Weierstrass Institute for Applied Analysis and Stochastics
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Leibniz Group 1: Coupled Flow Processes in Energy and Environmental Research

The PAKT Network

- ▷ Weierstrass Institute for Applied Analysis and Stochastics
- ▷ Free University Berlin
- ▷ Friedrich-Alexander-University Erlangen–Nuremberg
- ▷ Potsdam Institute for Climate Impact Research
- ▷ University Potsdam

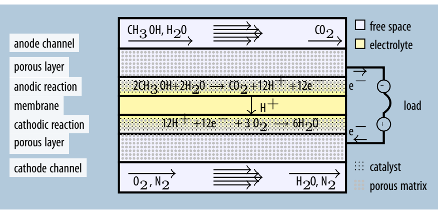
The mathematical modelling and numerical solution of coupled flow processes is an important and challenging interdisciplinary problem:

- ▷ **Appearance of coupled flow processes:** energy research, geo sciences, environmental and climate research, civil engineering, materials science
- ▷ **Research topics of the network:** reactive transport of dissolved species, coupling of free flow and porous media flow, exchange processes in multi–phase flows
- ▷ **Mathematical models:** free flow: (incompressible) Navier–Stokes equation, porous media flow: Darcy and Brinkman model, soil hydrology: (stochastic) Richards equation, species transport: reaction–diffusion–convection equation, interface conditions: boundary layer theory, Beavers–Joseph jump condition,...

The Leibniz Group 1

- ▷ **Project leader:** J. Fuhrmann
- ▷ **Work package I:** Divergence–free Finite Volume Methods for Flows Coupled with Transport Processes (A. Linke)
- ▷ **Work package II:** Interface Conditions Between Free Flow and Porous Media Flow in Fuel Cells (M. Ehrhardt)

Numerical simulation of coupled flows in porous media and free flow situations is essential for many industrial and environmental problems. Both kinds of flows appear together e.g. in proton exchange membrane (PEM) fuel cells. The transport of the fuel to the active zones, and the removal of the reaction products are realized by channels and porous diffusion layers. Mathematical models of PEM fuel cells aim at optimizing the important water management. For this issue a deeper understanding of the coupling of the flow processes is necessary.



The Coupling of Free Fluid and Porous Media Flow

- ▷ Different models for fluid–porous interfaces [1,2] (Navier–Stokes and Darcy/Brinkman)
- ▷ appropriate interface conditions for the coupling of free flow and porous media flow
- ▷ two and three layer models

▷ **Free Flow: incompressible isothermal Navier–Stokes equations** (or Stokes equations for creeping flow)

$$-\mu\Delta\mathbf{u}+(\rho\mathbf{u}\cdot\nabla)\mathbf{u}=\mathbf{f}_{\mathrm{NS}}-\nabla p,\qquad \nabla\cdot\mathbf{u}=0,\qquad \mathbf{x}\in\Omega_f \qquad \text{(NS)}$$

▷ **Different (Macroscopic) Mathematical Models for Saturated Flow in Porous Media in** Ω_p:

– **Darcy Model** of the flow rate is sufficiently low

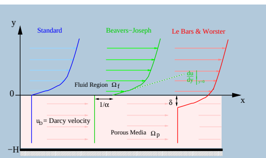
$$\mu\mathbf{K}^{-1}\mathbf{u}=\mathbf{f}_{\mathrm{D}}-\nabla p,\qquad \nabla\cdot\mathbf{u}=0,\qquad \mathbf{x}\in\Omega_p \qquad \text{(D)}$$

– **Brinkman Model** (in order to account for **high porosity** (i.e. $\phi\geq 0.6$) or to impose **no–slip conditions** on solid walls

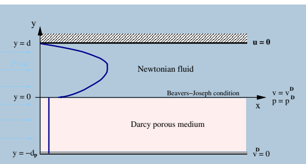
$$-\nabla\cdot(\mu_{\mathrm{eff}}\nabla\mathbf{u})+\mu\mathbf{K}^{-1}\mathbf{u}=\mathbf{f}_{\mathrm{B}}-\nabla p,\qquad \nabla\cdot\mathbf{u}=0,\qquad \mathbf{x}\in\Omega_p \qquad \text{(B)}$$

Fluid–Porous Interface Conditions and Exact Solutions

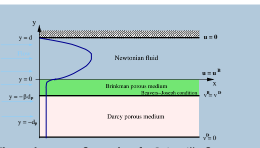
- ▷ **classification of flow:** near parallel flow , near normal flow
- ▷ Fluid–Porous Interface Conditions
  - – Beavers–Joseph jump condition (1967)
  - – Le Bars & Worster condition (2003)
  - – Transition Zone Approach by Hill & Straughan (2008)
- ▷ **exact solutions** for basic flow in two and three layer models
  - – to validate numerical code



standard case: no–slip condition on the fluid–porous interface
Beavers–Joseph condition: slip of size $1/\alpha$ on the interface
Le Bars & Worster condition: slip by δ into porous media



Two–layer configuration for Poiseuille flow overlying a porous medium (Darcy): velocity is significantly discontinuous at interface



Three–layer configuration for Poiseuille flow overlying a porous medium with Brinkman transition layer: still discontinuity in velocity between Brinkman and Darcy layers with relative error $\gamma\sim 1/\beta$ of lower order

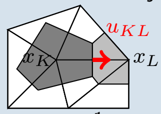
Finite Volume Methods and Discrete Maximum Principle

- ▷ **Goal:** preserve continuous properties for discrete viscous conservation laws
  - – discrete maximum principle
  - – positivity (important for nonlinearities)
- ▷ compatible divergence-free discretization of incompressible Navier–Stokes equations

- ▷ **Goal:** development of covolume methods for the incompressible Navier–Stokes equations in 2d and 3d customized for coupling to reaction-convection-diffusion equations
- ▷ **Idea:** $-\nabla\cdot(D\nabla c-c\vec{u})=0$ fulfills a maximum principle $\iff$ $\nabla\cdot\vec{u}=0$
- ▷ **Starting point:** divergence-free mixed Scott–Vogelius FEM for Navier-Stokes equations
- ▷ **New covolume method:** degrees of freedom: $\vec{u}^h\cdot\vec{n}$ located at edge center, $\vec{n}\perp$ Voronoi face
- ▷ use of duality between boundary conforming Delaunay [5] and Voronoi grids $\Longrightarrow$ appropriate discretization of differential operators ∇, $\nabla\cdot$ and $\nabla\times$ possible using Gauss' and Stokes' theorems
- ▷ discrete maximum principle preserved for some classes of nonlinear reaction-convection-diffusion equations

Discretization of the divergence

K, L: control volumes
V_{KL}: Voronoi face $\perp$ to edge $\overline{KL}$:

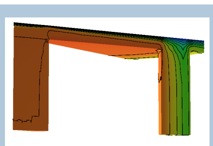


$$\mathrm{div}_h(x_K):=\frac{1}{|K|}\sum_{L\in\mathcal{N}(K)}u_{KL}|V_{KL}|$$

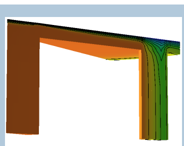
Numerical Results

Simulation of electrochemical experiments relevant for fuel cell modelling, done by partners from electrochemistry [4]
here: cooperation with WIAS Research Group 3 (Numerics)

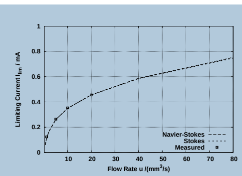
- ▷ mixed finite elements for the flow field
- ▷ finite volumes for reaction-convection-diffusion equations
- ▷ integration of the FEM velocity normals over faces of the FVM control volumes



Taylor–Hood flow (weakly divergence-free) yields to a violated discrete maximum principle for a coupled convection-diffusion equation



Scott–Vogelius flow (strongly divergence-free) yields to a fulfilled discrete maximum principle for a coupled convection-diffusion equation



The numerical simulated limiting current compares well to the experimental data

References

[1] M. Ehrhardt, J. Fuhrmann, E. Holzbecher and A. Linke, *Mathematical Modeling of Channel–Porous Layer Interfaces in PEM Fuel Cells*, in: B. Davat and D. Hissel (ed.), Proceedings of 'FDFC2008 – Fundamentals and Developments of Fuel Cell Conference 2008', Nancy, France, December 10–12, 2008, ISBN 978-2-7466-0413-1.

[2] M. Ehrhardt, J. Fuhrmann and A. Linke, *The Fluid–Porous Interface Problem: Analytic and Numerical solutions to Flow cell problems*, in Proceedings of MODVAL6 – 6th Symposium on Fuel Cell Modelling and Experimental Validation, Bad Herrenalb/Karlsruhe, Germany, March 25–26, 2009.

[3] R. Eymard, J. Fuhrmann and K. Gärtner, *A finite volume scheme for nonlinear parabolic equations derived from one-dimensional local Dirichlet problems*, Numer. Math. **102** (2006), 463–495.

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[5] H. Si, *Three–Dimensional Boundary Conforming Delaunay Mesh Generation*, Ph.D Thesis, Technical University Berlin, 2008. Webpage: http://tetgen.berlios.de/

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