Simulation-Based Optimization with Applications

Poster Session Abstracts

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Multiple Solutions for Variational Inequalities via Latent Variable Proximal Point and Deflation

Chenghao Dong, University of Oxford

Many problems in science, engineering, and finance involve solving variational problems subject to inequality constraints, such as simulations for contact mechanics, fracture, fluid flow with positivity constraints, and even American option pricing. Unlike standard PDE problems, VIs involve inequality constraints that introduce nonlinearity and nonsmoothness, making them significantly more difficult to solve numerically. An ideal algorithm for VIs should (i) return feasible approximations, (ii) be independent of discretisation choices, (iii) exhibit mesh-independent convergence, and (iv) compute multiple solutions. Existing methods satisfy only subsets of these properties, and none provides an efficient framework for systematically computing multiple solutions. Recent work introduced the Latent-Variable Proximal Point (LVPP) algorithm, which reformulates VIs as a sequence of nonlinear PDEs and achieves feasibility and mesh-independent convergence for single solutions. This project extends LVPP to compute multiple solutions. We propose a Voronoi–Bregman regularisation mechanism that enables multiple search directions per iteration and integrates naturally with deflation techniques for exploring distinct solution branches. The resulting framework aims to provide the first scalable approach for computing multiple high-resolution solutions of VIs in large-scale scientific applications.

Data-Driven Trajectory-Optimization-Based Model Reduction via Covariance Balancing for Optimal Control

Emmanuel Sunday Ameh, Cornell University

Robust data-driven reduced-order models (ROMs) could enable near-optimal control for very high-dimensional nonlinear dynamical systems, with applications in active flow control such as relaminarizing turbulent flows and recovering from aerodynamic stall. With initial conditions far away from the desired steady state, accounting for nonlinear effects becomes crucial — yet makes solving the resulting Hamilton-Jacobi-Bellman (HJB) equation, which defines the value function over the continuous state space, computationally intractable due to the curse of dimensionality. Reduced-order models (ROMs) can help in a variety of ways, but existing methods often fail to capture relevant dynamics for the control problem.To overcome these challenges, we first approximate the infinite-horizon optimal control problem with a large finite horizon to obtain a time-invariant version of the value function. We furthermore employ an indirect method of trajectory optimization (which is feasible in high dimensions) to obtain state and costate data offline, along locally optimal trajectories for estimating state and gradient covariance matrices. This method builds on the Pontryagin minimum principle and other related work that establishes the costate (adjoint variables) provided as generalized gradients of the optimal value function satisfying the HJB equation . An oblique projection obtained by balancing these matrices with initial conditions sampled uniformly from an uncontrolled attractor, is used to identify active directions in the state space along which the value function is most sensitive and states have large variance . The oblique projection obtained is used to build surrogate models for both the value function and the optimal feedback control law, which is validated on the full order model. ROM-based state estimators are also built with these projections for closed-loop feedback control. We assess the quality of the resulting ROMs across linear and nonlinear PDE control problems, benchmarking against existing ROM approaches.

Electromagnetic Source Cloaking with Optimization
Yaw Owusu-Agyemang, George Mason University

Maxwell's equations are an important modeling component in a variety of modern engineering applications, ranging from nanoscale optical devices to magnetic confinement fusion. Despite the significant advances in the mathematical analysis and numerical methods for the solution of Maxwell's equations, little progress has been made in our understanding of optimal control and optimal design problems governed by Maxwell's equations. In this work we study the mathematical and computational challenges associated with such optimization problems. We establish the well-posedness of the forward problem and optimization problems under minimal regularity. Next, we derive the first order necessary and sufficient optimality conditions. The discretization of electric and magnetic fields are carried out using Nedelec and Raviart-Thomas finite elements. We establish the convergence of this discretization to the continuous problems. Finally, the efficacy of the theoretical framework is illustrated via numerical simulations done in MrHyDE, an advanced electromagnetic software and ROL (the Rapid Optimization Library), both developed at Sandia National Laboratory.

Duality Framework for Flux Constrained Flow: Analysis and Numerics
Felipe Perez Silva, George Mason University

We consider Darcy's law for flow in a porous medium with bilateral flux constraints. Using Fenchel duality theory at the continuous level, we derive a posteriori error estimates for any conforming approximation at both the dual and primal (or predual) levels. At the discrete level, we establish a priori error estimates for the Raviart–Thomas approximation at the dual level and the Crouzeix–Raviart approximation for the primal (or predual) formulation, which yield quasi-optimal error decay rates. The discrete dual problem is solved using a semismooth Newton algorithm, while the solution to the discrete primal formulation is derived from the discrete dual solution via an inverse generalized Marini formula.

A proximal Galerkin method for the isometry constraint
Frederic Marazzato, University of Nevada, Las Vegas

Following the work of Friesecke, James, and M\"uller, certain nonlinear plate models have been formulated as energy minimization problems subject to an isometry constraint, whereby the first fundamental form of the mid-surface equals the identity tensor. Several numerical methods have been proposed to approximate minimizers of such constrained problems using gradient flows with tangent-space updates. However, this class of methods presents two main challenges. First, a preprocessing step is required to enforce the boundary conditions and generate an initial guess sufficiently close to an isometry. Second, each step of the gradient flow typically increases the isometry defect. We propose an alternative approach based on the proximal Galerkin framework, originally introduced for problems with convex inequality constraints. The method preserves and exploits the geometric structure of the feasible set to obtain a significantly more efficient algorithm in which each iteration produces an exact isometry at the barycenter of every mesh cell. In contrast to existing approaches, no preprocessing step is required, enabling broader applicability of these important computational models. Numerical experiments on several standard benchmarks demonstrate that the method converges to a prescribed error tolerance in an asymptotically mesh-independent number of iterations and requires fewer iterations than previous methods, even on coarse meshes.

Numerical Optimization of Experiments with Multiple Outputs

Jeffrey Larson, Argonne National Laboratory

Many scientific optimization problems involve expensive simulations that produce multiple outputs, while the ultimate quantity of interest is a function of those outputs. We present optimization methods that exploit this structure by directly modeling the vector-valued simulation outputs and composing them with the desired objective function. This approach enables efficient optimization with significantly fewer expensive simulations and has been successfully applied to problems in nuclear physics, plasma turbulence, accelerator design, and quantum metrology.

Multidimensional Structure-Preserving High-Order FDTD Methods for Maxwell's Equations in Kerr-Debye-Lorentz Media

Emmanuel Oguadimma, Oregon State University

We present a structure-preserving finite difference time domain (FDTD) method for the three-dimensional Maxwell-Kerr-Debye-Lorentz system. Built on the classical Yee staggered-grid discretization of Maxwell's equations and auxiliary differential equations for the Debye and Lorentz material responses, the method is designed to preserve key structural properties of the continuous model. In particular, a modified exponential update for the Kerr susceptibility handles the stiffness in the nonlinear material response, preserves nonnegativity, and is asymptotic-preserving in the Kerr relaxation limit, recovering the instantaneous Kerr-Lorentz model. We prove a discrete energy identity under a CFL-type stability condition and exact preservation of a discrete divergence constraint in the source-free case. The resulting nonlinear electric-field update is implemented efficiently through Newton-GMRES with matrix-free Jacobian-vector products, making the method practical for large-scale multidimensional simulations. Numerical experiments confirm second-order accuracy, verify the divergence-preserving property, and show that the scheme captures nonlinear optical phenomena including soliton propagation and harmonic generation. Overall, the proposed method provides a robust and efficient multidimensional FDTD scheme for nonlinear dispersive Maxwell models, with potential applications in computational photonics including simulation-based optimization.

Finite element approximation of a Stokes-Kirchoff plate fluid-structure interaction system

Lander Besabe, Clemson University

We study a finite element framework for a coupled fluid-structure interaction (FSI) system involving a three-dimensional (3D) Stokes flow and a two-dimensional (2D) fourth-order Kirchhoff plate. The interaction between the parabolic and hyperbolic partial differential equations occurs at the boundary interface, where coupling conditions enforce the matching of fluid and plate velocities and the Dirichlet trace of the fluid pressure. The main contribution is a domain decomposition (DD) framework for the FSI system in which the plate equation is reformulated as two coupled second-order PDEs. This avoids the use of -conforming elements and provides flexibility in the choice of discrete approximation spaces. We analyze well-posedness and temporal stability and present numerical results demonstrating the effectiveness of the proposed method.

Polarization-Induced Beam Bending: Mathematical Model, Discretization, and Algorithm

Sarswati Shah, George Mason University

We study a reduced hydrodynamic formulation of paraxial beam propagation in which the beam intensity, optical phase, and polarization phase are coupled through a nonlinear dispersive system. While prior analytical work has derived explicit beam-bending laws under short-distance asymptotic assumptions, a fully resolved numerical treatment of the resulting model over long propagation distances has not previously been available.

In this work, we first provide a generic form of theoretical bending behavior at short-distance. Next, the exact balance for energy is presented. Subsequently, we present a conservative numerical scheme for the coupled system, combining a finite-volume discretization of the intensity equation with monotone Hamilton--Jacobi (H-J) solvers for the phase dynamics and upwind transport of polarization. The method preserves the nonnegativity of the intensity and remains stable under long-distance propagation. We also present the merits of the scheme through a test case. We perform large-scale simulations over propagation distances of tens of meters, while resolving millimeter-scale transverse structure. The numerical results reproduce the analytically predicted and experimentally observed quadratic beam bending at short distances and reveal systematic deviations beyond the asymptotic regime. These deviations arise from nonlinear phase accumulation and dispersive effects captured by the full model but neglected in short-distance theory. To the best of our knowledge, this work provides the first fully resolved numerical study of the coupled hydrodynamic beam model over propagation distances that far exceed the range of validity of existing analytical approximations.