SimTech Cluster of Excellence

University of Stuttgart Germany

Coupling of micro- and macro models for complex flow and transport processes in biological tissue

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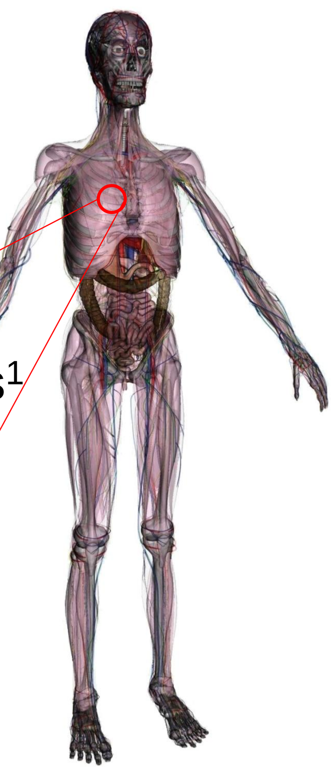
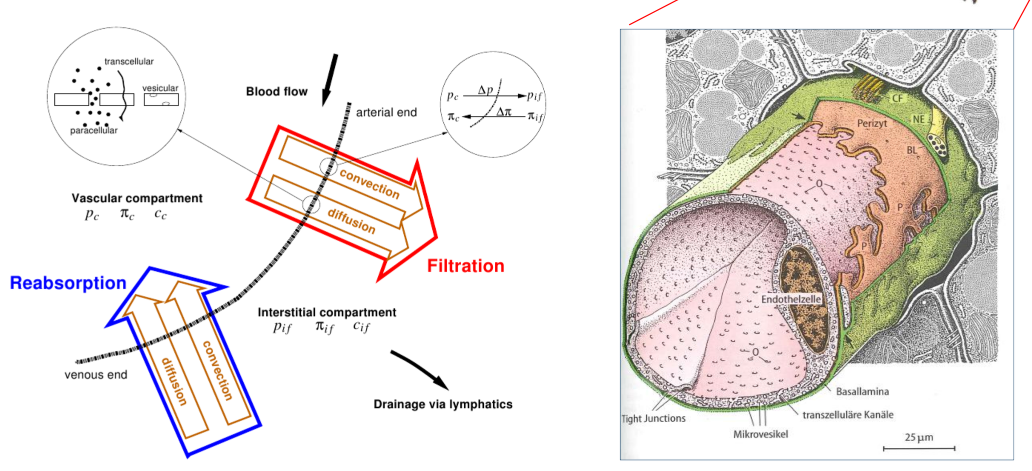
Motivation

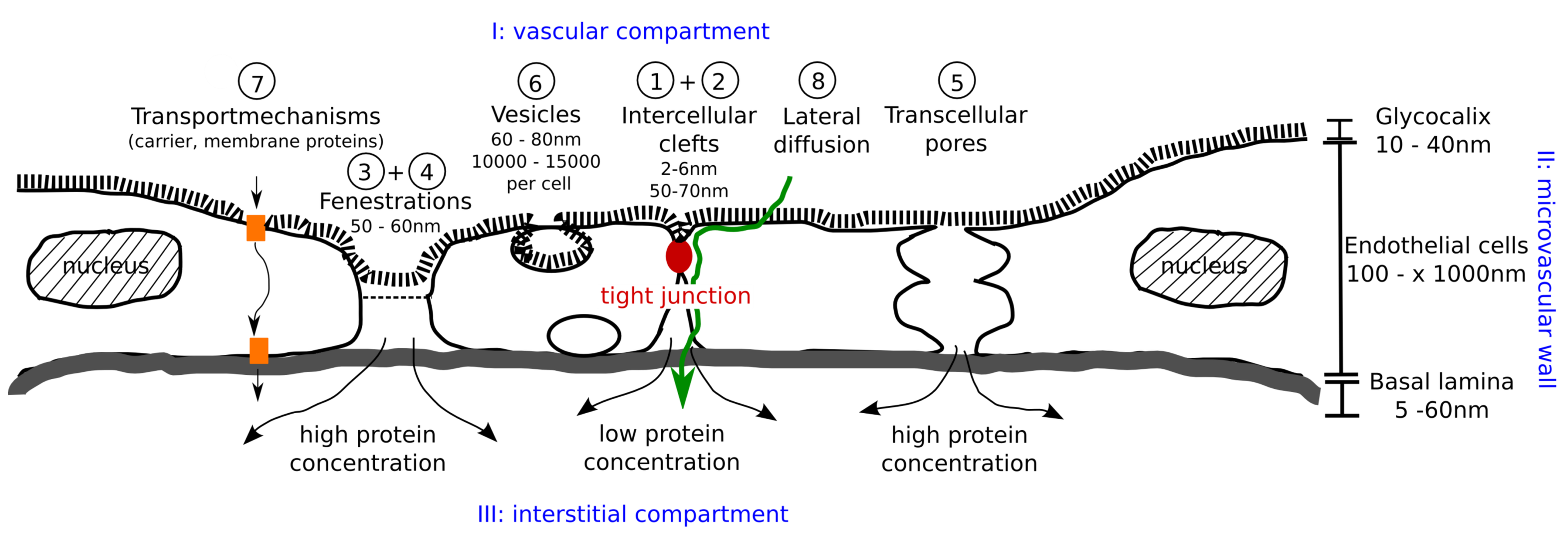
Goal: coupling free flow with flow in porous media
→ focus on the interface structure and processes
Application: transvascular exchange of therapeutic agents[1]





Transvascular flow and transport processes (Junqueira et al., 2005)

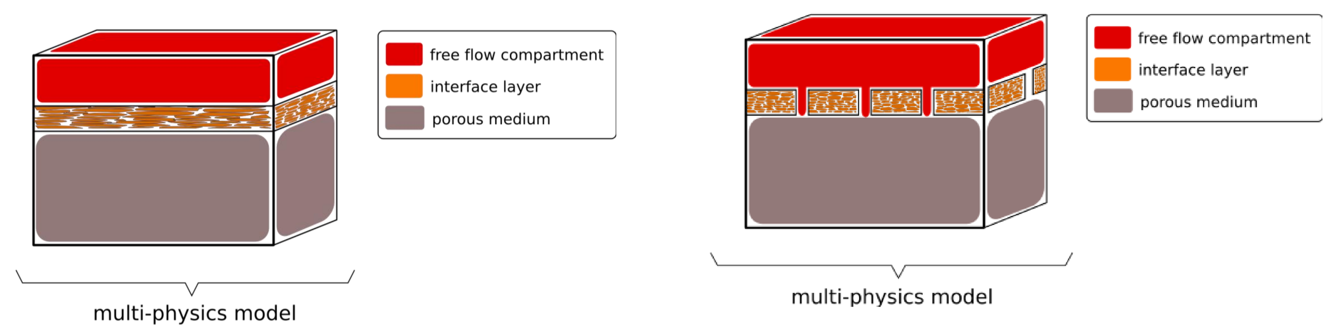
→ exchange processes strongly dependent on wall structure as well as on size and charge of transported substance



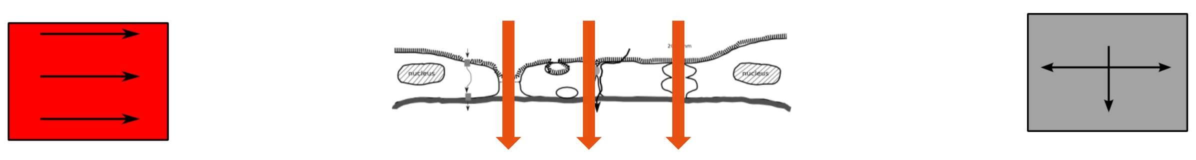
Structure of the capillary wall: variety of para- and transcellular pathways, structure strongly dependent on anatomic location as well as on physiological and pathological conditions

→ crucial to resolve the structure of the microvascular wall and the occurring transport processes

Description of capillary wall as porous medium



- continuum description, same scale for all compartments
- single phase, compositional flow (blood/plasma + therapeutic agent)
- incompressible, Newtonian fluids



$\mathrm{Re} = 0.0496$	$\mathrm{Re} \approx 10^{-10} - 10^{-4}$	$\mathrm{Re} = 4.3 \cdot 10^{-6}$
$\mathrm{Pe} = 800$	$\mathrm{Pe} \approx 10^{-2} - 10^{6}$	$\mathrm{Pe} = 0.083$

- viscous flow, inertial forces negligible
⇨ applicability of Stokes and Darcy
- advective processes dominate in capillary, diffusion dominates in tissue
- no lateral flow in capillary wall ⇨ no-slip condition at wall surface

→ **coupled model for free flow and flow in porous media**[2]

Continuity of normal forces:

$$[((p\mathbf{I} - \mu\nabla \boldsymbol{v})\mathbf{n}) \cdot \mathbf{n}]^{\mathrm{ff}} = [p]^{\mathrm{pm}}$$

Continuity of mass fluxes:

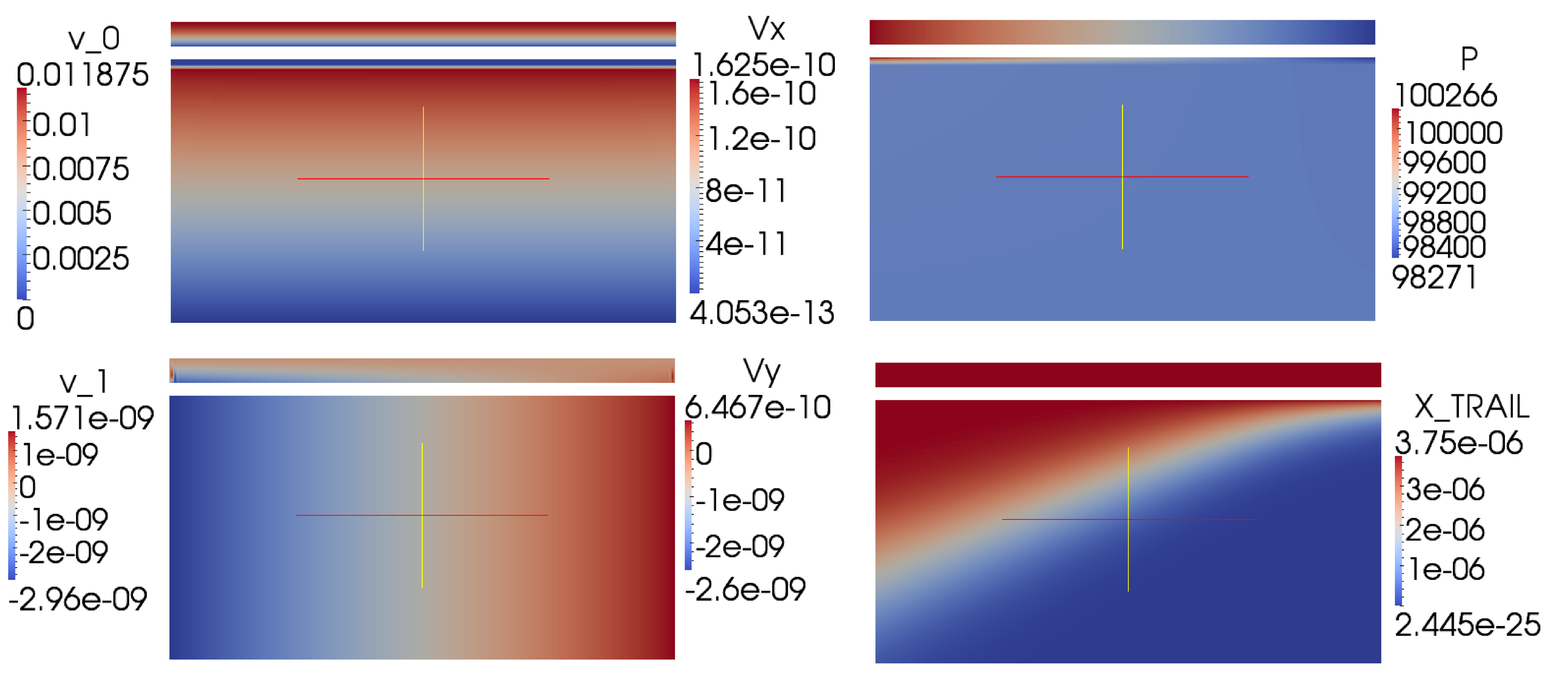
$$[\rho \boldsymbol{v} \cdot \mathbf{n}]^{\mathrm{ff}} = -[\rho \boldsymbol{v} \cdot \mathbf{n}]^{\mathrm{pm}}$$

$$[(\rho \boldsymbol{v} X^\kappa - \rho D^\kappa \nabla X^\kappa) \cdot \mathbf{n}]^{\mathrm{ff}} = -[(\rho \boldsymbol{v} X^\kappa - \rho D^\kappa \nabla X^\kappa) \cdot \mathbf{n}]^{\mathrm{pm}}$$

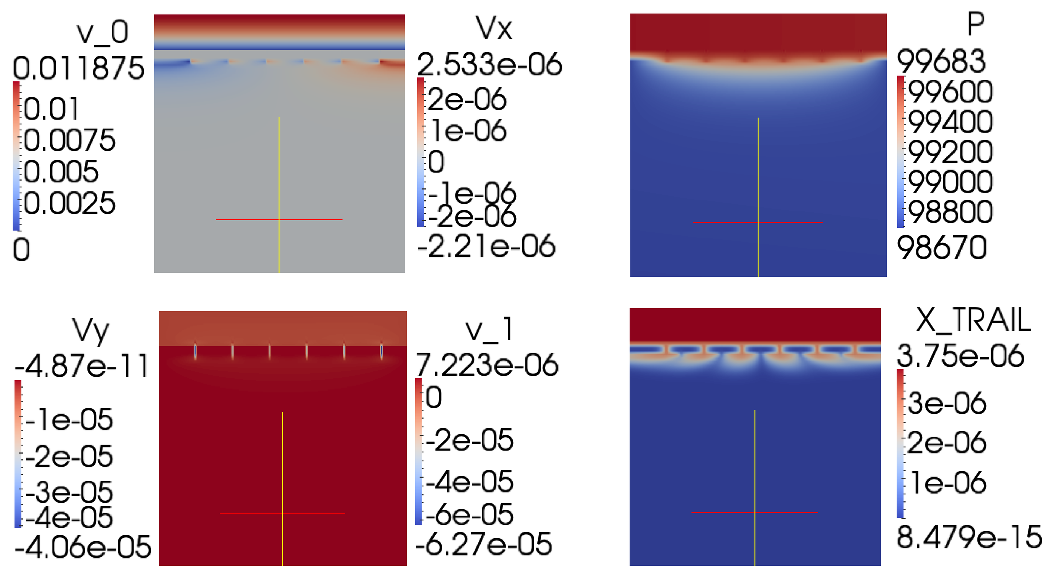
Continuity of mass fractions:

$$[X^\kappa]^{\mathrm{ff}} = [X^\kappa]^{\mathrm{pm}}$$

First results



Homogeneous capillary wall: Distribution of pressure [Pa], x- and y-velocity [m/s] and mass fractions of a dissolved substance



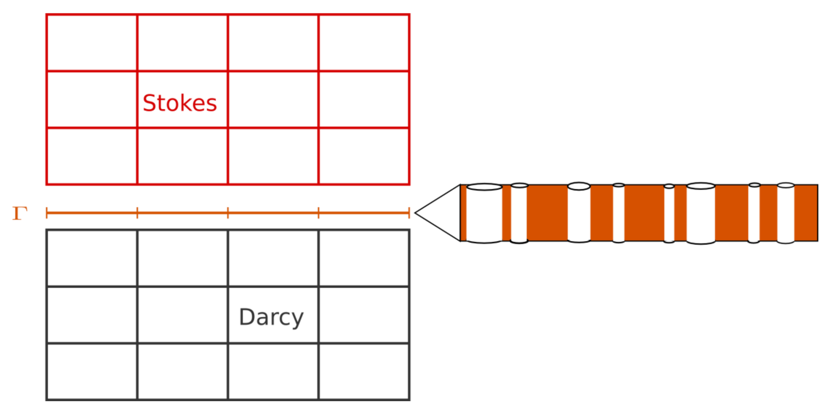
Heterogeneous capillary wall: Distribution of pressure [Pa], x- and y-velocity [m/s] and mass fractions of a dissolved substance (K_{pores} = 3.125e-16 m^2 calculated with Poisseuille)

- fails to resolve structures and processes of capillary wall
- volume-averaged models not applicable to a thin, heterogeneous structure like the capillary wall

Description of capillary wall as bundle-of-tubes model

- macro-models for vascular and interstitial compartment
- micro-model for capillary wall:
  paracellular pathways = straight, rigid, cylindrical tubes
- influence of electro-chemical processes at glycocalyx can be included
- no adsorption, desorption or retardation processes

→ **coupled micro-/macro-model**



free flow	pore model	porous medium
$\nabla p - \mu \nabla \cdot (\nabla \boldsymbol{v}) = 0$	$\bar{u}_k = \underbrace{\left(\frac{R_k^2}{8\mu} + \frac{1}{2}\frac{L_s}{R}\right)}_{K(R_k,\mu,L_s)} \frac{\partial p}{\partial z}$	$\nabla \cdot \left(-\frac{\mathbf{K}}{\mu}\nabla p\right) = 0$

$$\Phi_r \, \rho \frac{\partial X^\kappa}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}_r X^\kappa - \rho D_r^\kappa \nabla X^\kappa) = 0$$

→ coupled with mortar method[3] for non-conforming meshes
→ monolithic coupling envisaged

References

[1] Curry, F. E. Mechanics and thermodynamics of transcapillary exchange. Handbook of Physiology, Section2: The Cardiovascular System, Vol. IV, Part1, 308-374, American Physiological Society, (1984).
[2] Mosthaf K.; Baber, K.; Flemisch, B.; Helmig, R.; Leijnse, T.; Rybak, I. and Wohlmuth, A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow. Submitted to Water Resources Research (2011).
[3] Balhoff, M. T. ; Thomas, S.G.; Wheeler, M. F.: Mortar coupling of pore-scale models. Comput Geosci. 12, 15-27 (2008).

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