

**PDEs and Geometry: Numerical Aspects**  
**Poster Session Abstracts**  
**Wednesday, March 13, 2024**

**Nested Iteration and Nonlinear Methods for Liquid Crystal Shape Optimization Applications**

Anca Andrei, Tufts University

Anisotropic fluids, such as nematic liquid crystals, can form non-spherical equilibrium shapes known as tactoids. Predicting the shape of these structures as a function of material parameters is challenging and paradigmatic of a broader class of problems that combine shape and order. Here, we develop a discrete shape optimization approach with finite elements to find the configuration of a two-dimensional tactoid using the Landau de Gennes framework and a Q- tensor representation. Efficient solution of the resulting constrained energy minimization problem is achieved using a quasi-Newton and nested iteration algorithm. Numerical validation is performed with benchmark solutions and compared against experimental data and earlier work. We explore physically motivated subproblems, whereby the shape and order are separately held fixed, to explore the role of both and examine material parameter dependence of the convergence. Nested iteration significantly improves both the computational cost and convergence of numerical solutions of these highly deformable materials.

**Hodge decomposition finite element method for the 3D quad curl problem**

Casey Cavanaugh, Louisiana State University

We present a finite element method for the quad-curl equation in three dimensions. Using the Hodge decomposition for divergence-free fields, the fourth-order problem is reformulated as three standard second-order saddle point systems. Furthermore, the Hodge decomposition approach allows for the finite element method to handle domains with general topology. Analysis and numerical results are presented using a variety of domains with different topological properties.

**GPT-PINN: Generative Pre-Trained Physics-Informed Neural Networks toward non-intrusive Meta-learning of parametric PDEs**

Yanlai Chen, UMass Dartmouth

Physics-Informed Neural Network (PINN) has proven itself a powerful tool to obtain the numerical solutions of nonlinear partial differential equations (PDEs) leveraging the expressivity of deep neural networks and the computing power of modern heterogeneous hardware. However, its training is still time-consuming, especially in the multi-query and real-time simulation settings, and its parameterization often overly excessive.

This poster presents the recently proposed Generative Pre-Trained PINN (GPT-PINN). It mitigates both challenges in the setting of parametric PDEs. GPT-PINN represents a brand-new meta-learning paradigm for parametric systems. As a network of networks, its outer-/meta-network is hyper-reduced with only one hidden layer having significantly reduced number of neurons. Moreover, its activation function at each hidden neuron is a (full) PINN pre-trained at a judiciously selected system configuration. The meta-network adaptively “learns” the parametric dependence of the system and “grows” this hidden layer one neuron at a time. In the end, by encompassing a very small number of networks trained at this set of adaptively-selected parameter values, the meta-network is capable of generating surrogate solutions for the parametric system across the entire parameter domain accurately and efficiently.

**Error analysis of BDF 1-6 time-stepping methods for the transient Stokes problem: velocity and pressure estimates**

Alessandro Contri, NTNU — Norwegian University of Science and Technology

We present a new stability and error analysis of fully discrete approximation schemes for the transient Stokes equation. For the spatial discretization, we consider a wide class of Galerkin finite element methods which includes both inf-sup stable spaces and symmetric pressure stabilized formulations. We extend the results from Burman and Fernández [*SIAM J. Numer. Anal.*, 47 (2009), pp. 409-439] and provide a unified theoretical analysis of backward difference formulae (BDF methods) of order 1 to 6. The main novelty of our approach lies in the use of Dahlquist's G-stability concept together with multiplier techniques introduced by Nevannlina-Odeh and recently by Akrivis et al. [*SIAM J. Numer. Anal.*, 59 (2021), pp. 2449-2472] to derive optimal stability and error estimates for both the velocity and the pressure. When combined with a method dependent Ritz projection for the initial data, unconditional stability can be shown while for arbitrary interpolation, pressure stability is subordinate to the fulfillment of a mild inverse CFL-type condition between space and time discretizations. Authors: Alessandro Contri, Balázs Kovács, André Massing Link: <https://arxiv.org/abs/2312.05511>

## **Modeling hypothermia with a multiscale model coupling partial differential equations for temperature with ordinary differential equation.**

Tyler Fara, Oregon State University

We present a computational model simulating body temperature in extremities subject to extreme cold (hypothermia). The phenomenological description of the problem is that the body responds to hypothermia by vasoconstriction, whereby the body restricts blood flow to the extremity, preserving core body temperature even at the expense of sacrificing tissue in the extremity. Our model includes: (i) a parabolic partial differential equation (PDE) with an energy exchange term modeling blood perfusion through tissue, and this term is derived by multiscale analysis, and (ii) a constrained ODE representing the body's metabolic and vasoconstrictive responses. We approximate the solution to the model with mixed finite element method on Cartesian grids for the PDE with an immersed boundary approach to handle complex geometries.

## **The Restriction of the Laplace Operator**

Padi Fuster Aguilera, University of Colorado Boulder

On a Riemannian manifold, there is no canonical Laplace operator for vector fields or forms, and it is not clear what is the "correct" Laplacian to use when formulating fluid dynamics equations. In this poster, we will present different approaches for obtaining a viscosity operator when considering a Riemannian hypersurface in the Euclidean space, as well as show some concrete examples.

## **Computing Smooth Surfaces via Nets of Geodesics**

Tom Gilat, Bar-Ilan University

The poster presents my study concerning the computation of smooth surfaces given a network of curves in 3d, such that the curves given are geodesics on the computed surface. The motivation for this work originated in considering CAD interfaces, sketch-to-3d methods, and how artists illustrate 3d objects in 2d drawings. In this study I introduce the notion of a minimal Gaussian curvature (squared) surface: a surface which spans a contour such that it is a geodesic and the integral of  $K^2$  is minimized. I compute an approximation of such surface for each patch in the net. For this, I use isothermal coordinates and obtain approximately a biharmonic equation for the conformal factor of the metric of each such patch. I explain in the poster how I compute the boundary conditions, Dirichlet and Neumann, for these equations.

## **Solving Parabolic PDEs on Discrete Domains**

Leticia Mattos Da Silva, Massachusetts Institute of Technology

We introduce a framework for solving a class of parabolic partial differential equations on triangle mesh surfaces, including the Hamilton-Jacobi equation and the Fokker-Planck equation. PDEs in this class often have nonlinear or stiff terms that cannot be resolved with standard methods on curved triangle meshes. To address this challenge, we leverage a splitting integrator combined with a convex optimization step to solve these PDEs. Our machinery can be used to compute entropic approximation of optimal transport distances on geometric domains, overcoming the numerical limitations of the state-of-the-art method. In addition, we demonstrate the versatility of our method on a number of linear and nonlinear PDEs that appear in diffusion and front propagation tasks in geometry processing.

## **Shape Optimization with an Unfitted Finite Element Method**

Jeremy Shahan, Louisiana State University

We present a formulation of a PDE-constrained shape optimization problem that uses an unfitted finite element method (FEM). The geometry is represented (and optimized) using a level set approach and we consider objective functionals that are defined over bulk domains. For a discrete objective functional (i.e. one defined in the unfitted FEM framework), we show that the exact shape derivative can be computed rather easily. In other words, one gains the benefits of both the optimize-then-discretize and discretize-then-optimize approaches.

We illustrate the method on a simple model (geometric) problem with known exact solution, as well as shape optimization of structural designs. We also give some discussion on convergence of minimizers.

This is joint work with Shawn W. Walker (walker@math.lsu.edu, LSU)

## **Inf-Sup Stability of Parabolic TraceFEM**

Mansur Shkipov, University of Maryland, College Park

This manuscript presents an inf-sup analysis of continuous-in-time, discrete-in-space TraceFEM discretization of the (fixed) surface heat equation. The analysis relies on two components. First is the modification of the normal derivative volume stabilization, wherein in addition to stabilizing the solution one also stabilizes the time derivative with a different stabilization scaling. We refer to this scheme as "total stabilization". The second component is the study of the "stabilized  $L^2$ -projection". This analysis leads to convergence to minimum regularity solutions, symmetric error bound in an energy error functional, and "textbook" condition number estimates. The analysis does not take into account the error in approximating the geometry and time discretization.

## **Efficient Computation of Higher Dimensional Mean field Control based Barycenters from Reaction-Diffusion Systems**

Arjun Vijaywargiya, University of Notre Dame

In this work, we address a class of mean field optimal control problems arising in the computation of the Wasserstein barycenters of multi-density systems with reactive-diffusive dynamics. The primary objective is to present a comprehensive framework for efficiently solving these control problems. Our approach involves the utilization of high-order finite element discretizations of the spacetime domain to achieve improved accuracy. The discrete optimization problem is then solved using the primal-dual hybrid gradient (PDHG) algorithm, a powerful first-order optimization method known for its effectiveness in addressing a wide range of constrained optimization problems. The efficacy and robustness of our proposed framework are illustrated through several numerical examples in three dimensions, such as the computation of the barycenter of multi-density systems consisting of Gaussian distributions and of reactive-diffusive multi-density systems involving 3D voxel densities. Additional examples highlighting shape interpolation, where one object is continuously transformed into another, are also supplied.