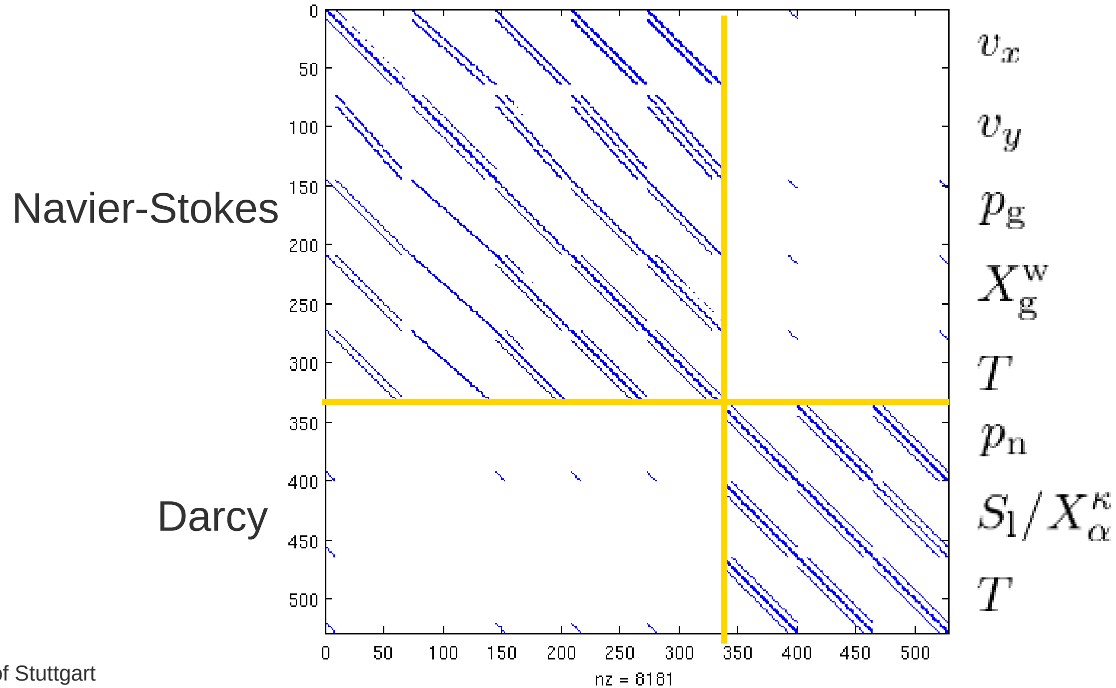

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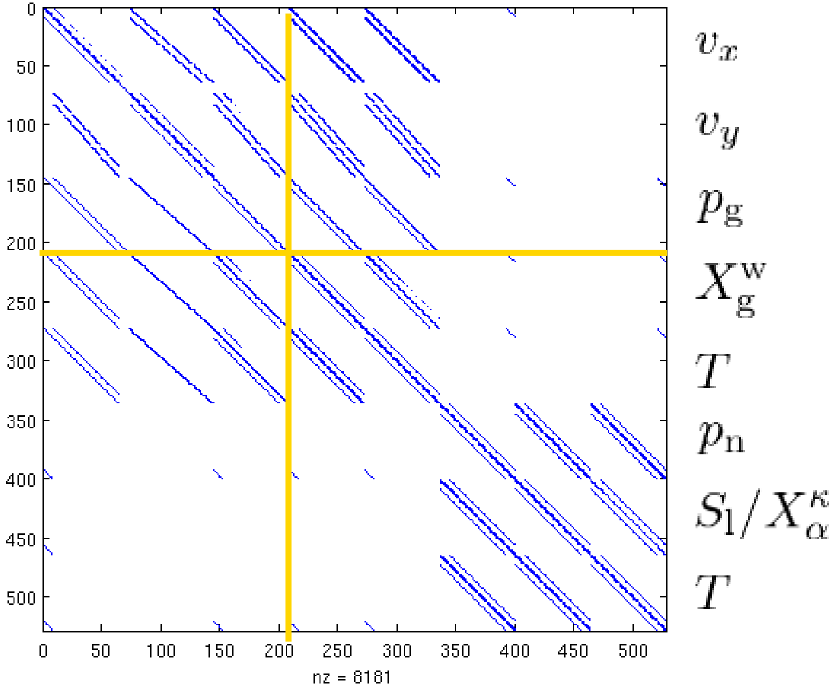
Navier-Stokes

Darcy



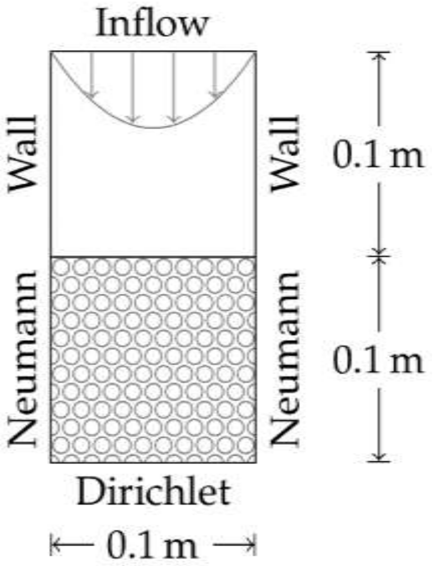
Implementation

- Darcy: porous-medium simulator DuMu^x
- Navier-Stokes: written with DUNE-PDELab
- Coupling: DUNE-MultiDomain
- Linear solver: UMFPack or SuperLU

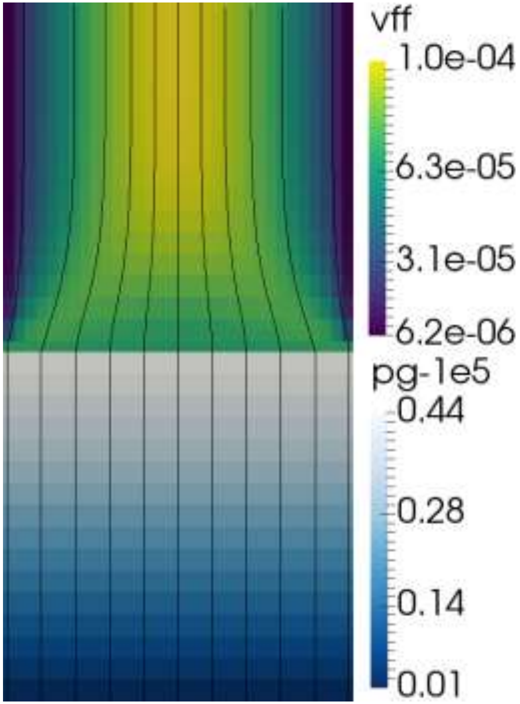
Code will be available for download and use under open source license

Numerical results: Conservation

- normal flow from top to bottom
- closed to left and right
- single-phase, isothermal
- compare inflow to outflow

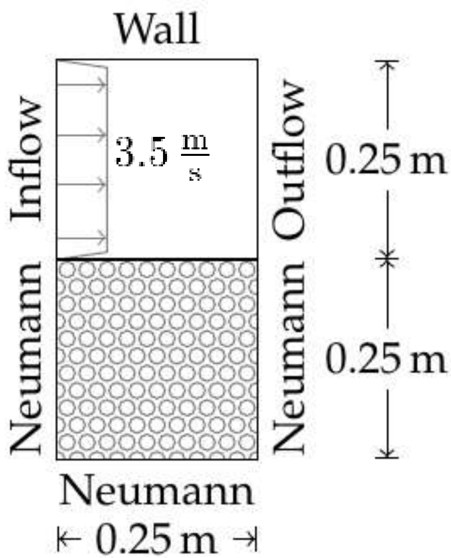


Grid	Flux difference
8^2	$5.22 \cdot 10^{-10}$
16^2	$5.11 \cdot 10^{-10}$
32^2	$5.07 \cdot 10^{-10}$
64^2	$5.05 \cdot 10^{-10}$

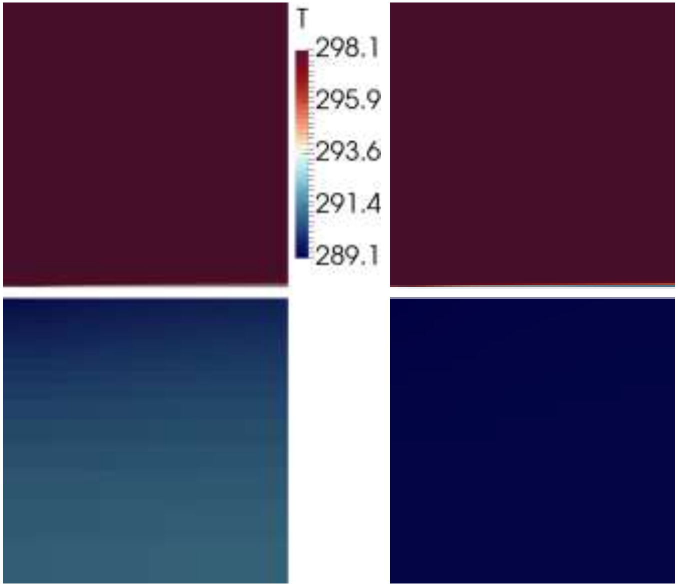


Numerical results: Windtunnel

- motivated from lab experiment, Mosthaf et al. 2014
- air flows over water-filled box
- box on top of balance
- 1024 elements per subdomain



Temperature

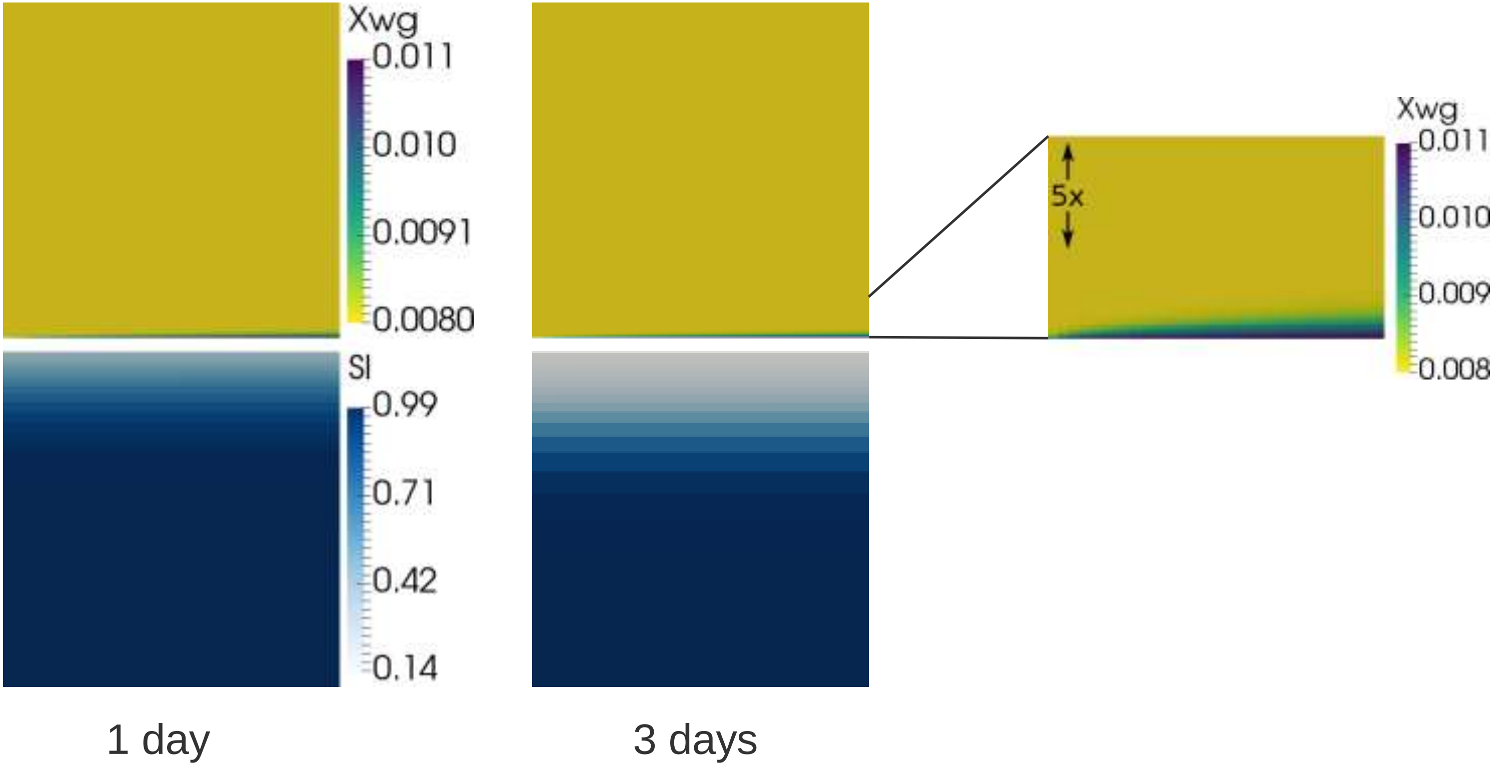


1 day

3 days

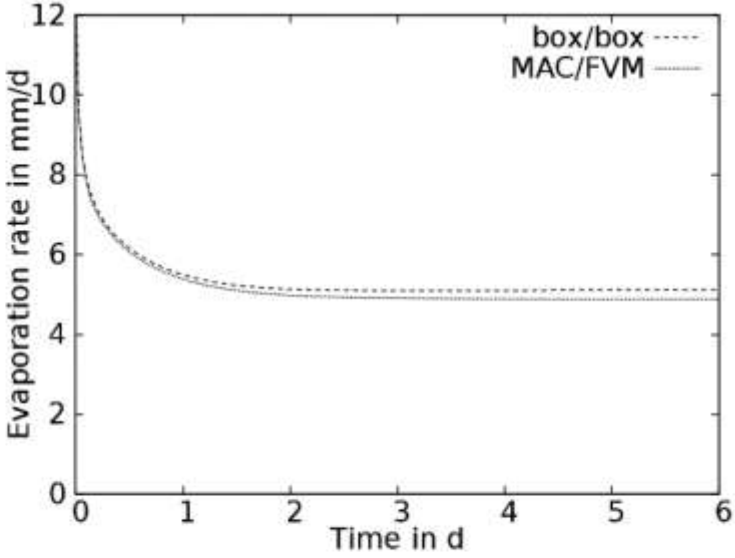
Numerical results: Windtunnel II

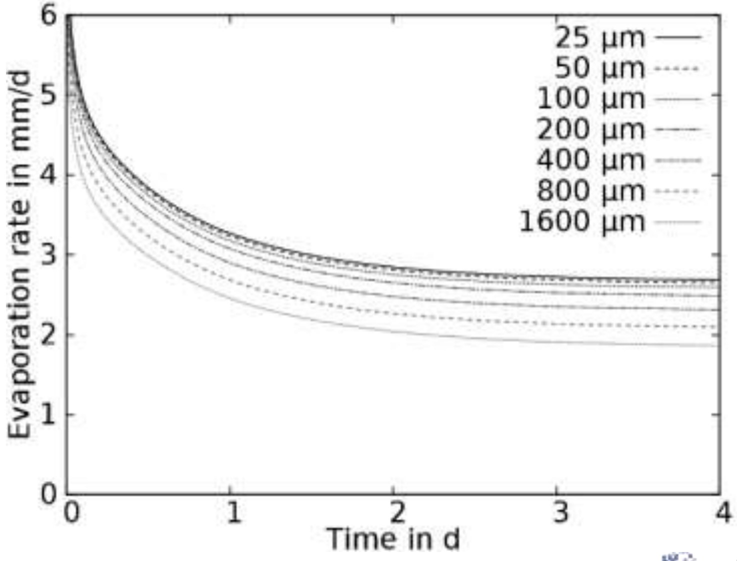
Vapor mass fraction, water saturation



Numerical results: Comparison and convergence

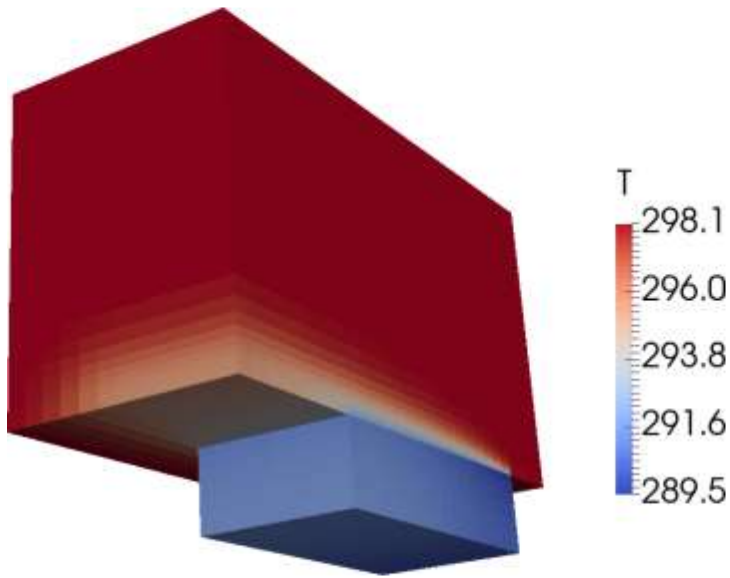
- evaluate overall evaporation rate
- compare to box/box scheme
- check behavior for thinner grid cells around interface, use Stokes flow





Numerical results: 3d

- extended to three dimensions
- enlarged free-flow domain
- symmetry boundary condition



Linear solver

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

Schur complement

$$\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right) x_2 = b_2 - A_{21}A_{11}^{-1}b_1$$

$$A_{11}x_1 = b_1 - A_{12}x_2$$

Block Jacobi

$$\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} x_1^n \\ x_2^n \end{pmatrix} = \begin{pmatrix} b_1 - A_{12}x_2^{n-1} \\ b_2 - A_{21}x_1^{n-1} \end{pmatrix}$$

- all tested combinations 10 times slower compared to direct methods
- asymmetry prevents use of many preconditions and solvers
- stick to direct solvers

Outlook

Further investigate coupling conditions

Speedup

- assembly: simplify physics
- linear solver: parallelize, GPU

Improve decoupling

- algebraic level
- model decoupling

Applications

- more sophisticated setups
- third-party users