

Mathematical Models and Numerical Methods for Multiphysics Systems

May 1-3, 2024,
O'Hara Student Center, University of Pittsburgh

Conference Schedule

Wednesday, May 1st

8:30 - 8:50 Registration

8:50 Opening

Session 1

9:00 - 9:45 Gabriel Gatica

Banach spaces-based mixed formulations for multiphysics systems in fluid mechanics

9:45 - 10:30 Luca Formaggia

Application of model order reduction technique to subsurface flows

10:30 - 11:15 Coffee Break

Session 2

11:15 - 12:00 Martin Vohralík

An application of the Gronwall lemma avoiding exponential of the final time: a posteriori error estimates for the Stefan and Richards problems

12:00 - 14:00 Lunch Break (lunch provided)

Session 3

14:00 - 14:45 Jan Nordbotten

Momentum-balancing discretizations of linearized Cosserat materials and elasticity

14:45 - 15:30 Martina Bukač

A diffuse interface method for fluid-poroelastic structure interaction

15:30 - 16:15 Coffee Break

Session 4

16:15 - 17:00 Sorin Pop

Linear iterative schemes for degenerate parabolic equations

17:00 - 17:45 Costanza Aricó

Solution of the (Navier)-Stokes-Brinkman equations using $H^{(div)}$ -velocity fields and recent extensions in the framework of multipoint flux mixed finite element method

18:00 - 21:00 Conference Dinner – University Club Gold Room

Thursday, May 2nd

Session 1

9:00 - 9:45 Erik Burman

An abstract framework for heterogeneous coupling: stability approximation and applications

9:45 - 10:30 Annalisa Quaini

A FEM for a phase-field model of two-phase incompressible surface flow with electrostatic interaction

10:30 - 11:15 Coffee Break

Session 2

11:15 - 12:00 Miguel Fernández

Mechanically consistent modeling of fluid-structure-contact interaction

12:00 - 14:00 Lunch Break and Poster Session (lunch provided)

Session 3

14:00 - 14:45 Sunčica Čanić

From vascular stents to bioartificial organs: multi-layered poroelastic media interacting with incompressible fluids

14:45 - 15:30 Marcio Murad

A fixed-stress-split scheme for a black-oil multiphysics flow model in poroelastic media

15:30 - 16:15 Coffee Break

Session 4

16:15 - 17:00 Ingeborg Gjerde

Network models for the flow of CSF in the brain

17:00 - 17:45 Johnny Guzmán

A second-order correction method for loosely coupled discretizations applied to parabolic-parabolic interface problems

Friday, May 3rd

Session 1

9:00 - 9:45 Martin Schneider

Coupling free and porous media flows at the pore and the REV scales

9:45 - 10:30 TongTong Li

An augmented fully-mixed formulation for the quasistatic Navier-Stokes-Biot model

10:30 - 11:00 Coffee Break

Session 2

11:00 - 11:45 Miroslav Kuchta

Robust iterative solvers for brain glymphatics

11:45 - 12:30 Sergio Caucao

Velocity-vorticity-pressure mixed formulation for the Kelvin-Voigt-Brinkman-Forchheimer equations

12:30 - 14:00 - Lunch Break (lunch provided)

14:00 - 14:30 Closing Discussion

Speakers

Costanza Aricó, *University of Palermo*

Martina Bukač, *University of Notre Dame*

Erik Burman, *University College London*

Sunčica Čanić, *UC Berkeley*

Sergio Caucao, *Universidad Católica de la Santísima Concepción*

Miguel Fernández, *Inria Paris*

Luca Formaggia, *Politecnico di Milano*

Gabriel Gatica, *Universidad de Concepción*

Ingeborg Gjerde, *Simula and Norwegian Geotechnical Institute*

Johnny Guzman, *Brown University*

Miroslav Kuchta, *Simula*

TongTong Li, *Dartmouth College*

Marcio Murad, *Laboratorio Nacional de Computação Científica*

Jan Nordbotten, *University of Bergen*

Sorin Pop, *University of Hasselt*

Annalisa Quaini, *University of Houston*

Martin Schneider, *University of Stuttgart*

Martin Vohralik, *Inria Paris*

Solution of the (Navier)-Stokes-Brinkman equations using $H(\text{div})$ -velocity fields and recent extensions in the framework of multipoint flux mixed finite element method

Costanza Aricò^{*1}

¹Department of Engineering, University of Palermo, Italy

*contact: costanza.arico@unipa.it

The present talk is devoted to a new numerical continuum *one-domain* approach (ODA) solver, recently presented for the simulation of the transfer processes between a free fluid and a porous medium [1]. The solver is developed in the *mesoscopic* scale framework, where a “fictitious” equivalent single medium replaces the fluid and solid phases and one set of governing equations, valid everywhere in the domain, is used to model the transfer processes. The transition from the bulk fluid to the bulk porous region is modelled using a transition zone located in between these two regions (e.g., [3, 2]). Within this transition zone, the change of the effective macroscopic properties of the permeable medium, such as porosity and permeability, is modelled with appropriate continuous transition functions. The set of governing equations, the Navier-Stokes-Brinkman equations, are derived by averaging the governing pore-scale equations over a Representative Elementary Volume (REV) [6], and are solved along with the continuity equation, under the hypothesis of incompressible fluid. The porous medium is assumed to be fully saturated and can potentially be anisotropic. The domain Ω_T is discretized with unstructured grids (or meshes) \mathcal{M} allowing local refinements.

A fractional time step procedure is applied, where one predictor and two corrector steps are solved within each time iteration. The predictor step is solved in the framework of a marching in space and time procedure, with some important numerical advantages. The two corrector steps require the solution of large linear systems, whose matrices are sparse, symmetric and positive definite, with \mathfrak{M} -matrix property over Delaunay-meshes. A fast and efficient solution is obtained using a preconditioned conjugate gradient method. The discretization adopted for the two corrector steps can be regarded as a Two-Point-Flux-Approximation (TPFA) scheme, which, unlike the standard TPFA schemes, does not require the grid mesh to be \mathbf{K} -orthogonal, (with \mathbf{K} the anisotropy tensor).

Inside each cell $e \in \mathcal{M}$, the velocity vector computed at the end of each time iteration \mathbf{u}_e is assumed $\mathbf{u}_e \in \mathfrak{R}_e$, where \mathfrak{R}_e is the lowest-order Raviart-Thomas (**RT0**) space function [7]. Thanks to the **RT0** properties, the velocity components are piecewise constant inside each cell e if $\sum_{j=1}^{nf} Q_j^e = 0$ (where nf is the number of the interfaces of cell e and Q_j^e is the DOF of the space \mathfrak{R}_e associated with interface j). If this condition is satisfied, $\nabla \cdot \mathbf{u}_e = 0 \quad \forall \mathbf{x} \in e$, $\forall e \in \Omega_T$. The fluid pressure is assumed to be piecewise linear inside each cell e according to the nodal values [1].

As demonstrated with the presented numerical test cases, the proposed scheme correctly retains the anisotropy effects within the porous medium. Furthermore, the proposed solver overcomes the restrictions of most other ODA solvers at the mesoscale recently presented in the literature, such as low Reynolds numbers, 1D flow or linearization of the convective inertial terms (e.g., [4, 8]).

A serious limit of the presented algorithm is related to the Delaunay mesh constraint to obtain positive definite symmetric matrices of the two corrective problems. A new numerical technique is currently in progress to overcome this issue. At the present time it is applied for the solution of the standard form of the Stokes equations in 2D problems. As in the previously described algorithm, a fractional time step procedure is applied, where a prediction and a correction problem are sequentially solved. In the framework of the multipoint flux approximation method, the Raviart-Thomas-1 (**RT1**) mixed finite element method is considered, and a special quadrature rule, as proposed in [9], is employed. The basis functions of the local **RT1** space are derived from the ansatz spaces defined by [5]. This allows second order approximation for the velocity components and pressure. The proposed procedure leads to the local elimination of the viscous stresses, in the prediction problem, and of the velocity, in the correction problem, with symmetric and positive definite systems in the prediction and correction problems, respectively. Details of this multipoint flux approximation extension will be presented and discussed, as well as preliminary results obtained over mildly and strongly distorted grids.

References

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A diffuse interface method for fluid-poroelastic structure interaction

Martina Bukač¹, Francis Aznaran¹, Boris Muha², Abner Salgado³

¹Applied and Computational Mathematics and Statistics, University of Notre Dame, USA

²Department of Mathematics, University of Zagreb, Croatia

³Department of Mathematics, University of Tennessee, Knoxville, USA

*contact: mbukac@nd.edu

The interaction between a free flowing fluid and a poroelastic structure, commonly formulated as a (Navier-) Stokes/Biot coupled system, has been used to describe problems arising in many applications, including environmental sciences, hydrology, geomechanics and biomedical engineering. Many existing numerical methods for this problem are based on a sharp interface approach, in the sense that the interface between the two regions is parametrized using an exact specification of its geometry and location, and the nodes in the computational mesh align with the interface. However, the exact location is sometimes not known, or the geometry is complicated, making a proper approximation of the integrals error-prone and difficult to automate. Hence, in this talk, we present a diffuse interface method for the coupled fluid-poroelastic structure interaction. The method uses a phase-field function which transitions from 1 in one region to 0 in the other region. We will first present the analysis of convergence of the discrete diffuse interface solution to the continuous sharp interface solution for the Stokes-Darcy problem. Then, we will discuss the extensions to Stokes-Biot system. The performance of the method will be demonstrated on a series of numerical examples.

An abstract framework for heterogeneous coupling: stability, approximation and applications

Erik Burman¹, Silvia Bertoluzza²

¹Department of Mathematics, University College London

²IMATI-CNR, Pavia

*contact: e.burman@ucl.ac.uk

With the advent of exascale high performance computing in multiphysics applications, there is an increasing interest in fast methods for the solution of linear systems resulting from the discretization of coupled partial differential equations. Such heterogeneous problems where systems are coupled, either over an interface or on a bulk overlap, may be challenging because of different properties of the coupled physical systems. There may also be an interest in using separate optimized codes for the different subproblems, prompting the need of efficient coupling methods that are agnostic to the different solvers to be coupled. In this talk we will take a recent computational project on the electrostatic potential in molecular solvation as starting point for the discussion. For this problem a heterogeneous Poisson-Boltzmann equation close to the molecule must be coupled to a homogeneous Poisson equation in the far field. This prompts the coupling of finite element and boundary element methods. We will then introduce an abstract theoretical framework for heterogeneous coupling that is agnostic to the numerical methods used for the different subsolvers [1]. This naturally leads to a set of assumptions which must be satisfied by the bulk and coupling operators for the well-posedness of the reduced system, where the bulk fields have been eliminated. Having established the theory on the continuous level we consider discretization of the systems, under minimal assumptions on the local solvers and discuss the stability, stabilization and preconditioning of the reduced formulation. Finally we will show how the framework applies to some different heterogeneous coupling problems such as FEM-BEM coupling, the Arlequin method and mixed dimensional problems.

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From vascular stents to bioartificial organs: multi-layered poroelastic media interacting with incompressible fluids

Suncica Čanić¹, Yifan Wang², Martina Bukac³, Andrew Scharf¹, Jeffrey Kuan⁴, Boris Muha⁵

¹Department of Mathematics, University of California, Berkeley

²Department of Mathematics, Texas Tech University

³Department of Applied Mathematics, Notre Dame University

⁴Department of Mathematics, University of Maryland

⁵Department of Mathematics, University of Zagreb, Croatia

*contact: canics@berkeley.edu

From vascular stents to bioartificial organs, multi-layered poroelastic media play a crucial role in modeling the mechanistic aspects of the interaction between biological tissue and fluids such as blood or blood plasma. In this talk we will summarize the derivation of two multiphysics models: (1) a model describing the behavior of drug-eluting stents within arterial walls interacting with blood flow, and (2) the design of encapsulated bioartificial organs, like the pancreas, interacting with plasma flow delivering oxygen and nutrients to the transplanted pancreatic cells. Crucial for the mathematical and physical understanding of these models and for the design of the corresponding numerical schemes to solve them, is the analysis of their well-posedness. We will summarize recent results addressing the well-posedness for this class of problems. Namely, we will talk about fluid-structure interaction problems involving the interaction between the flows of incompressible, viscous fluids (Stokes or Navier-Stokes flows) interacting with multi-layered poroelastic structures consisting of a thick (Biot) layer and a thin poroelastic layer (Biot or reticular plate) located at the interface between the thick Biot structure and the fluid flow. Both linear [1] and nonlinear coupling [5] will be discussed. We will introduce a new partitioned scheme to solve this problem [6]. We will discuss numerical results revealing the regularizing nature of the interface with mass in the case of poroelastic structures and talk about the implications of the numerical results on the design of bioartificial pancreas [7, 2] and drug-eluting stents [3, 4, 8].

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Velocity-vorticity-pressure mixed formulation for the Kelvin–Voigt–Brinkman–Forchheimer equations

Sergio Caucao^{*1}, Ivan Yotov²

¹GIANuC² and Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción

²Department of Mathematics, University of Pittsburgh

*contact: scaucao@ucsc.cl

We propose and analyze a mixed formulation for the Kelvin–Voigt–Brinkman–Forchheimer equations for unsteady viscoelastic flows in porous media. Besides the velocity and pressure, our approach introduces the vorticity as a further unknown. Consequently, we obtain a three-field mixed variational formulation, where the aforementioned variables are the main unknowns of the system. We establish the existence and uniqueness of a solution for the weak formulation, and derive the corresponding stability bounds, employing a fixed-point strategy, along with monotone operators theory and the well-known Schauder and Banach theorems. Afterwards, we introduce a semidiscrete continuous-in-time approximation based on stable Stokes elements for the velocity and pressure, and continuous or discontinuous piecewise polynomial spaces for the vorticity. Additionally, employing backward Euler time discretization, we introduce a fully discrete finite element scheme. We prove well-posedness and derive the stability bounds for both schemes, and establish the corresponding error estimates. We provide several numerical results verifying the theoretical rates of convergence and illustrating the performance and flexibility of the method for a range of domain configurations and model parameters.

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Mechanically consistent modeling of fluid-structure-contact interaction

Miguel A. Fernández¹

¹Inria, Sorbonne Université, CNRS, Laboratoire Jacques-Louis Lions, Paris, France,

*contact: miguel.fernandez@inria.fr

The numerical simulation of systems where several solids immersed in a fluid can come into contact is a complex problem that raises many modeling, mathematical and numerical difficulties. It is crucial for many biomedical applications such as, for instance, the simulation of cardiac valve dynamics (native or artificial), where contact modeling is of fundamental importance. Fluid-structure interaction (FSI) without contact is already challenging due to the moving geometries and the potential strong coupling between the solid and the fluid subsystems. If contact between solids is to be modeled as well, several additional difficulties that have to be faced: (i) In some configurations and with no-slip boundary conditions, FSI models are unable to predict contact (see, e.g., [1, 2, 3]); (ii) The simple addition of a contact constraint (variational inequality) to a FSI model which allows for contact yields a mechanically inconsistent fluid-structure-contact interaction model (see [4, 5]); (iii) Fluid-structure-contact interaction involves non-linearly changing interface conditions (e.g., from fluid-solid to solid-solid) and different space and time scales.

The first difficulty requires a modification of the boundary and interface conditions on the contacting walls (see, e.g., [6, 7, 8]) that reproduces the physically observed contact phenomena. However, as highlighted in the second point, this is not necessarily enough to deliver a mechanically consistent model, due to unphysical void creation (e.g., when an elastic solid releases from contact) or to unbalanced stress at contact. A favored approach to circumvent these two difficulties consists in considering a poro-elastic modeling of the roughness layer of the contacting solid (see, e.g., [4]). The price to pay is a model with a high computational complexity (notably, with respect to traditional FSI without contact). Moreover, very small fluid regions can get trapped between the solid and the contacting wall, which are difficult to treat numerically. An alternative simplified model has recently been reported in [11], but which requires a bulk description of the porous layer in the fluid.

In a simplified setting, we will show how the above-mentioned issues can be overcome by combining a relaxed contact formulation with a reduced surface Darcy-type model of the porous layer attached to the contact wall (see [5]). By building on the arguments reported in [2, 9], a theoretical result on the capability of the proposed model to encompass contact will be provided (see [10]). We will also discuss the asymptotic behavior with respect to the porous layer parameters. Numerical evidence of these results will be presented.

This is joint work with E. Burman, M. Champion, S. Frei, F. Gerosa, C. Grandmont, F. Vergnet and M. Vidrascu.

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Application of model order reduction technique to subsurface flows

Luca Formaggia^{*1}, Enrico Ballini¹, Alessio Fumagalli¹, Anna Scotti¹, Paolo Zunino¹

¹MOX, Department of Mathematics, Politecnico di Milano, Italy

*contact: luca.formaggia@polimi.it

In this talk, we present some recent research activities in the `compgeo@mox` group focusing on the development of reduced-order models for subsurface flow in the presence of fractures. After an introduction to the problem of flow in fractured porous media, we discuss the necessity of developing fast surrogate models for use in multiquery situations.

We then illustrate some recent results concerning the simulation of flow in fractured porous media, including uncertainties in the fault position. We will illustrate how the application of data-driven model order reduction, a combination of supervised learning, deep neural networks, and numerical simulations, provides effective model reduction strategies that are intrinsically nonintrusive and, as a consequence, particularly adequate to handle models with geometric nonlinearities, like those induced by the uncertainties in the position of the fractures.

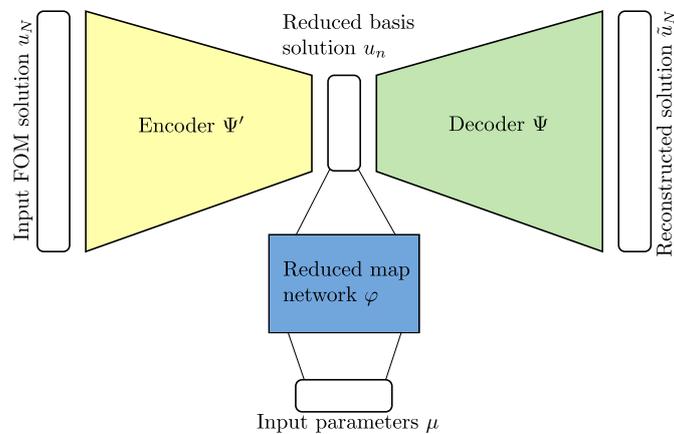


Figure 1: A schematic illustration of the DL-ROM neural network architecture used in this work

We will also illustrate some results on techniques to enforce local mass conservation in reduced models.

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Banach spaces-based mixed formulations for multiphysics systems in fluid mechanics

Gabriel N. Gatica^{*1}, Sergio Carrasco¹, Sergio Caucao², Salim Meddahi³, Nicolás Núñez¹, Ricardo Ruiz-Baier⁴

¹CI²MA and Departamento de Ingeniería Matemática Universidad de Concepción, Concepción, Chile

²GIANUC² and Departamento de Matemática y Física Aplicadas, UCSC, Concepción, Chile

³Departamento de Matemáticas, Facultad de Ciencias, Universidad de Oviedo, Oviedo, España

⁴School of Mathematics, Monash University, Melbourne, Australia

*contact: ggatica@ci2ma.udec.cl

In this talk we refer to some mathematical aspects regarding the application of Banach spaces-based mixed variational formulations to diverse nonlinear and coupled nonlinear problems in fluid mechanics. As illustrative examples we consider the coupled Darcy and heat equations, the Navier-Stokes Brinkman problem, and the coupled Brinkman-Forchheimer/Darcy model. The discussion includes, in particular, the derivation of the right spaces to which the unknowns and test functions need to belong, the structure of the resulting continuous and discrete schemes, and the approaches adopted for their solvability analyses. Some numerical results are also reported.

This work was partially supported by ANID-Chile through CENTRO DE MODELAMIENTO MATEMÁTICO (FB210005), and ANILLO OF COMPUTATIONAL MATHEMATICS FOR DESALINATION PROCESSES (ACT210087).

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Network models for the flow of CSF in the brain

Ingeborg Gjerde^{*1,2}, Miroslav Kuchta¹, Marie Rognes¹, Antonio Sanchez³, Barbara Wohlmuth⁴

¹SCAN department, Simula Research Laboratory

²NGI Digital, Norwegian Geotechnical Institute

³Jacobs School of Engineering, University of California San Diego

⁴Numerical Analysis, Technical University of Munich

*contact: ingeborg.gjerde@ngi.no

Our brain uses approximately 20% of the body's energy in resting state. Yet, the brain lacks a traditional lymphatic system for metabolic clearance. This raises the question of how the brain clears metabolic waste. This question is of key importance as several neurological diseases, such as Alzheimer's and Parkinson's disease, are characterised by the accumulation of toxic proteins in the brain.

According to the glymphatic theory, cerebrospinal fluid (CSF) flows in a network of perivascular spaces surrounding the arteries of the brain. This allows for a bulk flow of CSF through the brain that can remove metabolic waste. There are, however, several unanswered questions regarding the physical driving forces of this flow.

In this talk, we present a Stokes type network model for simulating pulsatile glymphatic flow. We further introduce the concept of graph calculus and graph Sobolev spaces, and show how these can be used to formulate suitable discretization methods. With the numerical methods in hand, we show how network simulations can be set up to match experimental results, allowing us to probe the driving forces of CSF flow. In particular, our simulations show the importance of vasomotion associated with sleep.

A second-order correction method for loosely coupled discretizations applied to parabolic-parabolic interface problems

Johnny Guzmán¹, Erik Burman², Rebecca Durst³, Miguel Fernandez⁴, Sijing Liu⁵

¹Division of Applied Mathematics, Brown University

²Department of Mathematics, University of College London

³Department of Mathematics, University of Pittsburgh

⁴Sorbonne Université and INRIA

⁵ICERM and Brown University

*contact: johnny_guzman@brown.edu

We consider a parabolic-parabolic interface problem and construct a loosely coupled prediction-correction scheme based on the Robin-Robin splitting method. We prove second order convergence in the case the the interface is perpendicular to two sides of the domain. The proof hinges on estimates of the discrete time derivatives of the prediction step. Numerical results are shown to support our analysis.

Robust iterative solvers for brain glymphatics

Miroslav Kuchta^{*1}

¹Simula Research Laboratory

*contact: miroslav@simula.no

Mathematical models of the waste clearance mechanisms of the brain constitute coupled multiphysics problems where the components interact across a common interface, which is a lower-dimensional manifold. The coupling and wide ranges of physical parameters are among the challenges encountered when constructing iterative solvers for the resulting PDE systems. In this talk I will review our earlier work which led to parameter-robust preconditioners for certain formulations of Darcy/Biot-Stokes [1, 2] and coupled 3D-1D Darcy-Darcy models [3]. Here, the uniform stability estimates require parameter-weighted, fractional order or interface perturbed norms. Efficient solvers for Riesz maps with respect to the related inner products will be discussed. I will finally present our recent efforts addressing the sensitivity to geometry and, in particular, the difficulties that the current preconditioners face when applied to practically relevant geometries.

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An augmented fully-mixed formulation for the quasistatic Navier–Stokes–Biot model

Tongtong Li¹, Sergio Caucao², Ivan Yotov³

¹Department of Mathematics, Dartmouth College

²Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción

³Department of Mathematics, University of Pittsburgh

*contact: tongtong.li@dartmouth.edu

We present a partially augmented fully-mixed formulation and a mixed finite element method for the coupled problem arising in the interaction between a free fluid and a poroelastic medium. The flows in the free fluid and poroelastic regions are governed by the Navier–Stokes and Biot equations, respectively, and the transmission conditions are given by mass conservation, balance of fluid force, conservation of momentum, and the Beavers–Joseph–Saffman condition. We apply dual-mixed formulations in both domains and impose the transmission conditions weakly by introducing the traces of the structure velocity and the poroelastic medium pressure on the interface as the associated Lagrange multipliers. Furthermore, since the fluid convective term requires the velocity to live in a smaller space than usual, we augment the variational formulation with suitable Galerkin type terms. Existence and uniqueness of a solution are established for the continuous weak formulation, as well as a semidiscrete continuous-in-time formulation with non-matching grids, together with the corresponding stability bounds and error analysis with rates of convergence. Numerical experiments are presented to verify the theoretical results and illustrate the performance of the method for applications to arterial flow and flow through a filter.

A fixed-stress-split scheme for a black-oil multiphysics flow model in poroelastic media

Marcio Murad^{*1}, Maicon Correa^{1,2}

¹Department of Computational Modeling, LNCC Brazil

²Institute of Mathematics, Statistics and Scientific Computing, Unicamp, Brazil

*contact: murad@lncc.br

We propose a new computational model for solving the Black-Oil flow model incorporating geomechanical coupling within the framework of the fixed stress split scheme. Flow and transport subsystems are rephrased in terms of compositions, and a suitable choice of the evolving sequential scheme is constructed and combined with the full resolution of a three-equation system of hyperbolic equations showing remarkable properties of capturing gas phase appearance/disappearance. Flow and mechanics subsystems are discretized by mixed finite element formulations, whereas the system of conservation laws for the compositions is solved by an innovative semi-discrete central-upwind finite volume scheme for hyperbolic conservation laws. The innovative numerical model remarkably shows the ability to capture the meticulous interaction between geomechanical effects and phase change in the vicinity of the bubble point along with handling multiphysics scenarios wherein the overburden formation displays nonlinear viscoelastic behavior typical of a rock salt. Numerical experiments are performed, including an undrained setting upon cyclic loading and water-flooding problems illustrating precisely the influence of the bubble point pressure upon the evolution of the poromechanical variables and hydrocarbon production.

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Momentum-balancing discretizations of linearized Cosserat materials and elasticity

Jan Martin Nordbotten^{1,2}, Wietse Boon², Omar Duran¹, Eirik Keilegavlen¹

¹University of Bergen, Bergen, Norway

²Norwegian Research Center (NORCE), Bergen, Norway

*contact: jan.nordbotten@uib.no

The Cosserat formulation of linearized elasticity contains an explicit constitutive law for the asymmetry of the stress tensor. This leads to a new field variable, the couple stress. Moreover, the constitutive law for the couple stress naturally deviates from the constitutive law of the linear stress by the length-scale squared, thus the Cosserat formulation can be seen as a two-scale formulation of elasticity. With this perspective, displacement is decomposed in (large scale) strain and (small scale) deviations in rotation, and the stress can be similarly interpreted. The above modeling considerations motivate the common description of materials modeled by the Cosserat equations as “micro-polar”.

In this talk, we highlight that the Cosserat equations are attractive from the perspective of developing discretization methods. Of particular relevance is to develop robust methods, both in the classical sense of incompressible materials, but also more importantly in the sense of a vanishing Cosserat length scale. This latter requirement allows for a seamless transition between Cosserat and linear elastic models of the same physical object, which is attractive if a Cosserat formulation is only of relevance for certain regions of the domain.

We construct explicitly two families of mixed-finite element methods, as well as a finite volume method, all developed within the same framework as outlined above.

Linear iterative schemes for degenerate parabolic equations

Sorin Pop¹, Koondanibha Mitra², Ayesha Javed¹

¹Faculty of Sciences, Computational Mathematics Group, Hasselt University

²Mathematics and Computer Science, Eindhoven University of Technology

*contact: sorin.pop@uhasselt.be

Degenerate parabolic equations appear as mathematical models for many processes appearing in the real life. Typically, such type of equations are nonlinear and parabolic, but may degenerate into elliptic, or hyperbolic ones, depending on the value of the unknown in the model.

A prominent example in this sense is the unsaturated flow in a porous medium (the Richards equation), which, upon choosing the main unknown properly, can be written in the general form

$$\partial_t b(u) - \Delta B(u) = f, \quad (t, x) \in (0, T] \times \Omega. \quad (1)$$

Here $T > 0$ is a maximal time and $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) is a Lipschitz domain. For simplicity, the boundary conditions are assumed homogeneous Dirichlet, and the initial condition completes the problem. The functions b and B are Lipschitz continuous and may have vanishing derivatives,

$$0 \leq b'(u) \leq L_b, \quad \text{and} \quad 0 \leq B'(u) \leq L_B,$$

for all $u \in \mathbb{R}$, for some $L_b, L_B > 0$. Boundary and initial conditions complete the model.

With $N \in \mathbb{N}$ a given number of time steps, and $\tau = T/N$, and with u^k being an approximation of u at $t = k\tau$, the Euler-implicit discretization of (1) gives

$$b(u^k) - b(u^{k-1}) - \tau \Delta B(u^k) = \tau f(k\tau), \quad x \in \Omega, \quad (2)$$

where $k \in \{1, \dots, N\}$, and with homogeneous Dirichlet boundary conditions.

In this presentation, we discuss some iterative schemes for approximating the solution of (2). Essentially, the schemes use a split formulation, in which the nonlinear terms are handled separately, but require no regularization. More precisely, with $u^{k,0} = u^{k-1}$ and for $i \in \mathbb{N}$, $i > 0$, we obtain a triple $(u^{k,i}, v^{k,i}, w^{k,i})$ by solving

$$\begin{aligned} v^{k,i} - \tau \Delta w^{k,i} &= b(u^{k-1}) + \tau f(k\tau), \\ v^{k,i} - L_b^{k,i-1} u^{k,i} &= b(u^{k,i-1}) - L_b^{k,i-1} u^{k,i-1}, \\ w^{k,i} - L_B^{k,i-1} u^{k,i} &= B(u^{k,i-1}) - L_B^{k,i-1} u^{k,i-1}. \end{aligned} \quad (3)$$

The choice of $L_b^{k,i-1}, L_B^{k,i-1}$ is specific to the scheme, and can lead to either the Newton scheme (when $L_b^{k,i-1} = b'(u^{k,i-1})$ and $L_B^{k,i-1} = B'(u^{k,i-1})$), or to the L-scheme (when $L_b^{k,i-1} = L_b$ and $L_B^{k,i-1} = L_B$) or the M-scheme (for a combination of the previous two). Note that, if convergence is achieved as $i \rightarrow \infty$, for the limit triple (u^k, v^k, w^k) one gets that $v^k = b(u^k)$, $w^k = B(u^k)$, and therefore u^k solves (2).

For these schemes, we prove the linear convergence under a mild restriction (if any) on the time step. This convergence is proved at the level of the elliptic problems, so it is not restricted to any spatial discretization or mesh. Moreover, it is obtained under a mild restriction (if any) on the time step. Numerical experiments show that the schemes are linearly convergent in cases when the Newton scheme diverges, and require a comparable number of iterations whenever the Newton scheme also converges.

A FEM for a phase-field model of two-phase incompressible surface flow with electrostatic interaction

Annalisa Quaini¹, Maxim Olshanskii¹, Yerbol Palzhanov¹

¹Department of Mathematics, University of Houston, 3551 Cullen Blvd, Houston TX 77204, USA

*contact: aquaini@uh.edu

We consider a thermodynamically consistent phase-field model of a two-phase flow of incompressible viscous fluids with electrostatic interaction. The model allows for a nonlinear dependence of the fluid density on the phase-field order parameter. Driven by applications in biomembrane studies, the model is written for tangential flows of fluids constrained to a surface and consists of (surface) Navier–Stokes–Cahn–Hilliard type equations. We apply an unfitted finite element method to discretize the system and introduce a fully discrete time-stepping scheme with the following properties: (i) the scheme decouples the fluid and phase-field equation solvers at each time step, (ii) the resulting two algebraic systems are linear, and (iii) the numerical solution satisfies the same stability bound as the solution of the original system under some restrictions on the discretization parameters. We provide numerical examples to demonstrate the stability, accuracy, and overall efficiency of the approach and provide validation against experimental data.

Coupling free and porous media flows at the pore and the REV scales.

Martin Schneider¹, Hanchuan Wu¹, Rainer Helmig¹, Sorin Pop²

¹Hydromechanics and Modelling of Hydrosystems, University of Stuttgart, Stuttgart, Germany

²Data Science Institute, Hasselt University, Hasselt, Belgium

*contact: martin.schneider@iws.uni-stuttgart.de

Exchange processes across a porous-medium free-flow interface occur in a wide range of environmental, technical, and biomechanical systems. In the course of these processes, flow dynamics in the porous domain and in the free-flow domain exhibit strong coupling, often controlled by mechanisms at the common interfaces.

In this talk, we will focus on presenting recent developments for such coupled systems at both the pore and the REV scale. The focus is set on the two-domain approach, which decomposes the problem into two disjoint subdomains. The free-flow region is described by the Navier-Stokes equations, while for REV-scale coupling, Darcy's or Forchheimer's law is used in the porous-medium subdomain, whereas the so-called pore-network modeling approach is chosen on the pore scale. Appropriate coupling conditions are formulated at the common interface, which enforce the conservation of mass, momentum, and energy.

Specific focus is set on two recent developments:

(1) A new approach is proposed for improving fully-implicit two-phase pore-network models by utilizing generalized flux functions and incorporating additional throat variables. These additional throat variables can be used for predicting invasion or snap-off events. A link to our recent work [3] can be achieved by eliminating them through a regularized Heaviside function. The improved robustness, accuracy, and efficiency is demonstrated through various test cases.

(2) A novel mass and momentum conservative control-volume finite-element (CVFE) framework [2] for the discretization of the free-flow subdomain. Furthermore, a new approach to couple this CVFE scheme, which is used in the free-flow subdomain, with a vertex-centered finite-volume method (Box method) used for solving Darcy flow in the porous medium, is presented. This work is therefore an extension of the work presented in [1], where a staggered grid approach has been used to discretize the free-flow region. The advantages of the novel control-volume finite-element scheme and the new coupling approach are discussed based on various test cases.

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An application of the Grönwall lemma avoiding exponential of the final time: a posteriori error estimates for the Stefan and Richards problems

Martin Vohralík^{*1,2}, Daniele A. Di Pietro³, Koondanibha Mitra⁴, Soleiman Yousef⁵

¹Inria, 2 rue Simone Iff, 75589 Paris, France

²CERMICS, Ecole des Ponts, 77455 Marne-la-Vallée, France

³Institut Montpellierain Alexander Grothendieck, CC051, place Eugène Bataillon, 34090 Montpellier, France

⁴Eindhoven University of Technology, De Rondon 70, 5612 AP Eindhoven, The Netherlands

⁵IFP Energies nouvelles, 1-4 Av. du Bois Préau, 92852 Rueil-Malmaison, France

*contact: martin.vohralik@inria.fr

In a priori analyses, one sometimes employs the Grönwall lemma in a form making appear exponential of the final time T , i.e., e^T . In a posteriori error analysis, appearance of any such a term in the estimator makes it hugely imprecise and practically useless for error control, with exploding effectivity indices. We review here the idea from [1], where a sharp employment of the Grönwall lemma avoids any appearance of e^T other than in the data oscillation term corresponding to the approximation of the initial condition, giving rise to time-integrated and exponentially weighted norms. We showcase its application to two model problems: the two-phase Stefan problem [1] which features a nonsmooth nonlinearity and allows to describe problems with evolving interfaces and phase changes, and the Richards problem [2] which exhibits both parabolic–hyperbolic and parabolic–elliptic degeneracies and serves as a gateway to model multiphase flows through porous media. Guaranteed a posteriori error estimates are derived and local space–time efficiency is discussed. Adaptive regularization, linearization, and algebraic resolution, in addition to adaptive steering of spatial meshes and time steps, is designed. Numerical results illustrate the sharpness of the estimates and the performance of the adaptive algorithms.

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Poster Presenters

Lucas Bouck, *Carnegie Mellon University*

Finite element approximation of a membrane model of liquid crystal polymer networks

Aytekin Cibik, *Gazi University*

Continuous data assimilation for a system of Darcy-Brinkman equations

Maicon Correa, *Unicamp - University of Campinas*

A semi-discrete central-upwind scheme for the transport of components in a poroelastic-black-oil model

Aashi Dalal, *University of Pittsburgh*

A Banach space formulation for the Navier–Stokes/Biot coupled problem

* *A Robin-Robin splitting method for the Stokes-Biot fluid-poroelastic structure interaction model*

Rui Fang, *University of Pittsburgh*

Numerical analysis of locally adaptive penalty methods for the Navier-Stokes equations

Connor Parrow, *University of Notre Dame*

Refactorization of Cauchy's method: a second-order partitioned method for fluid-poroelastic material interaction

Vedant Puri, *Carnegie Mellon University*

Nonlinear model order reduction with smooth neural fields

Andrew Scharf, *UC Berkeley*

Interaction between a fluid and a multilayered poroelastic structure with membrane

Farjana Siddiqua, *University of Pittsburgh*

Variable time step method of Dahlquist, Liniger, and Nevanlinna (DLN) for a corrected Smagorinsky model

Henry Von Wahl, *Friedrich Schiller University Jena*

A coupled fracture fluid-structure interaction framework

Ibrahim Yazici, *University of Pittsburgh*

Multipoint stress mixed finite element methods for elasticity

*presented by co-author Rebecca Durst

Finite element approximation of a membrane model of liquid crystal polymer networks

Lucas Bouck^{*1}, Ricardo H. Nochetto², Shuo Yang³

¹Department of Mathematical Sciences, Carnegie Mellon University

²Department of Mathematics, University of Maryland, College Park

³Yanqi Lake Beijing Institute of Mathematical Sciences and Applications, Tsinghua University

*contact: lbouck@andrew.cmu.edu

Starting from the classical 3D trace formula energy of liquid crystal polymer networks of Bladon, Warner and Terentjev [1], we derive a 2D membrane energy as the formal asymptotic limit of the 3D energy and characterize the zero energy deformations in the spirit of [2]. The membrane energy lacks convexity properties, which lead to challenges for the design of a sound numerical method. We discretize the problem with conforming piecewise linear finite elements and add a higher order bending energy regularization to address the lack of convexity. We prove in [3] that minimizers of the discrete energy converge to zero energy states of the membrane energy in the spirit of Gamma convergence; this includes the presence of creases. We solve the discrete minimization problem via an energy stable gradient flow scheme. We present computations showing the geometric effects that arise from liquid crystal defects as well as computations of nonisometric origami, including origami with incompatible stretching across creases that goes beyond theory [4].

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Continuous data assimilation for a system of Darcy-Brinkman equations

Aytekin Cibik^{*1}, Mine Akbas^{1,2}

¹Department of Mathematics, Gazi University, Turkey

²Department of Mathematics, Tarsus University, Turkey

*contact: abayram@gazi.edu.tr

In this study, we consider a continuous data assimilation scheme applied on a double-diffusive natural convection model. The algorithm is introduced with a second order time scheme along with a finite element discretization in space. We prove the long time stability and long time convergence of the proposed algorithm under restrictions of the time step size and data assimilation parameters. Two elaborative numerical test are given in order to confirm the theory and prove the promise of the algorithm.

A semi-discrete central-upwind scheme for the transport of components in a poroelastic-black-oil model

Maicon R. Correa^{*1}, Marcio A. Murad²

¹Department of Applied Mathematics, Unicamp, Brazil

²Department of Computational Modeling, LNCC, Brazil

*contact: maicon@ime.unicamp.br

In this work, we briefly discuss a Black-Oil model in Poroelastic media, where the conservation of the corresponding component densities replaces the traditional black-oil conservation volume equations at standard conditions [1, 2]. Such a model overcomes the necessity of keeping track of the dynamic hysteretic behavior of the bubble point pressure, treating the phase appearance by assessing the excess concentration relative to the saturation limit in the oil phase. The augmented concentration-based system (in terms of the compositions) of hyperbolic equations requires more sophisticated numerical schemes capable of handling more complex storativity behavior, which includes variations in the Lagrangian porosity [2]. Then, we present an innovative semi-discrete central-upwind finite volume scheme for the system of hyperbolic conservation laws capable of capturing spatial and temporal variability in porosity. This scheme obviates the necessity of adopting operation splitting schemes for the storativity in the transport equations, as performed in previous works [3]. The continuous-in-time semi-discrete formulation is then integrated using Strong Stability Preserving Runge-Kutta (SSPRK) schemes. We also comment on the use of this methodology as a block for coupling multiphase flows with geomechanics. The potential of the proposed scheme is illustrated in numerical simulations of black-oil flow problems in poroelastic media.

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A Banach space formulation for the Navier–Stokes/Biot coupled problem

Aashi Dalal^{*1}, Ivan Yotov¹, Sergio Caucao²

¹Department of Mathematics, University of Pittsburgh

²Departamento de Matemática y Física Aplicadas, Universidad Católica de la Santísima Concepción

*contact: aad100@pitt.edu

We introduce and analyse a fully-mixed formulation for the coupled problem arising in the interaction between a free fluid and a poroelastic medium. The flows in the free fluid and poroelastic regions are governed by the Navier-Stokes and Biot equations, respectively, and the transmission conditions are given by mass conservation, balance of stresses, and the Beavers-Joseph-Saffman law. We apply dual-mixed formulations in both Navier-Stokes and Darcy equations, where the symmetry of the Navier-Stokes pseudostress tensor is imposed in a weak sense. In turn, since the transmission conditions are essential in the fully mixed formulation, they are imposed weakly by introducing the traces of the fluid velocity and the poroelastic medium pressure on the interface as the associated Lagrange multipliers. Existence and uniqueness of a solution are established for the continuous weak formulation in a Banach space setting, employing classical results on monotone and nonlinear operators and a regularization technique together with the Banach fixed point approach. We then present well posedness and error analysis with corresponding rates of convergence for semidiscrete continuous-in-time formulation. Numerical experiments are presented to verify the theoretical rates of convergence and illustrate the performance of the method for application to flow through a filter.

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Numerical analysis of locally adaptive penalty methods for the Navier-Stokes equations

Rui Fang^{*1}

¹Department of Mathematics, University of Pittsburgh, PA

*contact: ruf10@pitt.edu

Penalty methods relax the incompressibility condition and uncouple velocity and pressure. Experience with them indicates that the velocity error is sensitive to the choice of penalty parameter ϵ . So far, there is no effective a priori formula for ϵ . Recently, Xie developed an adaptive penalty scheme for the Stokes problem that picks the penalty parameter ϵ self-adaptively element by element small where $\nabla \cdot u^h$ is large. Her numerical tests gave accurate fluid predictions. The next natural step, developed here, is to extend the algorithm with supporting analysis to the non-linear, time-dependent incompressible Navier-Stokes equations. In this report, we prove its unconditional stability, control of $\|\nabla \cdot u^h\|$ and provide error estimates. We confirm the predicted convergence rates with numerical tests.

Refactorization of Cauchy's method: a second-order partitioned method for fluid-poroelastic material interaction

Connor Parrow^{*1}, Martina Bukac^{1,2}

¹Department of Applied and Computational Mathematics and Statistics, University of Notre Dame

²Department of Applied and Computational Mathematics and Statistics, University of Notre Dame

*contact: cparrow@nd.edu

Poroelastic materials include both manmade and natural materials, with examples including biological systems found in bones, flesh, tissue, or blood clots; geological landscapes composed of rocks, soil, sand, or volcanic debris; and manmade substances such as ceramics, foams, or cements. They are often in contact with fluids. Hence fluid-poroelastic structure interaction models have been used to gain deeper insight in many applications. This work focuses on a development of a novel, strongly-coupled partitioned method for fluid-poroelastic structure interaction. The flow is assumed to be viscous and incompressible, and the poroelastic material is described using the Biot model. To solve this problem, a numerical method based on Robin interface conditions was used, combined with the refactorization of the Cauchy's one-legged ' θ -like' method. The finite element method is used for the spatial discretization. In this algorithm, a sequence of Backward Euler-Forward Euler steps is used to discretize the problem in time. In the Backward Euler step, the fluid and poroelastic structure sub-problems are solved iteratively until convergence. Then, the Forward Euler problems are solved using equivalent linear extrapolations. We prove that the iterative procedure is convergent, and that the method is stable provided $\theta \in [\frac{1}{2}, 1]$. Numerical examples are used to explore convergence rates with varying parameter values in the problem, and to compare our method to other strongly-coupled partitioned schemes from the literature.

Nonlinear model order reduction with smooth neural fields

Vedant Puri¹, Aviral Prakash¹, Levent Burak Kara¹, Yongjie Jessica Zhang¹

¹Mechanical Engineering, Carnegie Mellon University

*contact: vedantpu@andrew.cmu.edu

There has been heightened interest in model order reduction for predictive modeling in light of recent advances in machine learning (ML). Reduced order models (ROMs) follow a separation of variables approach. First a reduced state representation is learned from data. Then, the reduced state vector is evolved in time following the physics of the problem. ML-ROMs, which apply nonlinear transformations to obtain a powerful ROM representation, have been shown to outperform projection-based PCA-ROMs in advection-dominated fluid-flow problems. ML-ROMs, however, incur limitations as they are trained using autoencoders that learn to map high-dimensional simulation data from fixed grids to a reduced space.

In this work, we cut the training time in the offline stage by half by employing an encoder-less training approach where a decoder is learned along with reduced representations corresponding to trajectories in the training set. The decoder, a continuous neural field model, then learns a mapping from the reduced space to the space of continuous vector fields in a discretization-invariant manner. Our model is therefore able to learn ROMs from simulations on adaptive and evolving grids where interpolation to a fixed mesh may be infeasible.

Once a reduced representation is learned, the problem is time-evolved per the governing PDE system, which involves computing spatial derivatives of the solution field. Prior works suffer from nonsmooth neural representations whose derivatives are corrupted by noise, and resort to low-order finite differencing on a supplementary coarse mesh. We sidestep this problem by developing methods to learn smooth neural representations that can be differentiated exactly with automatic differentiation. Our key observation behind this improvement is that smooth neural representations can be learned by applying regularization to the decoder model during the offline training process.

In this presentation, we discuss our contributions which lead to faster offline-stage, and improved accuracy, performance during the online-stage. We demonstrate the efficacy of our methods on several 1D and 2D advection dominated traveling shock problems.

Interaction between a fluid and a multilayered poroelastic structure with membrane

Andrew Scharf¹, Sunčica Čanić¹, Martina Bukáč²

¹Department of Mathematics, University of California at Berkeley

²Department of Applied and Computational Mathematics and Statistics, University of Notre Dame

*contact: andrew.scharf@berkeley.edu

Multilayered poroelastic structures are found in many biological tissues, such as cartilage and the cornea, and find use in the design of bioartificial organs and other bioengineering applications. Motivated by these applications, we analyze the interaction of a free fluid flow modeled by the time-dependent Stokes equation and a multilayered poroelastic structure consisting of a thick Biot layer and a thin, linear, poroelastic membrane separating it from the Stokes flow. The resulting equations are linearly coupled across the thin structure domain through physical coupling conditions such as the Beavers-Joseph-Saffman condition. Previous work has been done in which weak solutions were shown to exist by constructing approximate solutions using Rothe's method. While a number of partitioned numerical schemes have been developed for the interaction of Stokes flow with a thick Biot structure, the existence of an additional thin poroelastic plate in the model presents new challenges related to finite element analysis on multiscale domains. We develop a novel, fully discrete partitioned method for the multilayered poroelastic fluid-structure problem based on the fixed strain Biot splitting method and show stability of the splitting scheme under a time-step condition. We also present numerical results showing convergence plots for manufactured solutions and validate the solver with a comparison to the Stokes-Biot model with no thin interface.

Variable time step method of Dahlquist, Liniger, and Nevanlinna (DLN) for a corrected Smagorinsky model

Farjana Siddiqua^{*1}, Wenlong Pei^{1,2}

¹Department of Mathematics, University of Pittsburgh

²Department of Mathematics, Ohio State University

*contact: fas41@pitt.edu

The classical Smagorinsky model's solution is an approximation to a (resolved) mean velocity. Since it is an eddy viscosity model, it cannot represent a flow of energy from unresolved fluctuations to the (resolved) mean velocity. This model has recently been corrected to incorporate this flow and still be well-posed. Herein, we first develop some basic properties of the corrected model. Next, we perform a complete numerical analysis of two algorithms (Backward Euler and Crank-Nicolson with linear extrapolation) for its approximation. They are tested and proven to be effective. Turbulent flows strain resources, both memory and CPU speed. Variable Time Step Method of DAHLQUIST, LINIGER AND NEVANLINNA (DLN) has greater accuracy and allows larger timesteps which means it requires less memory and fewer FLOPS. DLN can also be implemented adaptively. Hence, we also consider DLN method for the time discretization in Corrected Smagorinsky Model. We test that DLN gives best result.

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A coupled fracture fluid-structure interaction framework

Henry von Wahl^{1,2}, Thomas Wick³

¹Institute for Mathematics, Friedrich Schiller University, Jena, Germany

²Institute for Computational and Experimental Research in Mathematics, Brown University, Providence, RI, USA

³Institute for Applied Mathematics, Leibniz University Hannover, Germany

*contact: henry.vonwahl@uni-jena.de

We consider the propagation of a pressure-driven, fluid-filled, quasi-static brittle fracture inside an elastic material in which the crack develops. Applications for this can be found in porous media problems such as natural and induced fractures, groundwater flow, nuclear waste management, and fluid-filled biomaterials. For this crack-propagation problem, we model the fracture with well-known phase-field approach using an elliptic Ambrosio–Tortorelli functional. This approach is attractive due to the fixed background mesh and the possibility for the crack interfaces to move up to large deformations and topology changes. However, a drawback of this approach is that it is limited to simple physics at the crack interface between the fluid and the surrounding medium. Following our work in [2], we take a mesh reconstruction approach to switch from the interface-capturing phase-field model to an interface-tracking model in which the coupling conditions can be realized in a highly accurate fashion. Consequently, we model a Stokes flow inside the fracture coupled to the surrounding elastic medium using an Arbitrary Lagrangean-Eulerian (ALE) finite element method. However, the resulting fluid pressure is only available inside the fracture, which is incompatible with the standard pressurized phase-field fracture model. Consequently, we use a novel formulation for the pressure coupling in the phase-field fracture model, allowing us to use only the local pressure. A fully coupled approach is then obtained by iterating between the phase-field and the fluid-structure interaction models. The new phase-field fracture formulation is investigated using Sneddon's test, and the resulting coupled algorithm is demonstrated for several numerical examples of quasi-static brittle fractures.

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Multipoint stress mixed finite element methods for elasticity

Ibrahim Yazici^{*1}, Ivan Yotov¹

¹Department of Mathematics, University of Pittsburgh

*contact: iby2@pitt.edu

We develop multipoint stress mixed finite element methods for linear elasticity with weak stress symmetry on hexahedra and distorted quadrilateral grids. These methods can be reduced to a symmetric and positive definite cell-centered system. The methods on hexahedra utilize the lowest-order enhanced Raviart-Thomas finite element space, and the methods in 2D utilize the lowest-order Brezzi–Douglas–Marini finite element spaces for the stress. The symmetric vertex quadrature rule in 3D and non-symmetric vertex quadrature rule in 2D were used to localize the interaction of degrees of freedom, which allows for local stress elimination around each vertex. We develop two variants of the method in 2D and 3D. The first uses a piecewise constant rotation and results in a cell-centered system for displacement and rotation. The second employs a continuous piecewise bilinear (trilinear in 3D) rotation, allowing for further elimination of the rotation, resulting in a cell-centered system for displacement only. Stability and error analysis are performed for both methods. First-order convergence is established for all variables in their natural norms. A duality argument is employed to prove second-order superconvergence of the displacement at the cell centers. Numerical results are presented to confirm the theory.

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A Robin-Robin splitting method for the Stokes-Biot fluid-poroelastic structure interaction model

Aashi Dalal^{*1}, Ivan Yotov^{*1}, Rebecca Durst¹, Annalisa Quaini²

¹Department of Mathematics, University of Pittsburgh

²Department of Mathematics, University of Houston

*contact: aad100@pitt.edu, yotov@math.pitt.edu

We develop and analyze a splitting method for fluid-poroelastic structure interaction. The fluid is described using the Stokes equations and the poroelastic structure is described using the Biot equations. The transmission conditions on the interface are given by mass conservation, balance of stresses, and the Beavers-Joseph-Saffman condition. The splitting method uses Robin-Robin boundary conditions on the interface, which are defined using the transmission conditions. We prove the method is unconditionally stable and establish an error estimate showing that the time discretization error is $\mathcal{O}(\sqrt{T}\Delta t)$, where T is the end of the time interval of interest and Δt is the time step. Numerical experiments are presented to illustrate the theoretical convergence rate.