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NATURWISSENSCHAFTLICHE
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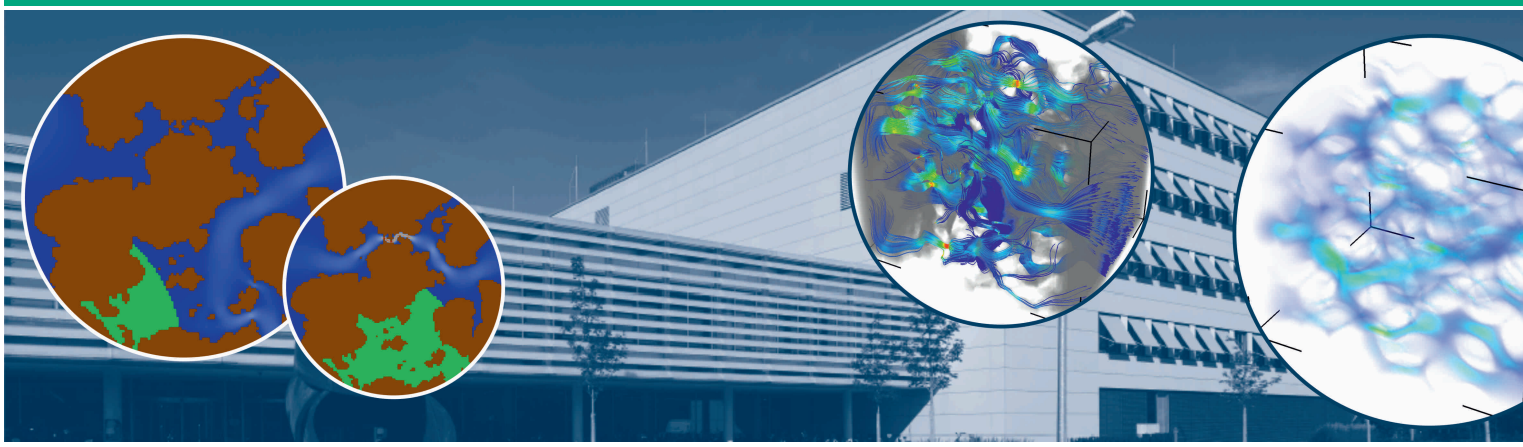
Workshop on Recent Developments in Modelling, Analysis and Simulation of Processes in Porous Media

On the Occasion of Peter Knabners 65th Birthday



Invited Speakers:

Hans van Duijn, Eindhoven University of Technology, The Netherlands
Rainer Helmig, University of Stuttgart, Germany
Mario Putti, University of Padova, Italy
Florin A. Radu, University of Bergen, Norway

Subjects of the workshop include:

Multiscale Phenomena, Algorithmic Developments, Digital Rock Simulations, Multiphase Problems, Homogenization, …

Deadlines:

Submission of Abstracts for Talks 31.01.2020
Registration for Participation 14.02.2020

pormed2020@math.fau.de

Announcement

March 05/06 2020

University
Erlangen-Nürnberg
Germany

More information & registration: math.fau.de/pormed2020

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Supported by Research Training Group 2339, IntComSin

Thursday, March 5th	
8:30 - 9:30	**Invited Presentation**
	Rainer Helmig, *Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart, Germany* Interfaces in porous media are (almost) everywhere: Do we need multi-scale concepts and strong cooperation between mathematicians and engineers?
9:30 - 10:00	**Coffee break**
10:00 - 12:00	**Minisymposium 1**
10:00 - 10:20	**Oleg Iliev**, *Fraunhofer ITWM* TBA
10:20 - 10:40	~~**Matteo Icardi**, *University of Nottingham*~~ ~~Upscaled models for heterogeneous reactions and conjugate transfer in porous media~~
10:40 - 11:00	**Lubomir Banas**, *Bielefeld University* Numerical homogenization of complex flow in porous media
11:00 - 11:20	**Renata Bunoiu**, *University of Lorraine, Metz* Homogenization of Bingham Flow in Thin Porous Media
11:20 - 11:40	**Malte Peter**, *University of Augsburg* Homogenisation of Stokes flow in a porous medium with evolving microstructure
11:40 - 12:00	**Angelika Humbert**, *Alfred Wegener Institute, Bremerhaven* Ice sheet hydrology - challenges and concepts
12:00 - 13:00	**Lunch break**
13:00 - 14:00	**Invited Presentation**
	Hans van Duijn, *Department of Mathematics and Computer Science, Eindhoven University of Technology, The Netherlands* Fronts in two-phase porous media flow: the effects of hysteresis and dynamic capillarity
14:00 - 16:00	**Minisymposium 2**
14:00 - 14:20	**Michel Kern**, *INRIA Paris* Space-time domain decomposition for two-phase flow between different rock types
14:20 - 14:40	**Markus Knodel**, *University of Erlangen* Global implicit solver for multiphase multicomponent flow in porous media with multiple gas phases and general reactions
14:40 - 15:00	**Ernesto Monaco**, *ESS Engineering Software, Steyr* Numerical Simulation of Supercritical Carbon Dioxide Flow with Finite Elements and Lattice Boltzmann Methods
15:00 - 15:20	**Darrell Tang**, *Wageningen University & Research* Performance of Aquifer Storage Systems
15:20 - 15:40	**Sorin Pop**, *Hasselt University* Flow and reactive transport in porous media
15:40 - 16:00	**Lukas Unglehrt**, *Technische Universität München* Flow regimes in oscillatory porous media flow
16:00 - 16:30	**Coffee break**
16:30 - 18:10	**Minisymposium 3**
16:30 - 16:50	**Marvin Fritz**, *Technical University of München* On the unsteady Darcy-Forchheimer-Brinkman equation in tumor growth models

16:50 - 17:10	**Salvatore Di Stefano**, *Politecnico di Torino* Biological tissues with evolving internal structure: modelling approach and numerical simulations
17:10 - 17:30	**Alice Lieu**, *University of Erlangen* Soils in silico - solutes, biofilms and structure formation
17:30 - 17:50	**Thomas Ritschel**, *University of Jena* Aggregate formation dynamics driven by 3D fluid flow in natural porous media
17:50 - 18:10	~~**Pavan Cornelissen**, *Wageningen University & Research*~~ ~~Salt transport in charged porous media~~
19:30	**Dinner**
Friday, March 6th	
8:30 - 9:30	**Invited Presentation**
	Mario Putti, *Department of Mathematics, University of Padova, Italy* Numerical L1 optimal transport via gradient flow
9:30 - 10:00	**Coffee break**
10:00 - 12:00	**Minisymposium 4**
10:00 - 10:20	**Olaf Ippisch**, *TU Clausthal* Efficient DG-based simulation of coupled surface subsurface flow
10:20 - 10:40	**Philipp Selzer**, *University of Tübingen* Postprocessing of Standard Finite-Element Velocity Fields and Semi-Analytical Particle Tracking Applied to Variably Saturated Flow in Porous Media
10:40 - 11:00	**Nicolae Suciu**, *University of Erlangen* Random walk solutions of the Richards equation
11:00 - 11:20	**Iryna Rybak**, *University of Stuttgart* Estimation of permeability for regular porous structures
11:20 - 11:40	**Peter Frolkovič**, *University of Technology, Bratislava* Level set methods in applications for porous media
11:40 - 12:00	**Stephan Gärttner**, *University of Erlangen* Efficiency and Accuracy of Micro-Macro Models for Mineral Dissolution/Precipitation
12:00 - 13:00	**Lunch**
13:00 - 14:00	**Invited Presentation**
	Florin A. Radu, *Deparment of Mathematics, University of Bergen, Norway* On iterative solvers for nonlinear, coupled problems in porous media
14:00 - 16:00	**Minisymposium 5**
14:00 - 14:20	**Andro Mikelić**, *University of Lyon 1* Mathematical theory and simulations of semi-linear thermoporoelasticity
14:20 - 14:40	**Jakub Both**, *University of Bergen* Robust iterative decoupling of poroelasticity models resulting from a gradient flow interpretation
14:40 - 15:00	**Johannes Kraus**, *University of Duisburg-Essen* On structure-preserving discretization of the fully dynamic multiple network poroelasticity model
15:00 - 15:20	**Markus Weimar**, *Ruhr University Bochum* New local higher order regularity shifts for the p-Poisson problem
15:20 - 15:40	**Markus Musch**, *University of Oslo* Well Posedness of Scalar Nonlinear Hyperbolic Conservation Laws on Networks
15:40 - 16:00	**Andreas Rupp**, *University of Heidelberg* C-E+G A survey of CG and DG leading to EG and back

Interfaces in porous media are (almost) everywhere: Do we need multi-scale concepts and strong cooperation between mathematicians and engineers?

Rainer Helmig, Sina Ackermann, Bernd Flemisch, Timo Koch, Kilian Weishaupt,
Dept. of Hydromechanics and Modelling of Hydrosystems, University of Stuttgart

Flow and transport processes in domains composed of a porous medium and an adjacent free-flow region appear in a wide range of industrial, bio-medical and environmental applications. Industrial applications range from flow in fuel cells to drying processes; possible bio-medical applications include the interplay of distribution processes in blood vessels and in the surrounding tissue. Applications in environmental systems include the infiltration of overland flow during rainfall, groundwater contamination due to infiltrating pollutants and evaporation from soil. Evaporation from soil is a good example from the immense variety of challenges. The corresponding patterns and evaporation rates strongly influence the water and energy balance of terrestrial surfaces, driving a multitude of climatic processes. To predict evaporative drying rates from porous media remains a challenge for several reasons.

REV-scale models for the exchange of fluids, momentum and energy between a porous medium and an adjacent free-flow domain do not yet accurately account for the true complexity of transfer processes during evaporation from a porous medium. The complexity is controlled by non-isothermal multi-phase flow and thermodynamically driven component transport in both the porous medium and the free-flow part. The exchange is affected by a variety of processes at different interfaces (fluid-fluid-solid contact line and boundary or viscous sub-layer) on different time and length scales, which are not all accounted for in continuum models on the REV scale. The challenge lies in the fact that the relevant interfaces have complex geometries and dynamics that depend on the state of the system. Current model concepts capture these effects empirically on the REV scale.

Ideas for the extension of the multi-physics towards more complex systems and possible interfaces with multiscale methods are discussed. In the presentation, we want to introduce and distinguish a multi-scale approach for coupling free flow and flow in porous media, ranging from a simple via a pore-scale to a complex interface approach. Furthermore, we will show that this development can be only successful if experimentalists and modelers or applied mathematicians and engineers work closely together.

TBA

Oleg Iliev, *Fraunhofer ITWM*

The catalytic membranes can degrade gaseous pollutants to clean gas via a catalytic reaction to achieve green emissions. A catalytic membrane is a three scale porous medium. The walls of catalytic filters are of size of centimeters or millimeters and consist of active (washcoat) particles, inert material and microscale, micron size pores. The washcoat particles are porous material with nanoscale pores. The catalytic reactions are heterogeneous (surface reactions) and they occur within the nanopores. Obviously, simulations at fully resolved pore scale are not feasible, and upscaling techniques have to be applied. It is known that the same microscale problem can be upscaled to different macroscale equations depending on the characteristic numbers. In this talk we present two studies: (A) Homogenization of reactive flow in the presence of strong absorption in the washcoat particles. Two flow regimes are studies, $Pe_f = O(1)$ and $Pe_f = O(\epsilon^{-1})$, and two different upscaled equations are obtained, respectively. The both derived upscaled equations are numerically validated comparing their solution to the solution of the microscale problem. (B) Three-way catalyst material was deposited inside the pores of a ceramic particulate filter and the pore geometry as well as the distribution of the catalyst in the pores was determined by xX-ray -microtomography (CT). On the resulting 3D geometry, the flow field through the pores was computed and the convection diffusion reaction equation in the open pores and the catalyst particles was solved assuming a first order reaction taking place in the catalyst. The conversion in the filter wall was compared to a homogeneous model with the same dimensions.

Upscaled models for heterogeneous reactions and conjugate transfer in porous media

Matteo Icardi, Federico Municchi, *University of Nottingham*

Most of the industrial problems involving fluid dynamics, and in particular multiphase flows and porous media possess an inherent multi-scale nature. Precise models for numerical simulations describing local, pore-scale, phenomena are generally of little practical use when studying large systems, due to the rapid oscillations of the fields (e.g., velocity, concentration, temperature, etc.). Furthermore, reactive systems are characterised by a complex interaction between distant scales fuelled by reactions taking place at the pore-scale.

A variety of methods can be employed to perform this procedure: asymptotic homogenisation is a powerful and versatile tool for the upscaling of transport and reaction equations in porous and heterogeneous media.

In this talk, we illustrate how homogenisation theory can be extended to scalar transport with heterogeneous reactive boundary conditions, of relevance, for example, in the modelling adsorption/desorption of nanoparticles from heterogeneous surfaces. Specifically, we present a C++ library developed in OpenFOAM for the upscaling of reactive transport in complex geometries capable of evaluating a set of effective parameters (e.g., effective diffusivity, transfer coefficients, etc.) employing the rigorous theoretical framework of homogenisation theory. After demonstrating the accuracy of our computational method against pore-scale simulations, we show how this can be applied to problems of adsorption/desorption to construct macroscopic models.

Finally, we show how these models can be extended to the case of conjugate transfer between a mobile region (where advection processes are relevant) and a set of immobile regions (where diffusion is dominant). We present an open-source implementation of the Generalised Multi-Rate Transfer Model (Municchi, Icardi, Phys Rev Res, 2020) in OpenFOAM and its applications to transport of contaminant in geological media.

Numerical homogenization of complex flow in porous media

Lubomir Banas, *Bielefeld University*

We present a multicomponent Cahn-Hilliard-Navier-Stokes (CHNS) model that describes incompressible flow of mixtures of arbitrary number of fluids with surface tension effects.
We propose a multiscale algorithm for the simulation of multiphase porous media flow with surface tension effects on the Darcy scale.
The numerical algorithm couples the CHNS model, which models the flow on the pore scale, to a discrete macroscale model.
We present numerical simulations to demonstrate the potential and the limitations of the presented numerical homogenization approach.

Homogenization of Bingham Flow in Thin Porous Media

Renata Bunoiu, *IECL and CNRS, University of Lorraine, Metz, France*

By using dimension reduction and homogenization techniques, we study the steady flow of an incompresible viscoplastic Bingham fluid in a thin porous medium which contains an array of bodies modelized as vertical cylindrical obstacles (the pores). A main feature of our study is the dependence of the yield stress of the Bingham fluid on the small parameters describing the geometry of the thin porous medium under consideration. Three different problems are obtained in the limit when a small parameter tends to zero, following the ratio between the height of the porous medium and the relative dimension of its periodically distributed pores. We conclude with the interpretation of these limit problems, which all preserve the nonlinear character of the flow.

This is a joint work with M. Anguiano, University of Sevilla, Spain; based on M.Anguiano, R.Bunoiu, Homogenization of Bingham flow in thin porous media, Networks and Heterogeneous Media, Vol. 15, No. 1 (2020), 87-110.

Homogenisation of Stokes flow in a porous medium with evolving microstructure

Malte Peter, *Universität Augsburg*

We consider the periodic homogenisation of the Stokes equation in a porous medium composed of solid matrix and pore space. Physical or chemical processes induce a (microscopic) evolution of the pore space, e.g. by reaction and precipitation. This evolution displaces fluid, which is modelled by a non-homogeneous Dirichlet boundary condition for the Stokes flow at the interface of the pore space and the solid matrix. The homogenisation of this problem is performed by utilising a transformation to a periodic reference domain and the macroscopic limit problem is determined using two-scale convergence. Compared to the well-known case without evolving microstructure, difficulties arise because the transformation of the domain induces a non-homogeneous divergence condition.

This is joint work with D. Wiedemann (Augsburg).

Ice sheet hydrology - challenges and concepts

Angelika Humbert, *Alfred Wegener Institute, Bremerhaven*

Surface melt in Greenland is providing a substantial amount of water and even by limiting global warming to 1.5°, temperatures will rise to about 3-4° over Greenland due to the polar amplification, leading to enhanced melt. This is a strong motivation to represent the formation, storage, and drainage of melt water in ice sheet models adequately.

The main pathways of surface melt are (i) water percolation into the porous firn, forming aquifers and refrozen melt layers at depth, (ii) surface run-off via rivers, (iii) formation supraglacial lakes and their (iv) drainage via englacial channels. Percolation of melt water into firn and refreezing is an effective mechanism for warming the upper layers. Aquifers of meters in vertical and kilometers in horizontal extent are in particular challenging for modeling. After the onset of melt, saturation of surface layers is a common phenomenon and the freeze-over in fall happens abruptly in just days. Lake drainage is rapid (hours to days), massive (up to 108 m^3) and often facilitated by formation of cracks, that turn into englacial channels.

Basal melting due to geothermal and frictional heat is contributing to the formation of a subglacial hydrological system. Subglacial channels have been modeled with an effective porous medium approach. Simulations are costly and often prone to numerical instabilities, as well as instabilities arising in the natural system. Here, we will present simulations showing the response to supraglacial water discharge on short time scales. Coupling between subglacial hydrology and sliding leads to additional complications of the problem.

Here, we will present conceptual developments for firn and englacial hydrology, as well as the established model for subglacial hydrology. We aim at fostering discussions, e.g. on the applicability of multi-scale FEM for ice sheet hydrology.

Fronts in two-phase porous media flow: the effects of hysteresis and dynamic capillarity

Hans van Duijn,
Department of Mathematics and Computer Science, Eindhoven University of Technology, The Netherlands

In this work, we study the behaviour of saturation fronts for two-phase flow through a long homogeneous porous column. The model includes hysteresis and dynamic effects in the capillary pressure and hysteresis in the permeabilities. Using a travelling wave analysis, entropy solutions are derived for Riemann problems that are arising in this context. These solutions belong to a much broader class compared to the standard Oleinik solutions, where hysteresis and dynamic effects are disregarded. Relevant cases are examined and the corresponding solutions are categorized. They include non-monotone profiles, multiple shocks and self-developing stable saturation plateaus. Numerical results are presented that illustrate the mathematical analysis. Finally, we discuss the implication of our findings in the context of available experimental results.

This is joint work with K. Mitra (Dortmund), T. Koppel (Munchen), I.S. Pop (Hasselt) and R. Helmig (Stuttgart).

Space-time domain decomposition for two-phase flow between different rock types

Michel Kern, *INRIA Paris*

We study a space–time domain decomposition method for two-phase flow in a porous medium where the capillary pressure field is discontinuous at the interface between the rocks. For this nonlinear and degenerate parabolic problem, with nonlinear and discontinuous transmission conditions on the interface, the Optimized Schwarz waveform relaxation method (OSWR) with Robin is considered. We provide a mathematical and numerical analysis of this space–time domain decomposition method. Complete numerical approximation is achieved by a finite volume scheme in space and the lowest order discontinuous Galerkin method in time. We prove the existence of a weak solution of the two-phase flow subdomain problem with Robin boundary conditions by analyzing the convergence of the finite volume scheme.

The domain decomposition algorithm is based on the solution of space-time nonlinear subdomain problems over the whole time interval, allowing for different time steps in different parts of the domain, adapted to the physical properties of each subdomain, and we show that such an algorithm is well-defined. Numerical experiments on three-dimensional problems with different rock types illustrate the performance of the domain decomposition method.

This is joint work with Elyes Ahmed and Caroline Japhet

Global implicit solver for multiphase multicomponent flow in porous media with multiple gas phases and general reactions

Markus M. Knodel, *FAU Erlangen*

Multiphase multicomponent flow processes in porous media have to be considered to study the efficiency of mineral trapping mechanisms for climate killing gas storage in deep layers. Robust predictions ask for the solution of large nonlinear coupled systems of diffusion-advection-reaction (partial differential) equations inheriting equilibrium reactions. In that we elaborate the fully globally implicit Kräutle-Knabner PDE reduction method for the case of multiple gas phases, we solve the arising Finite Element discretized / Finite Volume stabilized equations by means of a semismooth nested Newton solver. We present preliminary simulation results for the case of mutual injection of CO2 , CH4 and H2S into deep layers and investigate the arising mineral trapping scenario. Our methods are applicable also to other fields such as atomic waste storage or oil recovery.

Numerical Simulation of Supercritical Carbon Dioxide Flow with Finite Elements and Lattice Boltzmann Methods

Ernesto Monaco, *ESS Engineering Software Steyr GmbH*

Saline aquifers are chosen for geological storage of greenhouse gas CO2 because of their storage potential. A safe storage should prevent CO2 to leak into drinkable water reservoirs while it dissolves into water and finally precipitates forming carbonate minerals.

Numerical simulations can greatly help in studying this process, provided they are able to capture the different mechanisms of CO2 trapping and the flow regimes of CO2 at different length scales. This talk will present results of simulations conducted with Finite Element and Lattice Boltzmann Methods. The presented cases will range from CO2 flow at pore-scale to macro-scale flows in modeled multilayered saline reservoirs.

Performance of Aquifer Storage Systems

Darrell Tang, *Wageningen University & Research*

Solute and heat transport and recovery from cyclic injection-extraction wells with various radial flow geometries is studied. We derive approximate analytical solutions for the recovery efficiency of the first and subsequent cycles, in closed-form elementary functions, allowing for straightforward sensitivity analyses. The recovery efficiency increases monotonically as injection rates increase, dispersion decreases, and spatial dimensionality decreases. For most scenarios, recovery also increases monotonically as injection periods increase. However, recovery varies non-monotonically with cycle period in three dimensional flow fields, due to competing effects between diffusion and mechanical dispersion. The maximum recovery efficiency corresponds to an optimum period length, for which an expression is presented. It is well-known that linear chemical or thermal retardation implies a linear re-scaling of time. Therefore, the complex relationship between recovery and injection period implies that, whether an increase in retardation leads to an increase or decrease in recovery, depends on which hydrodynamic dispersion process dominates, and on flow field geometry. The dimensionless kinetic dispersion factor S is introduced, which enables identification of the dominant dispersion process. If a single hydrodynamic dispersion process dominates, the recovery efficiency is proportional to the newly introduced geometric dispersion factor G, that generalizes the concept of the area-to-volume ratio (A/V), by considering spatio-temporal interactions between dispersion and flow field geometry. Extensions to fractal flow fields and power-law mechanical dispersion are discussed.

Flow and reactive transport in porous media

Sorin Pop, *Hasselt University*

We discuss some mathematical models for flow and reactive transport in a porous medium. The emphasis is on dissolution and precipitation processes, and in particular the upscaling and numerical simulation of the related models.

Flow regimes in oscillatory porous media flow

Lukas Unglehrt, *Technische Universität München*

Oscillatory flow provides an ideal basis to study and model the behaviour of unsteady flow through porous media. Furthermore, oscillatory porous media flow occurs in various applications, for example acoustics or coastal engineering and marine sciences. We give an overview over the flow regimes that occur in oscillatory porous media flow and present the state of the art models for small amplitude flow in the time domain (Hill et al., 2001; Zhu et al., 2014) and in the frequency domain (Johnson et al., 1987; Pride et al., 1993, Lafarge, 2006). We then focus on the nonlinear, laminar, mid-frequency regime. Based on data obtained from Direct Numerical Simulation of flow in a hexagonally close-packed arrangement of spheres, we discuss the modelling challenges encountered in this particular flow regime. Finally, we present an extension of the model of (Hill et al., 2001; Zhu et al., 2014) and briefly demonstrate its capabilities and shortcomings.

References

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On the unsteady Darcy-Forchheimer-Brinkman equation in tumor growth models

Marvin Fritz, *Technical University of Munich, Chair for Numerical Mathematics*

A mathematical analysis of local and nonlocal phase-field models of tumor growth is presented that includes time-dependent Darcy-Forchheimer-Brinkman models of convective velocity fields and models of long-range cell interactions. In addition, a parameter-sensitivity analysis is described that quantifies the sensitivity of key quantities of interest to changes in parameter values. We employ the notion of active subspaces based on existing observational data. The work concludes with the presentation of numerical approximations of solutions of the governing equations and results of numerical experiments on tumor growth produced using finite element discretizations of the full tumor model for representative cases.

Joint work with Ernesto Lima (UT Austin), Barbara Wohlmuth (TUM) and J. Tinsley Oden (UT Austin)

Biological tissues with evolving internal structure: modelling approach and numerical simulations

Salvatore Di Stefano,
Dipartimento di Scienze Matematiche "G. L. Lagrange" - Politecnico di Torino

In this work, we would like to investigate the mechanical behaviour of a certain class of soft biological tissues, modelled as hydrated, statistically fibre-reinforced porous media, manifesting a rearrangement of their internal structure (see [1, 4]). For this purpose, we provide a constitutive framework in which we take into account the coupling among the deformation, the evolution of the interstitial fluid and remodelling, whose occurence contributes to the evolution of the internal structure of the tissues. In particular, with the term remodelling we denote the development of anelastic distortions, described by the introduction of a tensor quantity which is neither integrable nor compatible. In such case, we introduce a new degree of freedom and we obtain an evolution law as a result of a balance of generalised forces (see [2]). For the deformation and the evolution of the pore pressure, we refer to the standard equations of the Theory of Mixtures (see [3]).

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Soils in silico - solutes, biofilms and structure formation

Alice Lieu, Simon Zech, Alexander Prechtel, Nadja Ray, Raphael Schulz,
Applied Mathematics 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We assess the complex coupling of biological, chemical, and physical processes in soil with the help of a mechanistic modeling approach extending [1]. The aim is to gain a model-based understanding of dynamics in soils. The hybrid discrete-continuum model used explicitly represents the pore structure. The pore space consists of gas and liquid phases. There, the movement of interacting entities nutrients, bacteria and possibly charged chemicals is described by means of the diffusion and Nernst-Planck equations with Henrys law at the liquid/gas interfaces. Homogeneous chemical reactions are considered using for instance the mass action law whereas heterogeneous reactions on the solid surface are incorporated via a kinetic Langmuir isotherm. Moreover, a biomass phase can develop from agglomerations of bacteria and stabilising sticky agents may grow or decay at the solid surfaces. Root cells and an explicit phase of exudate as well as attachment properties of root hairs are included into our model. In addition to solving the continuous partial differential equations, a discrete cellular automaton method [2, 3, 4] is used, enabling dynamic structural organisation of the solid and biomass/mucilage phases at each time step. The partial differential equations are discretised with a local discontinuous Galerkin method [1] which is able to handle discontinuities induced by the evolving geometry. Upscaling techniques [5] are used to incorporate the information from the pore scale into the macroscale. We illustrate the capability of our approach in two examples. First, we investigate microaggregates which are the fundamental building blocks of soils and are thus important for soil structure, properties, and functions [6]. We study structure formation of microaggregates as a function of the size and shape of prototypic building units taking into account the effect of attraction and repulsion by charges. Second, biomass development and root exudate can significantly alter the macroscopic soil hydraulic properties. Using the model at hand, this effect can be quantified for different amount and spatial distribution of biomass/exudate within two- and three-dimensional geometries from CT-scans.

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Aggregate formation dynamics driven by 3D fluid flow in natural porous media

Thomas Ritschel, Kai Uwe Totsche, *Friedrich Schiller University Jena*

Fluid flow and reactive transport in natural porous media take place in a three-dimensional, hierarchically organized network of voids and pores in the size range of sub-micrometers inside small aggregates to several millimeters in, e.g., earthworm burrows or cracks. Thus, fluid flow regimes are manifold with consequences not only for the transport of solutes, but also for the displacement of colloidal particles and organic matter and thus, for their inclusion into soil aggregates. Therefore, we incorporated the simulation of three-dimensional fluid flow in pore networks typical for natural porous media into our recent approach to model soil aggregate formation using DLVO theory and diffusion-limited aggregation to overcome its previous limitations to suspensions at rest. To visualize the model capabilities, we simulated aggregation in pore networks that were synthetically designed to represent certain structural features such as pore junctions and dead-end pores. We explored the development of structural aggregated features that evolve in response to flow, transport and the topology of the soil pore space. The resulting three-dimensional arrangement of compounds and the entire aggregates were classified according to their morphological metrics, e.g. the pore space distribution, and functional properties, e.g. the water retention capacity, that are provided by these structures. By this fusion of complementary modeling approaches, we significantly contribute to the fundamental mechanistic understanding of the complex interplay and feedback of structure, interactions and functions on the scale of (micro-)aggregates.

Salt transport in charged porous media

Pavan Cornelissen, *Wageningen University*

Flow and transport may be significantly different in charged porous media such as clay, compared to regular porous media. The presence of charged surfaces results in a complex coupled system for water flow, salt transport, and the electric field. This coupled system plays a role in numerous applications, including enhanced oil recovery, radioactive waste storage in clay barriers, and irrigation with marginal water. Clay minerals generally have a negative surface charge. This leads to the formation of a diffuse double layer near the mineral surface, with a net surplus and deficit of cations and anions, respectively. Preferential transport of cations over anions therefore occurs. This results in the development of an electric potential to conserve electroneutrality, which decreases the effective diffusion coefficient compared to regular porous media. Additional transport processes that may occur in the coupled system are advection by both hydroynamic and electro-osmotic water flow. We quantified the effect of the double layer processes on salt transport through pore-network modelling. Such models are suitable for upscaling microscopic processes while including heterogeneous pore sizes and charge densities. While the pore space geometry is simplified in such models, the pore-network properties such as the pore size distribution and connectivity are based on realistic data. The impact of the diffuse double layer depends on the ionic strength. The double layers are thin at high ionic strength, which makes the effect of charged surfaces negligible. Contrarily, the double layers are thick at low ionic strength, and reductions of 25% of the effective salt diffusion coefficient were observed in charged porous media compared to uncharged porous media. These results indicate that the presence of charged mineral surfaces can significantly alter transport rates under certain conditions.

Numerical L^1 Optimal Transport via Gradient Flow

Enrico Facca, Federico Piazzon, Mario Putti,
Department of Mathematics "Tullio Levi-Civita", University of Padua - Italy

Recently we have introduced a dynamic formulation of the PDE-based optimal transport problem with linear cost (L^1), the so-called Monge-Kantorovich equations (M-K) proposed by Evans & Gangbo (1999). In our formulation the transport density μ and potential u are solutions of a nonlinearly coupled system consisting of a possibly degenerate elliptic equation in space and an autonomous ODE in time. The solution of this model is conjectureed to converge as $t \to \infty$ to the solution (μ^*, u^*) of the M-K equations. In partial support of this conjecture, we propose a Lyapunov-candidate functional, which we call Transport Energy. A combination of formal and rigorous results shows that this functional is strictly decreasing along the $\mu(t)$-trajectories and becomes stationary only for $\mu = \mu^*$, i.e., the optimal transport density of Evans & Gangbo.

We introduce a relaxed functional and show that our dynamics is a gradient flow for this functional with a unique asymptotic solution that coincides with μ^* when the relaxation parameter tends to zero.

We then develop a numerical approach based on a combination of Finite-Element inspace and an Implicit Euler method in time. We show that this approach is a discrete gradient flow method for the relaxed functional that converges quadratically towards the unique steady state solution for any sequence (in particular diverging) of time step sizes. Because of the implicitness of our approach, at each time step we employ an uncoupled Newton method for the solution of the nonlinear system. We prove that an inf-sup like condition, providing a relationship between the FEM spaces discretizing the transport potential and density, maintains the positive-definiteness of the Newton Jacobian, ensuring quadratic convergence at every time step.

Several experiments are used to verify the expected properties of our method. In particular, our approach is very efficient in calculating the Wasserstein-1 distance between two densities.

Efficient DG-based simulation of coupled surface subsurface flow

Olaf Ippisch, *TU Clausthal*

The simulation of coupled surface subsurface flow is a topic of high scientific and social relevance for flood protection, agriculture and weather prediction. Most existing numerical models use a kinematic wave approximation for the simulation of the surface runoff. We present an approach based on the diffusive wave approximation for surface and Richards' equation for subsurface flow. An operator splitting approach is used with a special boundary condition to achieve a mass conservative solution. The approach does not require tracking of the dry/wet boundary of the surface like other existing approaches. Spatial discretization of both flow equations is done with a Weighted Interior Penalty Discontinuous Galerkin scheme, while for the temporal discretization a semi-implicit scheme is used for the surface runoff and a diagonally implicit Runge-Kutta scheme for the subsurface flow. We present results obtained with the parallel numerical solver based on DUNE-PDELab and advanced in computational efficiency within the scope of EXA-DUNE project. A code generation framework developed by Dominic Kempf in the group at IWR Heidelberg was used to obtain an optimized version of the (expensive) subsurface solver. The replacement of the original material model including power functions by a cubic spline approximation allows a fast vectorized incorporation of flexible material functions. Sum-factorisation is used in the operator evaluations. On a 32 core Intel Haswell node, 20-35% of peak performance of the Dune-Codegen generated DG solver for subsurface flow is reached. The fully coupled model was tested in parallel simulations on unstructured grids with up to 4-th order DG spatial discretization and Alexander3 scheme in time.

Postprocessing of Standard Finite-Element Velocity Fields and Semi-Analytical Particle Tracking Applied to Variably Saturated Flow in Porous Media

Philipp Selzer, Ren Therrien, Olaf A. Cirpka, *University of Tübingen*

Particle tracking is the most direct and a computationally fast method to determine travel times and trajectories in subsurface hydrology. Consistent particle tracking requires a conforming velocity field, which ensures continuity of the normal flow component on element boundaries and element-wise mass conservation. These requirements are not met by the standard Galerkin Finite Element Method (FEM) which is often used nonetheless in subsurface flow simulations because it yields a continuous approximation of the primary unknown, and is able to handle unstructured grids and full material tensors easily. We present two different approaches to achieve conforming velocity fields in lowest-order Raviart-Thomas-Ndlec (RTN0) space, ensuring continuity and local mass conservation, from standard FEM solutions. The first method is based on a projection which maps a velocity field originating from a non-conforming solution, obtained by standard FEM, onto a velocity field in RTN0-space, requiring the solution of a saddle-point problem. The second approach is based on a cell-centered Finite Volume Method yielding a symmetric, positive-definite system of equations of considerably lower dimensionality, making use of a preceding standard FEM solution. Both methods are implemented as postprocessing codes and can be coupled to any existing finite element code. Based on the properties of the velocity field in RTN0-space, we derive element-wise analytical solutions for the particle trajectories and their associated travel times. We apply our framework to variably saturated flow on unstructured grids of triangular prisms including heterogeneous boundary conditions to meet the needs of applied subsurface hydrological modeling.

Random walk solutions of the Richards equation

Nicolae Suciu (1,2), Davide Illiano (3), Alexander Prechtel (1), Florin A. Radu (3),
(1) Department of Mathematics, Friedrich-Alexander University of Erlangen-Nuremberg, Germany
(2) Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy, Romania
(3) Department of Mathematics, University of Bergen, Norway

The elliptic and parabolic equations governing the pressure head for flows in saturated / unsaturated porous media are essentially diffusion equations with second order operator in Stratonovich form. They can be recast as Fokker-Planck equations, with drift augmented by the row derivative of the coefficient tensor, and further solved by random walk approaches. The alternative approach proposed here starts with the staggered finite difference scheme used to derive biased random walk rules governing the movement on a regular lattice of a system of computational particles. The particle density at lattice sites provides a numerical approximation of the solution. The procedure is implemented as a Global Random Walk (GRW) algorithm which simultaneously moves all the particles from a lattice sites to neighboring sites, according to the local jump probability. Consequently, the algorithm is orders of magnitude faster than classical sequential particle tracking approaches. Moreover, the GRW procedure can be applied to arbitrarily large numbers of particles, which ensures highly accurate numerical solutions. Non-linear and non-steady flow problems are solved with an iterative scheme which consists of performing, at fixed time steps, iterations with a transient scheme for the same pressure equation with fixed initial and boundary conditions from the previous time and coefficients evaluated at the previous iteration until the solution becomes stationary within the desired tolerance. The transient scheme is equivalent to a consistent forward-time central-space finite difference scheme. Its convergence is implied by the von Neumann stability condition which is ensured by the GRW relation between jump probabilities, discretization steps, and diffusion coefficients. One- and two-dimensional benchmark problems for the Richards equation, which capture the transition from unsaturated to saturated flow regimes, are used to validate the GRW solutions by comparisons with mixed finite-element and finite-volume solutions.

Estimation of permeability for regular porous structures

Iryna Rybak, *University of Stuttgart*

Intrinsic permeability is a crucial parameter which characterises and quantifies fluid flow in porous media. This parameter is often uncertain, even if the pore geometry is available. We performed a comparative study of different analytical, numerical and experimental methods to compute the permeability of a porous structure with regularly positioned solid cylinders. We discuss the obtained results with respect to individual strength and limitations of all considered methods.

Level set methods in applications for porous media

Peter Frolkovič, *University of Technology, Bratislava*

Level set methods for numerical tracking of dynamic interfaces in several applications related to porous media will be described. The basic ingredients of the methods will be introduced together with some recent advanced numerical techniques like semi-implicit methods and Voronoi implicit interface methods.

Efficiency and Accuracy of Micro-Macro Models for Mineral Dissolution/Precipitation

Stephan Gärttner, *FAU Erlangen-Nürnberg*

This talk presents efficient algorithms based on micro-macro models to simulate mineral dissolution and precipitation processes, analyzing potentially degenerating bulk properties of the medium such as porosity, diffusivity and permeability.

Our model comprises transport equations at the scale of the porous medium (macroscale) including convection, diffusion and reaction. They feature averaged time- and space-dependent coefficients explicitly computed by means of auxiliary cell problems (microscale). Taking advantage of parallel computing and a tailored adaptivity scheme, computation times comparable to purely macroscopic simulations are achieved.

We validated our approach against the dissolution of an array of dolomite grains in the micro-macro context.

On iterative solvers for nonlinear, coupled problems in porous media

Florin Adrian Radu, *University of Bergen, Norway*

Despite of intensive research in the last decades, there is still a strong need for robust and fast solvers for nonlinear, coupled PDEs. In this talk we will discuss first solvers for the Richards equation [1,2] and then for the linear, quasi-static Biot equations [3,4]. Monolithic and splitting schemes will be considered.

Finally, efficient numerical schemes for nonlinear versions of Biot's model will be presented. This includes nonlinear Lame parameters or compressibility [5], large deformations [6] or unsaturated flow and deformation [7].

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Mathematical theory and simulations of semi-linear thermoporoelasticity

Andro Mikelić, *University of Lyon 1*

In this talk we present a study the equations of semi-linear incremental thermoporoelasticity. Starting point is the dimensionless formulation in van Duijn et al (C.J. van Duijn, A. Mikelić, M. F. Wheeler, T. Wick, Internat. J Engng Sci., Vol. 138, 2019), which was obtained by a two-scale expansion. Nonlinearities in the equations arise through the fluid viscosity and the thermal conductivity, both may depend on temperature and through the coupling in the heat convection by the Darcy discharge in the energy equation. The coupled system of equations involves as unknowns the skeleton displacement, Darcy discharge, fluid pressure and temperature. We treat the system in its incremental (i.e. time-discrete) form. We prove existence using the theory of pseudo-monotone operators. Moreover, we show that the free energy of the system acts as a Lyapunov functional. This yields global stability in the time-stepping process.

Our theoretical results are substantiated with two-dimensional numerical tests using a monolithic formulation. Temporal discretization is based on the backward Euler scheme and finite elements are employed for the spatial discretization. The semi-linear discrete system is solved with Newton's method. We will present several numerical examples, where different source terms are employed to generate flow and heating. The spatial mesh refinement studies show computational convergence.

This is a joint work with C.J. van Duijn (Darcy Center Eindhoven-Utrecht) and T. Wick (Hannover).

Robust iterative decoupling of poroelasticity models resulting from a gradient flow interpretation

Jakub Both, *University of Bergen*

Coupled flow and mechanical deformation of porous media has been of increased interest in the recent past with applications ranging from geotechnical to biomedical engineering. With increased model complexity a high demand in numerical solvers arises. In this context, physically-based iterative splitting solvers, sequentially solving the physical subproblems, are widely popular due to their simple implementation and the possibility of reusing existing solver technologies. For unconditional stability however suitable and model-dependent stabilization is typically required. In the previous literature, the main motivation for specific choices has mostly been based on physical intuition. In this talk, we give mathematical justification in its core based on a gradient flow perspective of poroelasticity. Various existing poroelasticity models are demonstrated to fall into the framework of generalized gradient flows, e.g., the linear Biot equations but also extensions involving viscoelastic, thermal, and/or nonlinear material laws. This enables the theory of convex optimization for the efficient numerical solution, since gradient flow formulations are naturally discretized in time using a series of (convex) optimization problems. In the spirit of splitting solvers, we propose applying the fundamental alternating minimization for a systematic and robust decoupling of the physical subproblems. By this we re-discover splitting solvers as the undrained and fixed-stress splits for the linear Biot equations, and we also provide novel iterative splittings for more advanced models. A priori convergence is established in a unified fashion utilizing abstract convergence theory for alternating minimization.

This is a joint work with Kundan Kumar, Jan M. Nordbotten, and Florin A. Radu (all University of Bergen).

On structure-preserving discretization of the fully dynamic multiple network poroelasticity model

Johannes Kraus, *University of Duisburg-Essen*

Multiple-Network Poroelastic Theory (MPET) describes the mechanical behaviour of a poroelastic medium permeated by one or several fluid networks. It thereby overcomes the problem of performing separate analyses of the individual fluid compartments and the solid (often called matrix) while still accounting for their interactions.

In this work we consider a fully dynamic MPET model. To discretize it in time we use the Crank-Nicolson scheme, or, alternatively, the implicit midpoint rule. For space discretization we use a massconserving $H(\mathrm{div})$-conforming ansatz. We show that the resulting semi-discrete and fully discrete variational problems are inf-sup stable with inf-sup constants independent of any model and discretization parameters.

New local higher order regularity shifts for the p-Poisson problem

Markus Weimar, *Ruhr University Bochum*

In this talk we discuss local regularity estimates related to the p-Poisson equation for $p > 2$. Quasilinear problems of this type arise in many applications such as, e.g., in non-Newtonian fluid theory, non-Newtonian filtering, turbulent flows of a gas in porous media, rheology, radiation of heat and many others. In the planar case we are able to transfer local interior Besov and Triebel-Lizorkin regularity up to first order derivatives from the force term (in divergence form) to the flux $A(\nabla u)$. In case of higher dimensions or systems we have a smallness restriction on the corresponding smoothness parameter. Apart from that, our results hold for all reasonable parameter constellations including quasi-Banach cases with important applications in the adaptive finite element analysis.

The presentation is based on recent joint work with Anna Kh. Balci and Lars Diening from Bielefeld University [1, 2].

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Well Posedness of Scalar Nonlinear Hyperbolic Conservation Laws on Networks

Markus Musch, *University of Oslo*

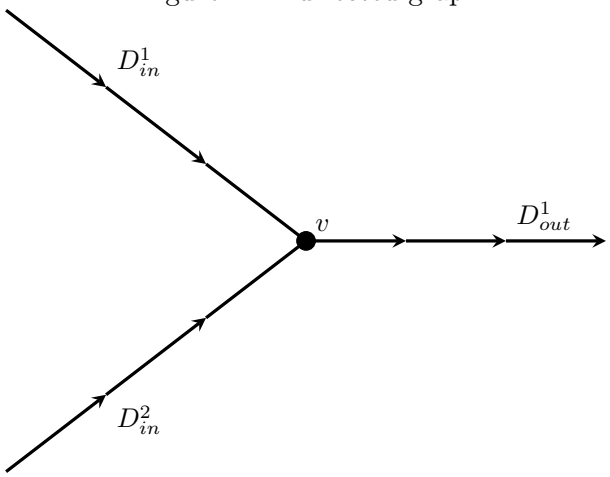
We consider a directed graph with one vertex v, along with N_{in} edges entering and N_{out} edges exiting the vertex as depicted in Figure 1. Each ingoing edge is resembled by an open interval $D^k_{in} = (-\infty, v), \forall k \in \{1, ..., N_{in}\}$ and each outgoing edge by an open interval $D^k_{out} = (v, \infty), \forall k \in \{N_{in} + 1, ..., N_{in} + Nout\}$. On each edge D^k we impose a scalar conservation law

$$u^k_t + f^k(u)_x = 0 \qquad \text{for } x \in D^k$$

and couple them on the vertex.

There are four points on our agenda: We want to show *stability, uniqueness* and *existence* of a solution as well as *approximability* of solutions by a numerical scheme

Figure 1: A directed graph



C-E+G — A survey of CG and DG leading to EG and back

Andreas Rupp, *University of Heidelberg*

We will discuss selected aspects of the analysis and implementation of continuous (CG), discontinuous (DG), and enriched Galerkin (EG) schemes for elliptic and parabolic equations. Moreover, we will briefly discuss ways of stabilizing the respective methods and their specific advantages to hyperbolic (conservative) equations. The standard EG method composes of the classical CG function space of the polynomial order k (originally k = 1) augmented by a piecewise constant at the center of each element. EG has the same interior penalty type bi-linear form as the interior penalty DG method and it inherits many advantages of DG. However, EG has fewer degrees of freedom than the DG method. It has been invented by Becker et al. (2003) and further developed and investigated by Wheeler and Lee in various publications.

The aforementioned properties motivate to construct a uniform analysis applicable to CG, DG, and EG by allowing arbitrary degree enrichment of the EG method which will be the basis of the presentation. Building on this, we will try to formulate criteria for an optimal choice of enrichment and ultimately for an optimal mixed primal EG scheme. Conservative stabilization and limiting techniques in terms of algebraic splitting, flux-corrected transport, and monolithic convex limiting are constructed. These techniques use aspects (and are ultimately build on techniques) of several publications by Kuzmin (and coauthors), while further (analytical) results can also be found in the books by Kuzmin and Hamalainen (2014), and Lohmann (2019).

This is joint work with Hennes Hajduk (TU Dortmund), Dmitri Kumzin (TU Dortmund), and Sanghyun Lee (Florida State University).