Weierstrass Institute for Applied Analysis and Stochastics

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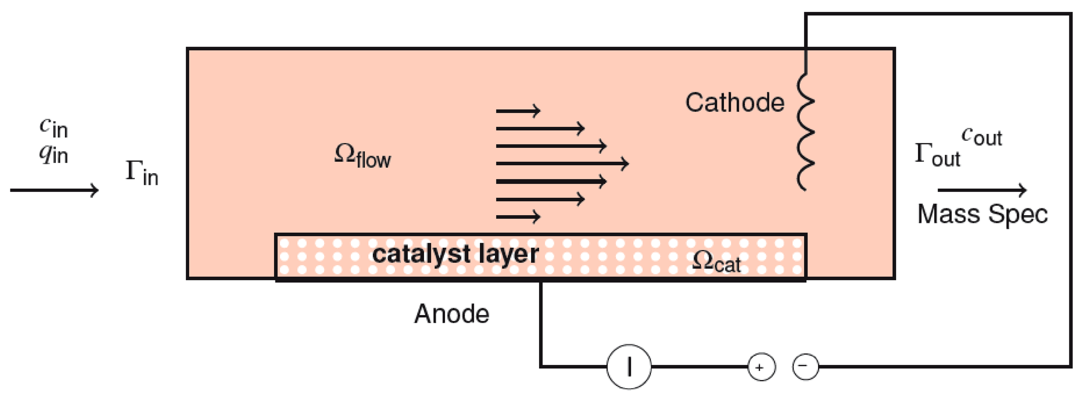
# Finite element - finite volume coupling for simulations of thin porous layer fuel cells

Leibniz Gemeinschaft

## Porous layer in fuel cells




- Physical background
  - Porous electrodes in fuel cells increase active area and improve reactant mixing [1]
  - Reactant supply through flow channels results in free-porous flow interface
- Goals
  - Investigate influence of free-porous interface on limiting current behavior

## Two-dimensional model: flow and reactant transport

- Stokes equations in the channel:

$$\nabla p_f - \operatorname{div}\left(\nu D(\mathbf{u}_f)\right) = 0, \text{ in } \Omega_f$$
$$\operatorname{div}\mathbf{u}_f = 0, \text{ in } \Omega_f$$

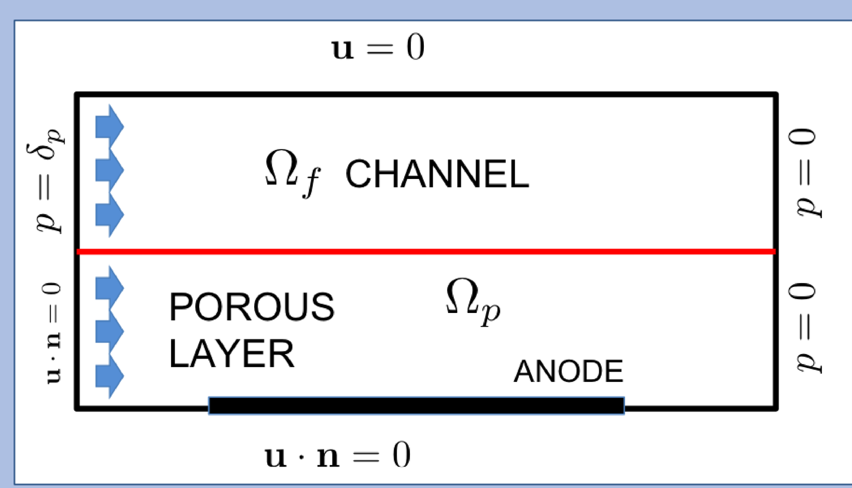
- Darcy's law in the diffusion layer:

$$K^{-1}\mathbf{u}_p + \nabla p_p = 0, \text{ in } \Omega_p$$
$$\operatorname{div}\mathbf{u}_p = 0, \text{ in } \Omega_p$$

- Interface conditions on $\Gamma$:
  - Mass conservation: $[\![\mathbf{u}\cdot\mathbf{n}]\!] = 0$
  - Efforts continuity: $p_f - \nu\mathbf{n}^T D(\mathbf{u}_f)\mathbf{n} = p_p$
  - Beavers-Joseph: $\nu\mathbf{n}^T D(\mathbf{u}_f)\mathbf{t}_j = -\alpha_j [\![\mathbf{u}_f\cdot\mathbf{t}_j]\!],\, j = 1,\ldots,d-1$
- Solute transport:

$$\partial_t c + \mathbf{u}\cdot(\nabla c) - D_c\Delta c = 0, \text{ in } \Omega$$

- Boundary conditions:
  - Injection at the inlet
  - $c = 0$ at the anode

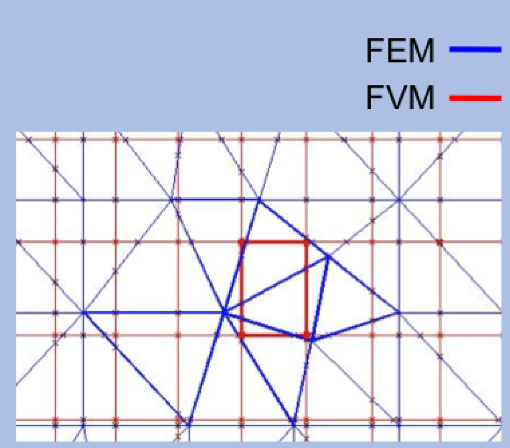



## Stokes-Darcy coupling in finite element framework

- Domain decomposition approach [2]
- Discretizations:
  - Taylor-Hood elements ($P_2/P_1$) for Stokes equations
  - $P_1/P_1$ stabilized finite elements for Darcy equations [3]
  - Nitsche penalty for velocity continuity at the interface
- Fixed point iteration:
  - Solve Stokes equations with given interface velocity
  - Solve Darcy equations with given pressure
- Direct sparse solver

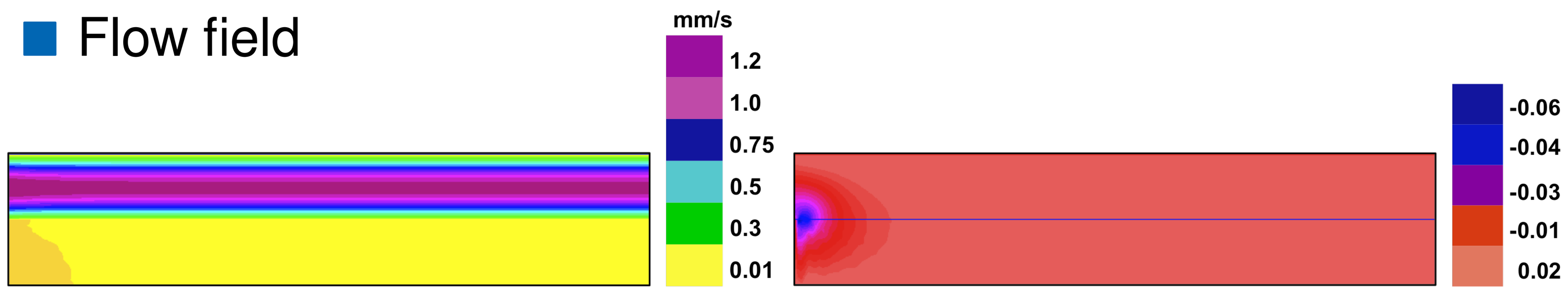
## Finite volume method for solute transport

- Upwind method based on Voronoi-boxes [4]
- Aligned grid with Delaunay triangulation
- Suitable for convection dominated problems with sharp layers [5]
- Solved with `pdelib2` (WIAS)
- Coupling with flow:
  - Independent discretization
  - FEM flux integration over Voronoi box boundaries




## Numerical results

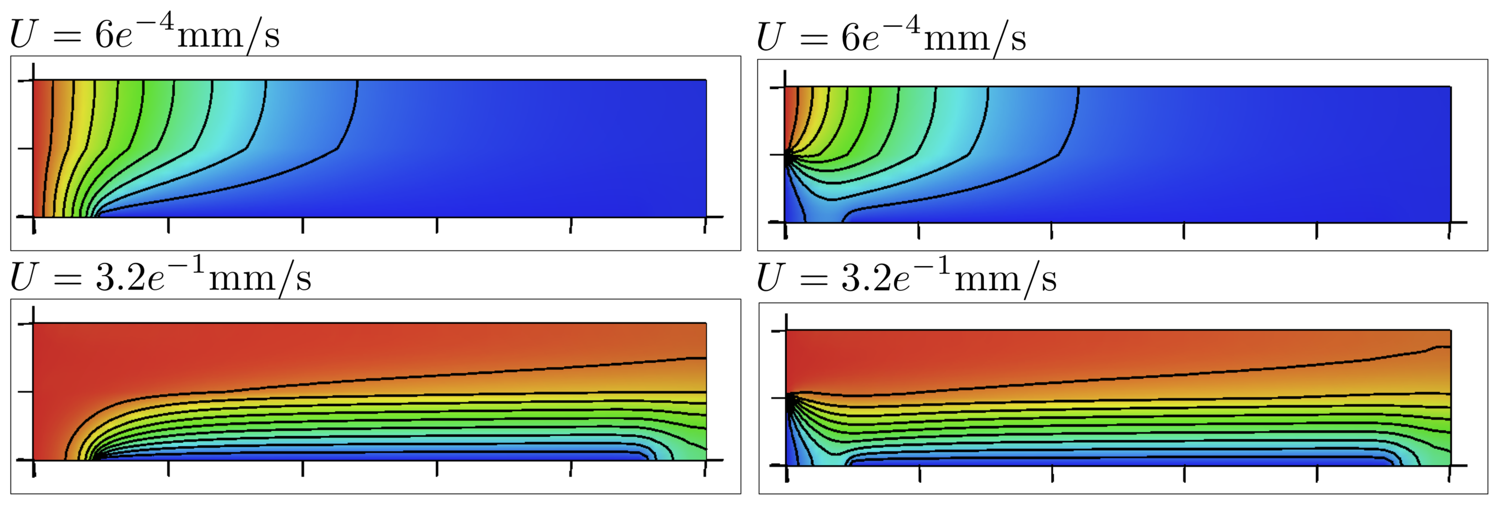
- Flow field




**Left.** Horizontal velocity. **Right.** Vertical velocity.

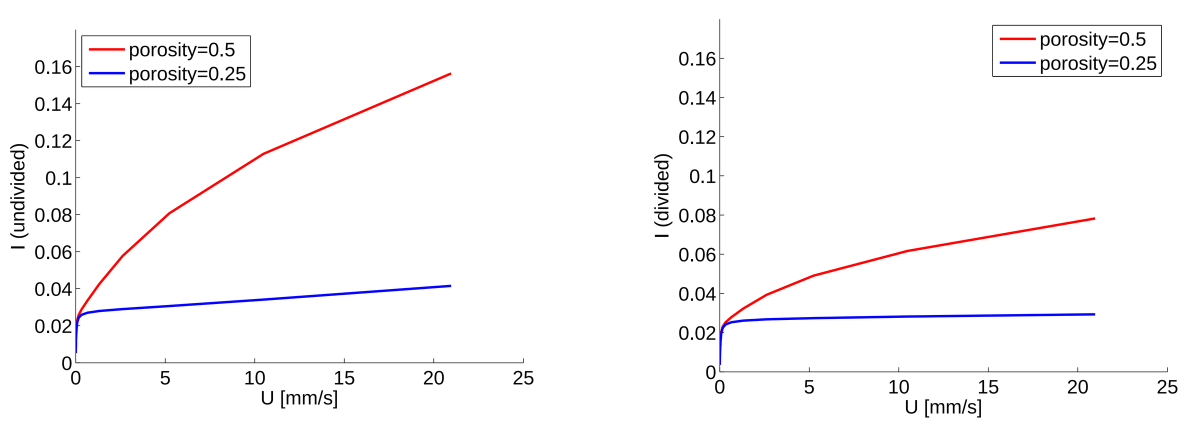
- Concentration field, for increasing injection velocities ($U$)

(red: $c = 1$, blue: $c = 0$)




**Left**: undivided input. **Right**: divided input.

- Limiting current




**Left**: undivided input. **Right**: divided input.

## Outlook

- Different discretizations for all equations
- Different coupling strategies
- Accelerated fixed point iterations
- 3D simulations
- Electrochemical reactions

## References

[1] J. Divisek, J. Fuhrmann, K. Gärtner, R. Jung, J. Electrochem. Soc., **150**(6) 2003.

[2] C. D'Angelo, P. Zunino, Math. Model. Numer. Anal. (M2AN), **45**(3), 2011.

[3] M.R. Correa, A.F.D. Loula, Comp. Meth. Appl. Mech. Engnr., **198**(33-36), 2009.

[4] J. Fuhrmann, A. Linke, H. Langmach, Appl. Num. Math., **61**(4) 2011.

[5] M. Augustin *et al.*, Comp. Meth. Appl. Mech. Engnr., **200**(47-48) 2011.

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