**FEniCS 2023** **June 14–16, 2023**

*Hotel Flamingo Resort, Pula (Cagliari), Italy*

# BOOK OF ABSTRACTS



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https://fenicsproject.org/fenics-2023/

# Welcome

The FEniCS 2023 conference is an opportunity for all those interested in the FEniCS Project and related projects to exchange ideas, communicate their results and network with the automated scientific computing community.

We welcome developers, existing and potential users of the FEniCS ecosystem as well as mathematicians, computer scientists and application domain specialists interested in numerical methods, their implementation and applications.

The FEniCS 2023 conference will emphasize an open and inclusive atmosphere, contributed talks from a diverse range of scientific areas, and dedicated time for discussions and coding.

Drew F. Parsons, Università di Cagliari, Italy (chair)
Francesco Ballarin, Università Cattolica del Sacro Cuore, Brescia, Italy
Chris Richardson, University of Cambridge, United Kingdom

# Oral presentations

## A structure-preserving upwind DG scheme for a degenerate phase-field tumor model

Daniel Acosta Soba (Universidad de Cádiz, Spain)
Francisco Guillén González (Universidad de Sevilla, Spain)
J. Rafael Rodríguez Galván (Universidad de Cádiz, Spain)

The aim of this talk is to present a well-suited approximation of a phase-field tumor model which consists of a Cahn-Hilliard equation with degenerate mobility for the tumor variable and a diffusion equation for the nutrient variable, coupled by proliferation and cross-diffusion terms. First, we introduce the tumor model and we discuss its properties. Then, we present a numerical approximation of the continuous model based on a convex-splitting time discretization and an upwind discontinuous Galerkin (DG) spatial scheme that preserves its physical properties (mass conservation, pointwise bounds and energy stability). Finally, we use FEniCSx to carry out several numerical experiments whose results are in accordance with the theoretical analysis. These tests compare our DG scheme with a continuous finite element spatial discretization, which presents numerical spurious oscillations due to the cross-diffusion terms. Moreover, they show the behavior of the model under different choices of parameters, mobility and proliferation functions.

## SimuStruct: An Integrated Approach of FEniCS and Machine Learning for Stress Prediction in Plates with Holes

João Alves Ribeiro (Massachusetts Institute of Technology, United States & University of Porto, Portugal & Inductiva Research Labs)
Bruno A. Ribeiro (Brown University, United States & Delft University of Technology, Netherlands & Inductiva Research Lab)
Faez Ahmed (Massachusetts Institute of Technology, United States)
Hugo Penedones
Jorge Belinha (Polytechnic of Porto, Portugal)
Luís Sarmento (Inductiva Research Labs)
Miguel A. Bessa (Brown University, United States)
Sérgio M. O. Tavares (University of Aveiro, Portugal)

In this talk, we introduce SimuStruct, an innovative integrated approach that combines FEniCS and machine learning for stress prediction in plates with holes. Building upon our previous research at ICLR 23 conference, we present SimuStruct as a comprehensive dataset of 2D structural parts, encompassing numerical solutions such as displacement, stress and strain fields, von Mises stress, as well as meshes and geometry for plates with holes.
The SimuStruct dataset serves as valuable training and evaluation data for machine learning-based methods, facilitating stress-strain field prediction and optimal mesh definition, thus supporting the development of ML-driven optimal mechanical design solutions.
Through this presentation, we will discuss the methodology employed in creating the SimuStruct dataset and explore its potential applications in the field of structural analysis. Additionally, we will present a case study demonstrating von Mises stress prediction using the SimuStruct dataset, highlighting the effectiveness of our integrated approach in predicting stress distribution in plates with holes under uniaxial loading conditions.
Furthermore, we will delve into the benefits derived from combining FEniCS, a powerful computational platform for solving partial differential equations, with machine learning techniques. This integrated approach holds the potential to surpass the limitations of traditional numerical methods, enhancing

the accuracy and efficiency of stress prediction in complex structures. It paves the way for innovative ML-based mechanical design solutions, fostering advancements in the field.
In conclusion, this presentation demonstrates the vast potential of SimuStruct as an invaluable resource for researchers and engineers engaged in ML-based structural analysis and design optimization. Through the synergistic utilization of FEniCS and machine learning, we strive to push the boundaries of structural analysis, enabling the development of more efficient and reliable engineering solutions.

## Implementation of an automatic locally-conformal Perfectly Matched Layer in FEniCSx

Antonio Baiano Svizzero (undaproject.com)

In this talk, I present the implementation of an automated locally-conformal perfectly matched layers (PML) method in FEniCSx for acoustic waves propagation. PML is a widely used technique for simulating unbounded domains in numerical simulations by absorbing outgoing waves at the boundary of the computational domain. While the "classical" PML can only be used on domains which boundary is defined throug a coordinate system (cartesian, spherical, etc.), the locally-conformal PML variant makes it applicable for arbitrary convex shapes, enhancing the accuracy of the method by matching the local direction of wave propagation with the direction of the PML layers. My implementation automates the process of generating the PML layers using the gmsh API, which allows for the extrusion of the layer and computation of all the needed geometric variables. I demonstrate the effectiveness of our approach on a range of benchmark problems, focusing on wave propagation in acoustics. This approach is expected to be extended in the future to a wide range of applications, such as seismology, electromagnetics, and fluid dynamics.

## High-Order Finite Element Schemes for the Stokes–Onsager–Stefan–Maxwell Equations

Aaron Baier-Reinio (University of Oxford, United Kingdom)
Patrick Farrell (University of Oxford, United Kingdom)

In this talk we consider the Stokes–Onsager–Stefan–Maxwell (SOSM) equations, which model the flow of concentrated mixtures of distinct chemical species in a common thermodynamic phase. The equations account for both the diffusive interactions between chemical species and the bulk convection. Our aim is to develop computationally efficient high-order finite element schemes that discretize these nonlinear equations in two and three spatial dimensions. Because the SOSM equations relate many unknown variables (e.g. the bulk and species velocities, pressure, concentrations, chemical potentials, etc.), this is a difficult task. In particular, there are many choices of which variables should be explicitly solved for in the formulation, and it is not clear which discrete finite element function spaces should be employed. To tackle this challenge, we derive a novel weak formulation of the SOSM problem in which the species mass fluxes are treated as unknowns. We show that this new formulation naturally leads to a large class of high-order finite element discretizations that are straightforward to implement and have desirable linear-algebraic properties. Moreover, from a theoretical standpoint, we are able to prove that when applied to a linearized version of the SOSM problem, the proposed finite element schemes are convergent. Our findings are illustrated with numerical experiments, which currently have been implemented using Firedrake, but we would like to investigate the advantages FEniCS may have to offer from an implementation standpoint.

## Modelling brain tumour growth and its impact on the surrounding tissue: a Continuum Mechanics approach with FEniCS-based simulations

Francesca Ballatore (Politecnico di Torino, Italy)
Chiara Giverso (Politecnico di Torino, Italy),
Giulio Lucci (Politecnico di Torino, Italy)

The mathematical modeling of brain tumours is a challenging problem with important implications for clinical predictions and personalized treatment planning. To achieve a realistic outcome, we propose a multiphase model based on Continuum Mechanics, treating both healthy and diseased regions as mixtures consisting of solid and fluid phases.
With the aid of patient-specific imaging data, we are able to reconstruct the preferential directions of nutrient diffusion, as well as the motion of fluids and cells, which all follow the orientation of white matter tracts. Subsequently, we modify the white matter fibers orientation, accordingly to the mechanical deformation induced by the tumour on healthy tissue. Our model also accounts for deformation of the cerebral ventricles caused by tumour growth.
To solve the mechanical model for brain tumour growth through numerical simulations, we obtain the weak formulation of the proposed model and solve it using FEniCS, as it allows for easy and flexible implementation of numerical methods. The numerical simulations are performed on real three-dimensional brain geometry using MRI and DTI data to build the computational domain and account for patient-specific anisotropy.
The combination of FEniCS and patient-specific imaging data enables a personalized approach to brain tumour modeling, which has significant implications for improving our understanding of brain tumours and developing more effective treatments. Indeed, our results demonstrate that tumour-induced displacements and stresses have a substantial impact on the surrounding tissue, even in regions distant from the tumour position. The proposed model also highlights relevant changes in the preferred directions of nutrient diffusion and cell motion caused by the spread of the cancer. Moreover, by incorporating imaging data specific to each patient, we accurately capture the shape and position of the ventricles in three-dimensional space and account for the mechanical deformation caused by the tumour on this critical brain structure. Finally, this framework may be a useful tool for the mechanical and computational modeling of other kinds of tumours growing in highly anisotropic environments and for estimating the effect of the expanding mass on the surrounding tissue.

## Efficient Preconditioning for Elliptic Problems: Implementing p-Multigrid with Dolfinx

Igor Baratta (University of Cambridge, United Kingdom)
Chris Richardson (University of Cambridge, United Kingdom)
Adrian Jackson (University of Edinburgh, United Kingdom)
Garth Wells (University of Cambridge, United Kingdom)

Traditional algebraic multigrid solvers often struggle to efficiently solve partial differential equations (PDEs) discretized with high-order finite element approximations. To overcome this limitation, alternative approaches such as p-multigrid preconditioners have been developed. By combining p-multigrid with high-order finite element approximations, it becomes feasible to tackle challenging PDE problems while simultaneously achieving high levels of accuracy and computational efficiency.
In this talk, we describe the key ideas behind p-multigrid preconditioners and show how Dolfinx's data-oriented design greatly simplifies their implementation. We show how the smoother has a significant

impact on the multigrid method's convergence rate and provide details on how to implement various polynomial smoothers that can be effectively combined with matrix-free operators. Finally, we show scalability results for elliptic problems across a variety of computing architectures, including AMD and Intel CPUs, as well as NVIDIA and AMD GPUs.

## Advanced material modeling in FEniCSx

Jeremy Bleyer (Ecole des Ponts ParisTech, France)

Solid mechanics involves studying the behavior of materials, and many of them exhibit complex nonlinear constitutive relations. While hyperelastic materials can be formulated using UFL operators and a free energy potential, materials with elastoviscoplastic behavior require solving for the evolution of internal state variables at the material point level. This approach involves a two-level nonlinear procedure in computational mechanics, where the stress state and internal state variables are solved for at each iteration of the global problem. The constitutive update must also provide the corresponding consistent tangent operator to achieve quadratic convergence of the global Newton algorithm. However, this two-level procedure is not easily enabled by FEniCSx, which is not designed for it.
This work aims to provide a simple way of defining such implicit constitutive equations, albeit with a slight computational and memory overhead. The library can handle various implementation types of constitutive equations, starting with user-defined constitutive updates using Numpy and Scipy, which are ideal for educational purposes. For better computational performance and behavior complexity, the library also supports material models defined by the MFront code generator. Additionally, two advanced material modeling techniques are presented in this work: highly non-smooth behaviors using conic optimization solvers such as CVXPY, and multiscale material models using Thermodynamics-based Artificial Neural Networks (TANN).

## FEM/BEM coupling using the Calderon projection and Nitsche's method

Michal Bosy (Kingston University London, United Kingdom)
Timo Betcke (University College London, United Kingdom)
Erik Burman (University College London, United Kingdom)
Christopher D. Cooper (Universidad Técnica Federico Santa María, Chile)
Matthew W. Scroggs (University College London, United Kingdom)

In this presentation, we will discuss a highly effective hybrid method for coupling FEM-BEM. Our approach involves coupling from both sides using a Nitsche-type method to couple to the trace variable. This results in a flexible and robust formulation, making it easy to combine with building blocks for other hybrid methods. We will showcase the method's efficacy through numerous computational examples and explore its application to the linear Poisson-Boltzmann problem. A popular tool for modelling electrostatics in molecular systems is the Poisson-Boltzmann equation. However, existing software options based on finite difference, finite element, and boundary element methods for solving it have their limitations. To address this, we suggest a methodology that combines finite and boundary element methods. All discussed approaches are implemented through the Python interfaces of the Bempp-cl and FEniCSx libraries.

[1] Betcke, T., Bosy, M., Burman, E., Hybrid coupling of finite element and boundary element methods using Nitsche's method and the Calderon projection. Numerical Algorithms (2022).
[2] Bosy, M., Scroggs, M. W., Betcke, T., Burman, E., Cooper, C. D., Coupling finite and boundary

element methods to solve the Poisson-Boltzmann equation for electrostatics in molecular solvation. Submitted to Journal of Computational Chemistry, 2023

## Blood flow modeling in brain aneurysms

Jana Brunátová (Charles University, Czech Republic)
Jaroslav Hron (Charles University, Czech Republic)

The application of computational fluid dynamics (CFD) in medicine is attracting growing attention, as patient-specific numerical models can help optimize clinical management.
CFD can be used to simulate blood flow in diseased human vessels, such as brain aneurysms.
Previous studies on patient-specific blood flow models have almost exclusively prescribed the no-slip boundary condition (BC) on walls. Although easy to implement, its validity at the interface between blood and the vessel wall is questionable. The novelty of our approach is prescribing a more general BC called Navier slip BC, which presumes a linear proportionality between the tangential part of the velocity on the wall and the shear stress using an additional parameter. We used a patient-specific aneurysm geometry and assumed that the vessel wall was impermeable, which is implemented using the Nitsche method. Blood flow is governed by generalized incompressible Navier-Stokes equations; thus, both Newtonian and non-Newtonian models were considered. We used the FEniCS module with a nonlinear solver adopted from the PETSc library to compute the velocity and pressure fields. From these quantities, we compute the wall shear stress (WSS), the oscillatory shear index, and the oscillatory velocity index. We show two numerical methods for computing WSS and evaluate differences in hemodynamics using different models and slip parameters.

## The influence of hypoxia on tumour growth, phenotypic heterogeneity and radiotherapy: mathematical modeling and simulations with FEniCS

Giulia Chiari (Politecnico di Torino/Università di Torino, Italy & Swinburne University of Technology, Australia)
Giada Fiandaca (Università di Trento, Italy)
Marcello Edoardo Delitala (Politecnico di Torino, Italy)

In the study of cancer evolution and radiotherapy treatments, scientific evidence shows that a key dynamic lies in the tumor-abiotic-factors interaction. In particular, oxygen concentration plays a central role in the determination of the phenotypic heterogeneity of the cancer cell population, both from a qualitative and geometric point of view.
Hypoxia acts as an environmental stressor promoting the selection of aggressive phenotypes and affecting therapeutic efficacy in a twofold way. On the one hand, selected cells are characterized by high resistance to hostile environments, resulting in the ability to survive in those areas in which the radiotherapy treatment is less effective because of the lack of oxygen (oxygen is responsible for the enhancement of the detrimental effect of ionizing radiation). On the other hand, selected cells present a low proliferative rate, thus being less exposed to radiotherapy action, which acts damaging the DNA of cells involved in the replication process.
In this talk, we present a continuous mathematical model to study the influence of hypoxia on the evolutionary dynamics of cancer cells. The model is settled in the mathematical framework of phenotype-structured population dynamics and it is formulated in terms of systems of coupled non-linear integro-differential equations. We consider a four-dimensional domain in which one dimension is dedicated to the time, two to the spatial representation, and the other one features the phenotypic state related

to the expression of the hypoxia-resistance gene. Numerical simulations are performed using Galerkin finite element methods, implemented in Python with FEniCS tool, with the aim to test different vessel dispositions, allowing to represent various biological situations (without the constraint of radial symmetry), such as cancer mass developing in well-oxygenated or highly inhomogeneous tissues and tumor cords growing around single vessels.
Then, the effects of radiotherapy treatment are included in the model and numerical simulations are driven to analyze the influence of the heterogeneity in oxygen concentration and phenotypic distribution of cancer cells on the treatment effectiveness. Various therapeutical protocols, differentiated per doses and timing, are considered. The computational outcomes show that the mutual interactions between the tumor mass and the oxygen distribution can result in a geometric characterization of tumor niches differentiated by phenotypic characteristics that determine a heterogeneous response to radiotherapy. The analysis of the study results provides suggestions about possible therapeutic strategies to optimize the radiotherapy protocol in light of the phenotypic and geometric inhomogeneities of the tumor.
The study constitutes the first step in the development of a mathematical tool for the delineation of patient-specific protocols which, in the perspective of personalized medicine, aim not only at the reduction (and in the best cases at the eradication) of the tumor mass, but also at the optimization, in case of relapse, of the phenotypic composition of the tumor so that resistance to subsequent treatments can be avoided as possible.

[1] G. Chiari, G. Fiandaca, M. E. Delitala, Hypoxia-resistance heterogeneity in tumours: the impact of geometrical characterization of environmental niches and evolutionary trade-offs. A mathematical approach. (MMNP preprint)
[2] G. Chiari, G. Fiandaca, M. E. Delitala, Hypoxia-related radiotherapy resistance in tumours: treatment efficacy investigation in an eco-evolutionary perspective. (Frontiers preprint)

## Direct Model of Electrical Impedance Tomography for the Peripheral Nervous System

Thomas Couppey (ETIS, France)
Olivier Romain (ETIS, France)
Olivier Français (ESYCOM, France)
Florian Kölbl (ETIS, France)

Electrical Interfaces the Peripheral Nervous System enable the design of implantable devices capable of treating symptoms for a large spectrum of diseases and enhance sensory-motor rehabilitation. Nerves consist in an ensemble of neural fibers, or axons, that carry electrical information related to various body functions (sensorial, motor and internal organs regulation). This information can be electrically recorded by sensing extracellular potential, however this technique suffers from poor spatial resolution and cell type identification is also limited. Electrical Impedance Tomography (EIT) has been experimentally shown as a technique enabling spatial mapping of nerves. Our research interest focuses on using EIT for fast imaging, spatial and type mapping of nervous spontaneous activity. Reaching this objective supposes a good understanding of the underlying physiological mechanisms and the development of in-silico models capables of assessing experimental results. Such models imply to couple simulation of axons' behavior using non-linear conductance-based Finite difference models with electrical conduction problems. The impedance or conductance change is located at the cell's membrane that results in a time-dependent 1D function containing membrane conductance values along the axon. A 3D nerve mesh based on realistic physiological dimensions is then generated with GMSH. To limit the element number and avoid needle-like elements in the mesh, the membranes are considered as surfaces inducing a discontinuity in the electric field. The electrical conduction

problems consist of solving Laplace equations in the whole mesh using Neumann boundary conditions at electrodes boundary to model current injections. Every time step, axons' membrane conductivity are updated by interpolating the result of 1D simulation. In other mesh domains, conductivity is constant in time with values commonly found in the literature for corresponding material. Using this principle, first results of impedance changes mimicking experimental results have been obtained, thus opening the way to quantitative in-silico evaluation of EIT possibilities for neural technologies.

## Multi-physics modelling of nuclear fusion device sub-components: The tritium breeding blanket

James Dark (CEA & LSPM/CNRS, France)
Rémi Delaporte-Mathurin (Massachusetts Institute of Technology, United States)
Etienne Hodille (CEA Cadarache, France)
Jonathan Mougenot (LSPM/CNRS, France)
Yann Charles (LSPM/CNRS, France)

The DEMOnstration fusion reactor is planned to be a first-of-a-kind nuclear fusion power plant to be built as the successor to ITER. The objectives of the design are the production of net electricity and operation with a closed fuel cycle. Replenishment of tritium fuel on-site will be imperative for the functioning of future commercial nuclear fusion reactors. Thus, accurate modelling of hydrogen transport and inventories within the reactor will be essential for safety issues and economic sustainability.
The open-source FEniCS-based hydrogen transport code FESTIM [1] is used to perform multi-material, multi-dimensional and multi-physics simulations of a reactor sub-component: the breeding blanket. The design showcased is the Water-Cooled-Lithium-Lead (WCLL) concept [2], which utilises a liquid metal (LiPb) tritium breeding material. A companion fluid dynamics solver has been developed with FEniCSx to model the flow of the breeding material, accounting for MHD effects. The solver was verified using published analytical solutions [3, 4]. The resulting velocity field was coupled with FESTIM to accurately simulate hydrogen transport in both the liquid and structural domains of the component.

[1] R.Delaporte-Mathurin, et al. NME, 21, 2019
[2] A.Del Nevo, et al. Fusion Eng. Des., 124, 2017
[3] J.Shercliff. Math. Proc. Camb. Philos. Soc, 49, 1953
[4] J.Hunt. J. Fluid Mech, 21, 1965

## Solving multiphysics problems in FEniCSx

Joseph P. Dean (University of Cambridge, United Kingdom)
Garth N. Wells (University of Cambridge, United Kingdom)

In science and engineering, the interaction between solid mechanical, fluid mechanical, thermal, and electromagnetic effects are critical to understanding the evolution of many physical systems. There is a growing interest in simulation techniques capable of analysing these multiphysics problems, with applications including predicting mantle convection within the Earth, the aerothermomechanical analysis of the flow around a spacecraft entering the Martian atmosphere, the thermomechanical and electromagnetic analysis of high power density electrical machines for (hybrid) electric propulsion, and the magnetohydrodynamic and thermomechanical analysis of liquid metal breeder blankets in nuclear fusion reactors, amongst a myriad of others.

We show how recent developments in the FEniCSx core libraries allow multiphysics problems to be solved in a single, unified framework, allowing for a flexible treatment of coupling conditions. In addition, the wide variety of finite elements available in FEniCSx allows methods to be used that preserve key properties of the governing equations in the discretisation.
We present an example demonstrating the coupled solution of the Navier-Stokes, Maxwell, and heat equations in a domain with both fluid and solid regions. The method conserves mass exactly, preserves a key invariance property of the Navier-Stokes equations, yields an exactly solenoidal magnetic field, and uses upwinding to stabilise advective terms in the fluid region.

## Checkpointing in DOLFINx

Jørgen S. Dokken (Simula Research Laboratory, Norway)

For large-scale time-dependent simulations, which can take thousands of CPU hours, it is crucial to be able to stop the simulation, then restart it at a later stage, without the need for starting all over again. Checkpointing has been lacking from DOLFINx for the last few years, and has been one of the reasons many users have been reluctant to migrate from legacy DOLFIN. In this talk, I will present an extension to DOLFINx, called adios4dolfinx [1] which makes it possible to do checkpointing with DOLFINx, using ADIOS2 [2] to read and write files. The current implementation is MPI compatible and supports reading and writing functions from any supported function space. The long term goal of this repository is to merge it into the DOLFINx main repository, starting with DOLFINx Pull Request 2618 [3].

[1] Dokken, J. S. (2023). ADIOS2Wrappers (Version 0.2.1), `https://github.com/jorgensd/adios4dolfinx/`
[2] William F. Godoy et al. ADIOS 2: The Adaptable Input Output System. A framework for high-performance data management, SoftwareX, 12, 2020, `10.1016/j.softx.2020.100561`.
[3] DOLFINx Pull Request 2618 `https://github.com/FEniCS/dolfinx/pull/2618`

## FEniCSx in Laser Hardening

Anton Evdokimov (Brandenburg University of Technology Cottbus-Senftenberg, Germany)
Filip Jasiewicz (Scansonic MI GmbH, Germany)
Nikolay Doynov (Brandenburg University of Technology Cottbus-Senftenberg, Germany)
Ralf Ossenbrink (Brandenburg University of Technology Cottbus-Senftenberg, Germany)
Vesselin Michailov (Brandenburg University of Technology Cottbus-Senftenberg, Germany)

This work presents an application case for FEniCSx in the field of metal processing. In this study, a simulation model was developed that allows for the computation of temperature distribution and the resulting hardness during the laser hardening of small-diameter holes. The developed model accounts for changes in laser inclination, distance to the focal plane, and the circumference of the irradiated area inside the hole during processing. This model was validated by comparing the computed temperature cycles and hardness profiles with experimental measurements. The study demonstrated the importance of these simulations for minimizing optimization costs, thereby facilitating the industrial application of this novel hardening technique.

## Slip Conditions in Fluid-Structure Interaction

Jakub Fara (Charles University, Czech Republic)

Slip conditions can improve the agreement of a mathematical model with real-world data. Although this topic has been studied a lot in a rigid domain, there has yet to be a result in fluid-structure applications. We will introduce our solver for discontinuous interface problems and demonstrate the results.

## Numerical treatment of diffusional phase transformations to predict damage in microelectronic solders

Wolfgang Flachberger (Montanuniversity Leoben, Austria)
Thomas Antretter (Montanuniversity Leoben, Austria)
Jiri Svoboda (Academy of Sciences of the Czech Republic)
Daniel Scheiber (Material Center Leoben, Austria)
Manuel Petersmann (KAI Villach, Austria)

This work presents a finite element variational formulation for the treatment of diffusional phase transformations using the Discontinuous Galerkin Finite Element Method (DGM). The diffusion model used is thermodynamically consistent and employs fundamental principles such as the vacancy mechanism of solid-body-diffusion. As vacancies are a non-conserved quantity, their evolution is described by a type of transport equation, which is generally associated with fluid- rather than solid-mechanics. This is one of the reasons why the continuous Galerkin Finite Element Method does not suffice for this type of model and the DGM needs to be employed. The model is characterized by sharp transitions between phases (sharp interface model) which is in strong contrast to other state-of-the-art methods for describing diffusional phase transformations like the Phase Field Method (PFM). A binary system is studied whose behaviour is described by two differential equations which are solved by an implicit, fully coupled scheme. The diffusion model is used to predict both the phase growth as well as damage relevant phenomena such as trapping of components at grain boundaries and other imperfections. Furthermore, the diffusion is coupled with a constitutive model for the mechanical material behaviour. The coupling is done in both ways considering the influence of diffusion on mechanics via phase-dependent material parameters as well as by considering the influence of stresses and strains on the diffusion. This enables a detailed investigation of the many phenomena that are observed at the small scales of microelectronic solders.

## Kinetic energy flow instability analysis applied to Poiseuille pipe flow

Chiara Giraudo (University of Oslo, Norway)
Ingeborg Gjerde (Simula Research Laboratory, Norway)
L. Ridgway Scott (University of Chicago, United States)

In this work, we present simulation results that shed light on the instability of Poiseuille pipe flow. While linearized instability analysis indicates that pipe flow is stable for any Reynolds number, laboratory experiments show the existence of a critical Reynolds number at which pipe flow becomes unstable. To address this discrepancy, we implemented the Kinetic Energy Flow Instability method, first introduced by Reynolds and Orr. This method is based on the variational formulation of the PDE and takes the form of an eigenvalue problem. Via solving this problem with FEniCS and SLEPc, we identified a critical Reynolds number which serves as an upper bound for stable pipe flow. Finally, we will also show early results obtained using an homotopy method, which provides insight on the development of turbulent pipe flow.

## Hitchhikers guide to coupled 1d-3d flow models in FEniCS

Ingeborg Gjerde (Simula Research Laboratory, Norway)
Miroslav Kuchta (Simula Research Laboratory, Norway)

Coupled 1d-3d flow models are used for a variety of applications, such as modeling fluid flow through vascularized tissue, modeling the flow of water and nutrients through soil embedded with a root system, or modeling the interaction between a well and reservoir. Veins, arteries, roots and wells all have in common that their radius is negligible compared to their length and the size of the domain as a whole. For this reason, we idealize them as being 1d geometries. The 1d structures are then endowed with a 1d flow equation, and coupled to the 3D flow equation by the use of a lower-dimensional source term. In this talk, we show how coupled 1d-3d flow models can be implemented in FEniCS using the mixed-dimensional library fenics_ii. This includes showcasing a new python library graphnics, which acts as an interface between FEniCS and networkx. We show how to implement different formulations of the coupled 1d-3d flow model, and illustrate how they affect the numerical properties of the discretization. Finally, we show some recent examples of how mixed-dimensional models have been used to answer medical mysteries related to cerebrospinal fluid flow in the brain.

## Advanced electromagnetism with FEniCSx

Stefano Greco (IIT CBN, Italy)
Michele Castriotta (IIT CBN, Italy)
Cristian Ciracì (IIT CBN, Italy)

The Finite Element Method (FEM) is ubiquitous in computational physics: it is a powerful and versatile method for solving Maxwell's equations, enabling the analysis and design of electromagnetic devices and systems. A key advantage of the FEM is its ability to handle a heterogeneous mesh refinement, allowing for higher accuracy in regions of interest, while keeping the overall computational cost contained. This feature is especially advantageous in nanophotonics. Moreover, the FEM is also very well suited for multi-physics problems, i.e., where electromagnetism is coupled with elasticity, heat transfer, fluid dynamics, etc. While some commercial options exist (which can be prohibitively expensive, have limited parallelization or scripting options and can be unreliable), open-source alternatives are very limited (often offering modules for electro- and magneto-statics only).
Here, we use FEniCSx to solve a series of common problems in electromagnetism, each requiring a specific set of boundary conditions (BCs), such as perfect electric and magnetic conductor BCs, perfectly matched layers, active ports, etc. We present some examples for calculating S-parameters of 3D periodic grating, scattering efficiencies for 3D and axis-symmetric. Finally, we show some examples of multi-physics coupling in which Maxwell's equations are coupled to a hydrodynamic-like equation for the description of advanced plasmonic effects in nanoparticles, in the limit of the Thomas-Fermi approximation and the quantum hydrodynamic theory.
Ultimately, our goal is to provide a higher-level simplified python interface for solving electromagnetic problems, in such a way that even inexperienced users could easily set up and customise a problem using FEniCSx, starting from the mesh building, for example using Gmsh, up to the computation of the output relevant physical quantities. This interface makes use of the Message Passing Interface (MPI) for parallelization, enabling the possibility to control and optimise the computation.

## Deep Learning Mesh Motion Techniques with Application to Fluid-Structure Interaction and Shape Optimization

Ottar Hellan (Simula Research Laboratory, Norway)
Johannes Haubner (University of Graz, Austria)
Miroslav Kuchta (Simula Research Laboratory, Norway)

Mesh degeneration is a bottleneck for fluid-structure interaction (FSI) simulations and for shape optimization via the method of mappings. In both cases, an appropriate mesh motion technique is required. The choice is typically based on heuristics and the exact choice of mapping is arbitrary from the continuous perspective, as long as the resulting mesh is not degenerate. Therefore machine learning may reasonably be adopted for the problem. We present machine learning-based mesh motion techniques integrated into FEM solvers implemented in FEniCS, with neural networks defined both inside the FEniCS stack in UFL and in PyTorch. We present a hybrid PDE-NN approach, where a UFL-defined neural network serves as parameterization of a coefficient in a second order nonlinear PDE solved in FEniCS. Existence of solutions for the nonlinear PDE is guaranteed by the choice of the neural network architecture. In addition, we present an approach where a neural network represented in PyTorch is integrated as an additive correction to a Laplace equation mapping solved in FEniCS. The quality of the learned mesh motion techniques is evaluated by applying them to an FSI benchmark problem.

## Modeling Cilia-Induced Flow of Cerebrospinal Fluid in Brain Ventricles with FEniCSx

Halvor Herlyng (Simula Research Laboratory, Norway)
Ada J. Ellingsrud (Simula Research Laboratory, Norway)
Marie E. Rognes (Simula Research Laboratory, Norway)
Nathalie Jurisch-Yaksi (Norwegian University of Science and Technology)

Research has demonstrated that regulation of cerebrospinal fluid (CSF) flow in the brain is important for healthy brain functioning, with abnormal flow patterns of CSF being related to various pathologies. Pulsations related to the cardiac cycle influence the CSF flow in the ventricles. Additionally, the inner walls of human brain ventricles are lined with cilia. These hair-like structures induce a complex flow pattern that aids in maintaining the chemical composition of CSF and facilitate CSF transport. Research also suggests that cilia are important for neural development. For the time being, a complete understanding of the interaction between cilia and CSF and the underlying mechanisms remains elusive.

This work investigates and quantifies the contribution of cardiac pulsations and cilia movement to CSF flow in brain ventricles. The flow is modeled and simulated with realistic brain ventricles geometries. Our computational model regards the flow as Stokes flow. A finite element method scheme is used to discretize the governing equations and solve the problem numerically. The solver is implemented in Python using FEniCSx. The numerical simulations are benchmarked to experimental image recordings of CSF flow in zebrafish ventricles, where cilia are present as in the human brain. From the same experiments a zebrafish brain ventricles geometry has been extracted, which was used in the computational study.

Our simulation results exhibit a compartmentalized flow structure where vortex patterns restrict flow to the different parts of the ventricles when cilia are present. In the absence of cilia, these vortex patterns vanish, supporting the conclusion of previous experimental work that cilia are crucial to establish vortex patterns in ventricular CSF flow. In future work, the flow model will be used to simulate transport in the brain ventricles to provide new insights on the contribution of cilia mechanics

and CSF flow to neural development, and how disruptions in cilia functioning can result in pathological conditions.

## Fluid-reduced-Solid Interaction (FrSI): Physics- and Projection-based Model Reduction for Cardiac Hemodynamics

Marc Hirschvogel (King's College London, United Kingdom)
Maximilian Balmus (King's College London, United Kingdom)
Mia Bonini (University of Michigan, United States)
David Nordsletten (University of Michigan, United States & King's College London, United Kingdom)

Fluid-solid interaction (FSI) plays a key role in many biomedical engineering applications, allowing one to model the adaptive interplay between fluid flow and tissue mechanics. Nevertheless, fully coupled FSI often poses challenges from a modeling and computational point of view. On the one hand, sparsity of patient data may render soft tissue geometry reconstructions from imaging intractable, and on the other hand, the computational demand for FSI is often orders of magnitude larger than that of classic CFD. Therefore, reduced hemodynamics models, simplifying the demand for solid mechanics, have been proposed for thin-walled arterial vessels undergoing small to moderate deformations. Leveraging recently proposed reduced membrane formulations for modeling of fluid flow in elastic arteries applied in a small-strain Eulerian framework, we propose a novel physics- and projection-based model reduction technique in an ALE reference frame suitable for a large range of cardiovascular applications, denoted as "fluid-reduced-solid interaction" (FrSI). In the FrSI approach, the solid physics are reduced to a 2-dimensional manifold at the fluid-tissue boundary, obtaining a nonlinear finite strain hyper-viscoelastic membrane model. This is complemented by a projection-based model reduction, performing a Galerkin projection of the fluid boundary momentum equations to a lower-dimensional subspace spanned by deformation modes from imaging (or full-order model motion) data. This projection allows the reduced-physics dynamics to evolve within the data state space, readily providing more realism to observed motion without losing adaptive fluid-tissue response, while filtering any low- to zero-energy membrane modes (wrinkling, buckling). We validate FrSI for an idealized left ventricle (LV) coupled to a lumped pre- and afterload model, showing excellent agreement between full- and reduced-order model in terms of overall flow and deformation pattern. Our results illustrate that FrSI is a highly relevant tool to streamline the simulation of hemodynamics in the heart and cardiovascular system, providing flexible-wall hemodynamics at a fraction of costs of full-order FSI models. FrSI is implemented as a monolithic system of incompressible Navier-Stokes ALE fluid mechanics using latest FEniCSx libraries in the open-source cardiovascular physics solver Ambit.

## Phase-field Modeling in FEniCS: Opportunities and Limitations

Pavan Inguva (Massachusetts Institute of Technology, United States)
Richard D. Braatz (Massachusetts Institute of Technology, United States)

Phase-field models are a powerful class of partial differential equation (PDE) models for studying multiphase systems and interfacial phenomena. Phase-field models introduce and track the evolution of an auxiliary field (the phase field) whose values specify which phase is in each spatial location in the system. The descriptive capability of phase-field models has resulted in their widespread use in many areas of science and engineering including multiphase fluid dynamics, solidification, fracture mechanics, microstructure evolution, image processing, vesicle formation, and tumor growth modeling. Depending on the application, phase-field models can be solved by themselves or coupled to species, momentum, and energy conservation equations which typically result in a nonlinear coupled PDE model that requires numerical methods for solution.

The FEniCS ecosystem has many capabilities such as simple syntax for many tasks such as coupling equations, and integration with powerful scientific computing libraries such as PETSc which facilitate the numerical solution of phase-field models. These capabilities have motivated FEniCS-based implementations of phase-field models by many groups, including for the simulation of fracture mechanics, two-phase electrohydrodynamic flows, and some common benchmarks such as the Cahn-Hilliard equation (e.g., see [1–3]). We demonstrate the FEniCS-based numerical solution of phase field models for a variety of physical systems, which point to limitations of FEniCS and other solvers in simulating some classes of phase field models with realistic parameter values. These results suggest directions for future developments of FEniCS to extend its applicability to a wider variety of phase field models. All code will be made available on a public Github repository for interested users.

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## Assimilation of 4D PC-MRI data into a blood flow model using dolfin-adjoint

Alena Jarolímová (Charles University, Czech Republic)
Jaroslav Hron (Charles University, Czech Republic)

The computational simulation of blood flow has been receiving increasing attention due to its potential to provide useful information in clinical practice. The model must be provided with sufficiently precise estimates of material parameters, boundary conditions, and the segmentation of the computational geometry. For that purpose, it is possible to use 4D phase-contrast magnetic resonance imaging (4D PC-MRI). However, the resolution and noisiness of the images make it hard to directly determine the required parameters. Therefore, it is feasible to use data assimilation instead. We created a model of blood flow in descending aorta containing several patient-specific parameters which are a priori unknown, one of them being the amount of Navier slip along the aortic wall. We solve the inverse problem to determine the most suitable boundary condition parameters using the variational data assimilation approach. The implementation was done in the FEniCS framework using the dolfin-adjoint library to deal with the PDE-constrained optimization which arises from the problem formulation.
The implementation of the method has been tested on artificially generated data in 3D. Then we proceeded to perform experiments with real patient data from several volunteers. The results suggest that the introduction of Navier's slip boundary condition can provide a much better fit to the 4D PC-MRI data than the standardly used no-slip boundary condition.

## On Evolution of Irreversible Systems: Computing Existence Analysis

Andres A. León Baldelli (Sorbonne Université, France)
Sebastien Neukirch (Sorbonne Université, France)

What happens to the stability of critical equilibrium states, as time goes by? In evolutionary problems, structural effects play a key role. We study evolving systems, singularly perturbed and under constraints. Picture fracture as a process: as a phenomenon of natural evolution, it offers an instance

of a particularly complex natural system showing pattern formation and jumps, unknown both in time and space.
From a mechanical perspective [1, 5] the structure of the incremental (quasistatic) evolution problem of fracture is cast in three statements: an irreversibility constraint (pointwise and stiff), an energetic stability criterion (a unilateral condition), and a power balance (in integral form).
Fully exploiting the stability statement provides a functional criterion of choice and a tool to correctly predict path bifurcations [4] and loss of stability of global structures under time-dependent loads. The problem is reduced to a variational constrained eigenvalue problem involving a nonlinear operator which handles both structural elasticity and an internal dissipative softening (damaging) process identifying fractures. In the perspective of large scale numerical experiments, I shall discuss some remarks on its energetic formulation as a variational problem driven by inequalities, relying on its purely energetic considerations.
Presenting a numerical FEniCS (dolfinx) implementation for this singular nonlinear evolution problem with several examples of its discrete approximation, I share the motivation and interest that lays at the intersection between mathematical analysis, theoretical mechanics, and advanced numerics, addressing the understanding of general mechanisms of evolution of irreversible systems, to find stable continuation paths.
The continuous-stability of a multiscale system along its nontrivial paths in phase space is a property that is difficult to check: numerically, at large scales with several material lengths involved, and analytically, in the infinite-dimensional setting.
Exploiting a connection with an existence theorem [3] stated for compact operators in a convex cone, a rigorous implementation of a general energetic statement for a complex system provides the challenge to deploy a fully transparent numerical experimental platform to address the prediction of large scale fracture events.
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## Modelling and numerical simulation of Veno-Venous Extra-Corporeal Membrane Oxygenation

Massimiliano Leoni (Johann Radon Institute for Computational and Applied Mathematics, Austria)
Johannes Szasz (Kepler University Klinikum, Austria)
Jens Meier (Kepler University Klinikum, Austria)
Luca Gerardo-Giorda (Johannes Kepler University)

Extra-Corporeal Membrane Oxygenation (ECMO) is a well-established procedure used in Intensive-Care Units (ICU) to treat patients with either pulmonary or heart failure. The blood of the patient is drawn via a cannula, oxygenated and injected via another cannula. The extraction cannula is normally located in the inferior vena cava. In the case of lung failure, but with a heart in good conditions, the injection cannula is placed in the superior vena cava (veno-venous, VV-ECMO). In the case of heart failure, the injection cannula is placed in the aorta (veno-arterial, VA-ECMO) to ensure that the blood is actually pumped across the arterial system. VV-ECMO is the standard procedure

in the case of Severe Acute Respiratory Syndrome and was routinely used for Covid-19 patients in ICU. A known clinical problem of VV-ECMO is recirculation, where a significant portion of the fully oxygenated blood appears to be recaptured by the extraction cannula in the inferior vena cava, instead of joining the normal circulation pathway. This results in a limited efficacy of the procedure: blood is inserted fully oxygenated but distal measurements show oxygen values as low as 80%. In this talk we will present our work on patient-specific modelling and simulation of VV-ECMO, a surprisingly uncharted territory in the current scientific literature. We will describe the major modelling challenges that ECMO poses, with a particular focus on the proper description of the blood flow. The patient geometry is reconstructed from a CT scan, while blood flow and oxygen diffusion are approximated by the Finite Element Method. We will present numerical results showing how poorly the standard VV-ECMO actually performs and we will discuss possible optimisation procedures or best practices to improve its effectiveness.

## Redefining the finite element with Implementation in mind

India Marsden (University of Oxford, United Kingdom)
David A. Ham (Imperial College London, United Kingdom)
Patrick E. Farrell (University of Oxford, United Kingdom)

The Ciarlet definition of a finite element has been used for many years to describe the requisite parts of a finite element. However, it can be considered that additional details incorporated into the definition would avoid the use of assumptions in the implementation that are currently required. One key example of these assumptions is how the degrees of freedom on shared entities are required to be equal, or not if a discontinuous element is desired. We will discuss how to solve this through amending the definition to include more information. In addition, we consider if there are more efficient ways to represent the degrees of freedom that enable a description of their structure.This talk will also show how these additions provide space for development in finite element implementations such as FEniCS and Firedrake.

## Poisson & Drift-Diffusion Equations Solver for Semiconductor Device Modelling

Jan Miklas (Brno University of Technology, Czech Republic)
Petr Prochazka (Brno University of Technology, Czech Republic)

We present an application example utilizing FEniCSx to solve the essential “semiconductor equations” modelling the electronic device operation. The device electrostatics is described by Poisson equation while charge transport of electrons and holes along with standard generation/recombination phenomena is governed by a classical drift-diffusion model. The equations constitute a system of coupled nonlinear elliptic and parabolic PDEs. The problem is solved numerically by use of DOLFINx methods for mixed function space formulation and Newton’s iterations. Precise estimation of switching loss in power semiconductor devices belongs to main challenges in power electronics applications design for several reasons; lack of simple yet accurate device models being of main ones. An ultimate goal of our FEM model - aside from improved understanding of internal device physics during switching transients - is to serve as an extensible modular validation tool for analytical assumptions applicable in simplified semi-analytical device models. Our particular research focus lies on derivation of insulated-gate bipolar power transistor (IGBT) one-dimensional device model covering the basic physics and precise switching waveforms prediction under arbitrary operating conditions at minimum computational cost. Graphic simulation outputs for basic semiconductor structures like PN junction

diode and NPN bipolar transistor and comparison with acquirable experimental data are presented to demonstrate the functionality of FEM model implementation.

## Elastodynamics with FEniCSx

Pierric Mora (Université Gustave Eiffel, France)

There already exist powerful free finite element codes for solving elastodynamics problems, but these are usually specialized in a single or few types of problems. With its flexibility in choosing basis polynomials, with the recent inclusion of complex numbers, and with its scalable architecture, FEniCSx has a great potential to be a unifying platform for treating a wide range of cases in an efficient manner: time domain (linear/nonlinear), frequency domain, normal modes, guided waves, periodic media...
Here I present 'Elastodynamicsx', a recent initiative to try to simplify the use of FEniCSx for such problems to people that are not experts in applied mathematics. The package consists of higher level classes representing material laws, boundary conditions, and solvers. I illustrate the presentation with examples relevant to the field of non-destructive evaluation using ultrasounds, namely: the radiation pattern of a wedge transducer (frequency domain), surface wave harmonics generation in concrete, and wave guiding in a civil engineering cable.

## A Design Process of Binary Stiffness Compliant Mechanism for Embodied Intelligence in Robotic Systems using FEniCS and gmsh

Parisa Omidvar (AMOLF, Netherlands)
Marc Serra-Garcia (AMOLF, Netherlands)
Paul Ducarme (AMOLF, Netherlands)

The conventional approach to designing the control unit of a robotic system involves the use of electronics. However, current trends in designing compliant metamaterials and soft robotics suggest that nonlinear structural responses of compliant parts, traditionally viewed as undesired behaviors, can be exploited to embody intelligent behavior in the system without relying on electronic chips. An example of this embodied intelligence can involve a soft robot that navigates a maze by executing a search algorithm.
An approach towards building systems with intelligent behavior and information processing consists in combining components with a well-designed and optimized response in a systematic way as if they were Lego blocks. These blocks will include nonlinear compliant mechanisms with variable or binary stiffness in which the stiffness changes over a range of values, or only between two values.
In this talk, we will explain our process of designing compliant mechanisms in which we use FEniCS and Gmsh. This numerical design process facilitates the creation of binary stiffness mechanisms with complex geometries and nonlinear material behavior and promotes the integration of these mechanisms into intelligent systems.

## Bread baking simulation with FEniCS

Laura Rinaldi (Università degli Studi di Padova, Italy)
Fabio Marcuzzi (Università degli Studi di Padova, Italy)
Giulio G. Giusteri (Università degli Studi di Padova, Italy)

A finite-element computational model for bread leavening and cooking will be presented. The partial differential equations considered describe heat exchange between the elements involved in the model and take into account the presence as well as the diffusion of moisture, yeast and their metabolism which implies some carbon dioxide production responsible for the volumetric growth of the dough. The temperatures evolution are coupled with the quasi-static deformation of the growing elastic dough. The application of FEniCS in our research allows to define numerically, to link together and to solve the above-mentioned coupled equations discretized in space and time. The results of the detailed simulations emulates the physical behavior of a bread dough during its baking process and allow to obtain an estimation of the resulting energy consumption. Moreover, this circumstantial model is the foundation for a surrogate/reduced modeling that can bring this simulation to run online with the real process, a main target of digital twins for Industry 4.0.

## Modeling and parameter estimation for tracer transport in the human brain

Jørgen Riseth (Simula Research Laboratory, Norway)
Kent Andrè Mardal (University of Oslo, Norway)

The talk will present the GRIP-study which aims to better understand the glymphatic system's role in clearing metabolic waste products in the brain and the potential role an alteration of the system may play in patients with Parkinson's disease. Parkinson's patients are known to exhibit aggregations of misfolded alpha-synuclein, possibly due to reduced waste clearance, making this study particularly relevant.
The study uses MRI-data from 15 Parkinson's patients and 10 healthy controls to model the spread and transport of tracers injected into the cerebrospinal fluid. Solute transport is modeled as a two-compartment diffusion model that describes homogenized transport through brain tissue and fluid-filled spaces surrounding blood vessels in the brain. We want to investigate whether potential differences between patients and controls may be identified through parameter estimation, based on concentration estimates from the MRI-data and PDE constrained optimization. The optimization procedure is implemented using FEniCS and dolfin-adjoint.

## ddfenics: a FEniCS-based (Model-Free) Data-driven Computational Mechanics implementation

Felipe Rocha (Ecole Centrale de Nantes, France)
Laurent Stainier (Ecole Centrale de Nantes, France)

Field equations are the cornerstone for mathematical modelling in several, if not all, branches of physics: gravitation, elasticity, fluid mechanics, electromagnetism, etc. Normally they are expressed in the form of PDEs, allowing to express the evolution of given physical systems according to underlying conservation principles. In this sense, we can consider such equations as the most fundamental ones since they remain unchanged with respect to specific media/material. On the other hand, additional closure relations such as constitutive models are needed for allowing unique solutions of such models. Naturally, the choice of such models is not unique and in some cases can give rise to non-optimal modeller bias. It is worth noticing that these drawbacks are still present even in the recent trend of ML-based surrogate models, even though the latter allows to slightly relax such bias. Circumventing these inconveniences, the so-called (model-free) data-driven computational mechanics (DDCM) method proposes a new paradigm that completely bypasses the need for constitutive laws to solve field equations, by accepting raw experimental datasets as inputs (e.g strain-stress, gradient-

flux pairs). The price to be paid: the solution of the generalised problem fits only partially in a PDE framework, therefore only part of the problem can be solved by FEniCS. While a PDE-like subproblem accounts for enforcing basic conservation principles and kinematical compatibilities, the second subproblem consists in a discrete optimization search (nearest neighbour) which ensures the optimal solution lies as close as possible to the experimental data. In this talk, we present ddfenics (https://github.com/felipefr/ddfenics), a library that aims at integrating the DDCM framework (with as few as possible changes from a user's perspective) into a typical FEniCS script. As a rule of thumb, the main design principle relies on mimicking the necessary FEniCS objects into ddfenics counterparts based on their functionality (instantiation of a variational problem, solver, etc). Some of the internal aspects and architectural choices used will be discussed, followed by numerical applications ranging from Darcy's flow to infinitesimal and finite strain elasticity demonstrating the full generality of ddfenics.

## Implementation of a modified Mitchell-Schaeffer model to describe the electrical activity in the heart

Jesus Jairo Rodríguez Padilla (Centre Inria d'Université Côte d'Azur, France)
Maxime Sermesant (Centre Inria d'Université Côte d'Azur, France)

The Mitchell-Schaeffer (MS) model belongs to the category of simplied ionic models of action potential (AP), regrouping fluxes of different ionic species together, depending on their effect on the transmembrane potential. Instead of representing the cell membrane permeability to the different ions involved, its limited parameters are related to the general shape of the cardiac AP.
The MS model consists of two ODEs and contains just two currents which mimic the sodium and potassium currents. It is complex enough to exhibit the restitution behavior of more physiological models, yet is simple enough that much of its behavior can be understood analytically.
In this model, two state variables are used: u, representing the scaled transmembrane potential; and h, acting as a gating variable: it controls the recovery of the virtual cardiac cell, by modulating its excitability and general response to an external current.
In this talk, we will present the weak formulation of the MS model, as well as the implementation in two and three dimensional domains using FEniCSx.

## newfl: working towards a new version of UFL

Matthew Scroggs (University College London, United Kingdom)
David Ham (Imperial, United Kingdom)
India Marsden (Oxford, United Kingdom)
Chris N. Richardson (University of Cambridge, United Kingdom)
Garth N. Wells (University of Cambridge, United Kingdom)

In the last few years, (almost) every component of FEniCS has been rewritten to create FEniCSx: every component except UFL, that is. In the last year or so, we have begun work to simplify and update parts of UFL. In this talk, I will present our progress and our future plans for UFL.

## SimCardEMS: A cardiac electromechanics solver to assess drug safety and efficacy

Ilsbeth van Herck (Simula Research Laboratory, Norway)
Henrik N. Finsberg (Simula Research Laboratory, Norway)

Cécile Daversin-Catty (Simula Research Laboratory, Norway)
Jørgen S. Dokken (Simula Research Laboratory, Norway)
Samuel Wall (Simula Research Laboratory, Norway)
Hermenegild Arevalo (Simula Research Laboratory, Norway)

Modelling and simulation of cardiac tissue are extensively used to describe electrical and mechanical processes in the heart. More recently, the coupling between these processes is also included in computational simulations, as well as the passive mechanical and electrical behaviour of the overall cardiac tissue. This opens up new avenues for simulating drug effects in cardiac tissue, including contraction as a cause of distress, but also as a possible treatment target. These fully coupled models require a dedicated electro-mechanical solver to connect the range of processes and scales. For this reason, we developed SimCardEMS, a FEniCS based cardiac electro-mechanical solver. This solver is available as open-source software and able to serve more applications in cardiac modelling.
In this talk, we present a fully coupled electro-mechanical model in the context of evaluating the effect of drugs on the heart. Our framework incorporates a modern human cell ordinary differential model (ODE) that describes cellular electrophysiology, embedded in a monodomain partial differential equation (PDE) representation of the electrical substrate and a continuum model to simulate contraction. This model represents the full cardiac cycle from electrical stimulus, internal calcium release, calcium induced activation of cross-bridge dynamics, active force and tissue contraction.
Bidirectional feedback between the electrical and mechanical models is achieved in two individual steps. Cellular parameters such as calcium concentration and cross-bridge states are projected to the continuum model, dictating the boundary conditions that govern the expansion and contraction. Changes in length and shortening velocity in the mechanical model is provided as feedback to the ODE model of electrical behaviour. Including this bidirectional coupling provides a model that can simulate drug effects on electrophysiology, but also assess changes in contraction or simulate drugs that target the contractile machinery specifically. Including both aspects of the cardiac cycle, as well as their influence on each other, improves drug modelling and possibly improves drug safety and efficacy prediction.

## Model order reduction of lattices by maximally localized Wannier functions

Sima Zahedi Fard (AMOLF, Netherlands)
Paolo Tiso (ETH Zürich, Switzerland)
Parisa Omidvar (AMOLF, Netherlands)
Marc Serra-Garcia (AMOLF, Netherlands) Final author (University, Country)

This work focuses on developing an efficient and precise finite element model for wave-based neural networks and their application to passive speech recognition. The elastic neural networks are constructed using a large nonlinear lattice made of hyperelastic material, which undergoes large deformations. The elastic neural network is required to perform precise information-processing tasks. Therefore, it is crucial to model it with a high degree of accuracy while also ensuring computational efficiency. To achieve this, we model the deformation using Wannier functions, that represent highly localized deformations. The resulting nonlinear models are sparse due to the localization. To consider changes in mode shapes induced by the nonlinearity, we include an additional modal derivative term.
FEniCS allows us to set up the necessary auxiliary problems to efficiently compute the Wannier functions and modal derivatives for a given geometry. This approach provides a method for accurate and computationally efficient simulations of highly nonlinear dynamical lattices, with potential applications in a range of fields such as phononic computing, photonics, microwave, etc.

## Netgen-DMPlex interface and FEniCS

Umberto Zerbinati (University of Oxford, United Kingdom)

As a result of a recent implementation of a Netgen-DMPlex interface inside Firedrake in this talk, we would like to explore possible applications of the Netgen-DMPlex interface to FEniCS.

# Poster presentations

## multiphenicsx - easy prototyping of multiphysics problems in FEniCSx

Francesco Ballarin (Università Cattolica del Sacro Cuore, Italy)

multiphenicsx is a python library that aims at providing tools in FEniCSx for an easy prototyping of multiphysics problems on conforming meshes. In particular, it facilitates the definition of subdomain/boundary restricted variables. multiphenicsx is the successor to multiphenics, a library with similar goals that used to target FEniCS. Within this poster, I will summarize the history behind multiphenics/multiphenicsx, provide technical insights on their implementation, and showcase their capabilities through several tutorials.

## Modelling Fluorescence Lifetime of Carbon Quantum Dots for Improved pH Sensitivity

Denise Dilshener (University of Bergen, Norway)
Drew F. Parsons (Università degli Studi di Cagliari, Italy)
Johannes Fiedler (University of Bergen, Norway)
Bodil Holst (University of Bergen, Norway)

We investigate a theoretical framework for predicting the fluorescence lifetime of carbon dots for improved pH sensitivity in pH sensors. Fluorescence lifetime is determined utilizing density functional theory and quantum mechanics to evaluate electronic transitions within carbon dots. The fluorescence lifetime of the carbon dot is sensitive to pH via the relative proportion of protonated and deprotonated sites. FEniCS will be used to evaluate the proportion of protonated to unprotonated charge sites, accounting for the electrostatic potential and adsorption of salt, H+ and OH- ions near the surface of the carbon dots. Theoretical predictions will be validate through comparison against experimental measurements, enabling refinement and optimization for diverse applications.

## Modelling the Impact of Chemisorption and Steric Forces in Cyclic Voltammetry Curves

Matteo Farci (Università degli Studi di Cagliari, Italy)
Drew F. Parsons (Università degli Studi di Cagliari, Italy)

Our study analyzes the phenomena of ion adsorption on charged surfaces immersed in an electrolyte solution. Understanding these phenomena is useful for the development of devices such as biosensors or batteries, as well as for simulating the results of electrochemical techniques such as cyclic voltammetry (CV). In equilibrium conditions the Poisson-Boltzmann (PB) model can be used, but this fails at large voltages or ion concentrations due to the fact that some effects, i.e. steric effects due to the finite size of ions, are not considered. For this reason more complex theories need to be used, also to include chemisorption phenomena that are important in the context of charge regulated surfaces. In addition we are interested in studying systems in non-equilibrium conditions, for this purpose we start from the Poisson-Nernst-Plank (PNP) model, the time dependent counterpart of the PB model. These complex models often have not analytical solution and required to solve non linear problems. Then we are developing a python library to solve them numerically by FEniCS. Our library can be used to study the CV curves of protein adsorption, supporting the development of electrochemical bionsensors.

## Solute adsorption in the wedge between charged surfaces

Alin Grigoras (Università degli Studi di Cagliari, Italy)
Drew F. Parsons (Università degli Studi di Cagliari, Italy)

In this study, we present a computational framework developed using the FEniCSx computing platform, capable of numerically solving the Poisson-Boltzmann equation and estimating the local electric potential and charge density distribution between charged surfaces. The implemented code employs the finite element method to simulate a wedge-shaped configuration, where an electrolytic solution resides between two surfaces, such as two glass plates. The system is represented as a triangular domain, with the base and hypotenuse representing charged glass surfaces. A Jacobian determinant enables separate scaling in X and Y directions, allowing a unit triangle to represent any wedge angle. We extract and integrate vertical profiles of concentration values at each x position, motivated by experimental optical data investigating ion adsorption[1]. The code allows for the variation of the angle between the two surfaces, providing insights into the effects of different angles on ion adsorption. The developed framework offers a valuable tool for exploring electrostatic phenomena in complex geometries and contributes to the understanding of charge distributions in wedge-shaped systems.

[1] Adsorption at Confined Interfaces, P. Gaddam, R. Grayson, and W. Ducker. Langmuir 2018, 34, 36, 10469–10479. doi:10.1021/acs.langmuir.8b01418

## Solving the Modified Poisson-Boltzmann Equation for Electric Double Layer Capacitors using FEniCS

Dagmawi B. Tadesse (Murdoch University, Australia)
Drew F. Parsons (Università degli Studi di Cagliari, Italy)

This poster presents our approach to solving the modified Poisson-Boltzmann equation for electric double-layer capacitors (EDLCs) using the FEniCS framework [1,2]. The equation incorporates ionic van der Waals (dispersion) interactions and incorporates finite ion sizes via the Carnahan-Starling steric force. Our work addresses the challenging nonlinear numerical complexities of high voltages and concentrations in EDLCs. The poster showcases the interplay between electric fields, ionic concentrations, and dispersion effects within the EDLC, highlighting the importance of accurate and efficient numerical methods. The outcomes of this study contribute to the advancement of EDLC modeling and demonstrate the potential of FEniCS for modelling complex electrochemical systems.

[1] The impact of steric repulsion on the total free energy of electric double layer capacitors. Dagmawi B. Tadesse, Drew F. Parsons. Colloids and Surfaces A, 648 (2022) 129134. DOI:10.1016/j.colsurfa.2022.129134
[2] Thermodynamics Beyond Dilute Solution Theory: Steric Effects and Electrowetting. Dagmawi Tadesse, Drew Parsons. Chapter 63, Encyclopedia of Solid-Liquid Interfaces. In press.

## Interactions between coarse and fine galena and quartz particles and their implications for flotation in NaCl solutions

Anna M. Nowosielska (Murdoch University, Australia)
Aleksandar N. Nikoloski (Murdoch University, Australia)
Drew F. Parsons (Università degli Studi di Cagliari, Italy)

In this study [1] we have investigated the interactions between coarse and fine galena and quartz particles and their implications for flotation in NaCl solutions. Tested were four different particle systems : (CC) Coarse galena/Coarse quartz, (CF) Coarse galena/Fine quartz, (FC) Fine galena/Coarse quartz and (FF) Fine galena/Fine quartz. The micro-flotation experiments were carried out in solutions containing 10 mM or 100 mM NaCl, at pH 9. It was found that galena recovery was the highest for the CC particle system, and the lowest for the FF particle system. The experiments also indicated that the recovery improved for the higher NaCl concentration. We calculated the total interaction free energy as a function of the separation distance for each test condition using FEniCS to solves a general Poisson-Boltzmann model employing pH-dependent charge-regulated surface charge (Neumann boundary conditions). It was established that for all particle systems, the galena/quartz interactions are dominated by repulsion. Galena/air bubble interactions in 10 mM were repulsive but became attractive in 100 mM NaCl salt solutions. The quartz/air bubble interactions were always repulsive, irrespective of the NaCl concentration. Based on these predictions, we postulate that the stronger repulsion of quartz particles towards air bubbles could be the driving force for galena recovery.

[1] Interactions between coarse and fine galena and quartz particles and their implications for flotation in NaCl solutions. Anna M. Nowosielska, Aleksandar N. Nikoloski, Drew F. Parsons Minerals Engineering 183 (2022) 107591. DOI:10.1016/j.mineng.2022.107591

## DefElement: an encyclopedia of finite element defintions

Matthew Scroggs (University College London, United Kingdom)

In this poster I will present `defelement.com`. It is a useful reference website that lists a huge range of finite elements and their definitions.

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