Simulation-Based Optimization with Applications
Poster Session Abstracts
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Optimal control for Darcy's equation in a heterogeneous porous media
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In this paper, we investigate optimal control problems in heterogeneous porous media. The optimal control problem is governed by the Darcy's flow equation; where the pressure is the state variable and the source/sink is the control variable. Then we introduce the reduced optimal control problem which contains only the state variable by replacing the control variable with a dependent quantity of the state variable based on the Darcy's equation. Here we employ interior penalty finite element methods for the spatial discretization to solve the reduced optimal control problem resulting in a fourth-order variational inequality. We use Lagrange finite elements for interior penalty methods, which require fewer degrees of freedom than finite element methods. We provide a priori error estimates and stability analyses by considering a heterogeneous permeability coefficient. Several numerical examples validate the given theories and illustrate the capabilities of the proposed algorithm.

MCMC Stepsize Selection for Neural Network Stochastic Approximation with Latent Variables
Federica Milinanni, ICERM

Factor analysis is a modeling approach that describes observed random variables through underlying latent variables. By using neural networks (NN) to map these latent variables to observables, we gain significant model flexibility. However, this also introduces the challenging problem of NN parameter estimation. In this work, we address parameter estimation in NN-based factor analysis using a stochastic approximation algorithm, based on the seminal work of Robbins and Monro. Implementing this algorithm requires sampling from the posterior distribution of the latent variables, conditioned on observations and current model parameters. We employ the Metropolis-Adjusted Langevin Algorithm (MALA) for this sampling step, a popular method within the class of Markov chain Monte Carlo Methods. Because the efficiency and stability of MALA are highly sensitive to the discretization stepsize, we provide a method for selecting a suitable stepsize value to ensure fast convergence to the target distribution. Our selection criteria leverage the interplay between the latent covariance structure and the properties of the neural network architecture. This approach reduces the need for manual tuning and improves the overall robustness of stochastic approximation in neural latent variable models. This poster is based on joint work with Dale S. Kim (UCLA).

Analysis of Bregman Proximal Point for the Obstacle Problem
Noe Reyes Rivas, Applied Mathematics, Brown University

We study the Bregman proximal point algorithm (BPP) for the obstacle problem, a fundamental variational inequality arising in contact mechanics, optimal design, and mathematical finance. At each iteration, BPP replaces the original problem with a regularized subproblem governed by a Bregman divergence, yielding a sequence of iterates whose convergence to the solution of the obstacle problem is the focus of this work. Our first contribution is a new technique for establishing the well-posedness of the BPP subproblems. Our second contribution concerns the algorithm's convergence analysis. In particular, we improve the best-known worst-case sublinear convergence rates for fixed step sizes and further show that linear convergence holds under additional regularity conditions. To our knowledge, these results provide the first optimal convergence rate guarantees for BPP applied to the obstacle problem. Numerical experiments illustrate the method's practical performance and corroborate the theoretical rates.

Infinite-dimensional spherical-radial decomposition for probabilistic functions, with application to constrained optimal control and Gaussian process regression

Kewei Wang, Courant Institute, New York University

The spherical-radial decomposition (SRD) is an efficient method for estimating probabilistic functions and their gradients defined over finite-dimensional elliptical distributions. In this work, we generalize the SRD to infinite stochastic dimensions by combining subspace SRD with standard Monte Carlo methods. The resulting method, which we call hybrid infinite-dimensional SRD (hiSRD) provides an unbiased, low-variance estimator for convex sets arising, for instance, in chance-constrained optimization. We provide a theoretical analysis of the variance of finite-dimensional SRD as the dimension increases, and show that the proposed hybrid method eliminates truncation-induced bias, reduces variance, and allows the computation of derivatives of probabilistic functions. We present comprehensive numerical studies for a risk-neutral stochastic PDE optimal control problem with joint chance state constraints, and for optimizing kernel parameters in Gaussian process regression under the constraint that the posterior process satisfies joint chance constraints.

Proximal Galerkin schemes for enforcing pointwise inequality constraints in de Rham complex finite element discretizations

Alexey Izmailov, Brown University Division of Applied Mathematics

This work introduces and analyzes Proximal Galerkin (PG) schemes for solving variational problems with pointwise inequality constraints in vector-valued function spaces. Natural discretizations for unconstrained problems of this type yield a saddle-point structure via the Finite Element Exterior Calculus (FEEC). This extends to a sequence of twofold saddle-point subproblems when applying the PG methodology to the constrained analogue. Here, we expand the PG framework across the de Rham complex, establishing the well-posedness of the general twofold saddle-point systems solved at each proximal iteration. Furthermore, we extend the analysis of PG schemes by providing a priori error analysis for inequality constraints in H(div) and H(curl). We demonstrate our approach by showcasing one of the first numerical methods for vector Laplacian obstacle problems associated with the 2D and 3D de Rham complexes. We also highlight possible applications to state-constrained optimal control and elastoplastic modelling. Finally, this framework yields a new approach to the numerical solution of the Hintermuller--Kunisch formulation of the BV-regularized image restoration problem.

The proximal Galerkin method for phase-field fracture

Biswajit Khara, Brown University

The phase-field method has emerged as a powerful tool for simulating fracture mechanics, yet it presents significant numerical challenges, particularly regarding the non-convexity of the energy functional and the enforcement of physical constraints such as crack irreversibility and the boundedness of the phase-field variable. This work uses the proximal Galerkin method as a robust and efficient framework for solving phase-field fracture problems. By reformulating the inequality-constrained optimization problem as a sequence of saddle-point problems via latent variables, the method rigorously enforces the physical bounds of the phase-field and naturally handles the irreversibility condition without the need for ad hoc penalty parameters or history variables. We validate the proposed approach through a series of numerical examples, including one-dimensional benchmarks with analytical solutions, standard two-dimensional quasi-static fracture tests such as the single-edge notched tension/shear tests, and dynamic cases such as crack branching and Kalthoff--Winkler tests. The results demonstrate that the method accurately reproduces theoretical predictions and aligns with standard staggered schemes, while offering a unified and mathematically consistent treatment of the constraints inherent to phase-field fracture modeling.

Efficient FDTD Modeling of Spatial Soliton Propagation and Scattering in Dispersive Nonlinear Optical Materials

Victory Obieke, Oregon State University

This work applies the auxiliary differential equation finite-difference time-domain (ADE–FDTD) method to model electromagnetic wave propagation in dispersive nonlinear materials. A coupled system of Maxwell's equations is developed that includes multipole linear Lorentz dispersion together with nonlinear Kerr and Raman polarizations. The Kerr polarization models the instantaneous intensity-dependent third-order nonlinear response of the medium. The Raman polarization models the delayed third-order nonlinear response arising from molecular vibrations in the medium.The approach is demonstrated through simulations of spatial optical solitons with two spatial components.The method avoids interpolation of the nonlinear staggered component terms, leading to a computationally efficient second-order accurate scheme.Using a realistic glass medium characterized by three-pole Sellmeier linear dispersion, instantaneous Kerr nonlinearity, and dispersive Raman nonlinearity, we investigate both the propagation of spatial solitons and their scattering by compact subwavelength air holes, which act as abrupt dielectric discontinuities along the soliton path. Our results reveal that after interacting with the air hole, the scattered electromagnetic field coalesces into a lower-energy propagating spatial soliton at a point many tens of wavelengths beyond the discontinuity. These findings demonstrate the effectiveness of the method and its potential for the design of soliton-based optical switching devices.

Reduced-Order Modeling and Hierarchical MPPI Control for Granular Terrain Shaping

Hassan Iqbal, The University of Texas at Austin

Autonomous terrain shaping in granular media is difficult because it requires long-horizon prediction of terrain evolution under repeated soil-tool interactions. High-fidelity continuum and particle-based simulators offer this predictive power, but are often too expensive for planning, and direct gradient-based optimization through them can become numerically unstable. Conversely, reduced-order purely geometric models can be efficient but may miss momentum-driven transport effects and struggle with continuous, multi-stage tasks. We present a hierarchical framework for autonomous excavation and terrain shaping that avoids direct long-horizon gradient optimization by combining a reduced-order granular dynamics model with task-conditioned macro proposal generation, fast surrogate physics scoring, and receding-horizon execution via derivative-free Model Predictive Path Integral (MPPI) control. The terrain is modeled by a depth-averaged simulator based on the Shallow Water Equations (SWE) augmented with frictional rheology and tool-induced forcing. For trench-shaping tasks, macro proposals are geometry-aware excavation strokes generated from the residual excavation field and local target geometry. For fill-aware tasks, macro proposals are transport corridors generated from source-demand couplings between excavated material and a desired fill region. Simulation results across connected, branched, mixed-geometry, disconnected, and fill-aware scenarios show that the framework qualitatively recovers the global structure of the target terrain across diverse task classes.