Numerical Optimization Activities

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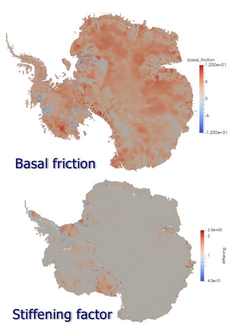
Numerical optimization is used in many applications to select parameters that minimize or maximize quantities of interest. Our focus is to develop methods for solving large-scale optimization problems that may include PDE constraints, sparse regularization, and discrete variables.

PDE-constrained Optimization

Goal: solve optimization problems with partial differential equation constraints that include nontrivial state and design constraints

$$\begin{aligned} \min_{u,w} \quad & f(u,v) \\ \text{subject to} \quad & g(u,v) = 0 \\ & c(u,v) \geq 0 \end{aligned}$$

- Applications include
  - Inverse problems
  - Sparse regression
  - Design optimization
- Support several packages
  - Toolkit for Advanced Optimization
  - Rapid Optimization Library
- Enable dynamic optimization
  - Use adjoints to compute derivatives
  - Utilize second-order adjoints



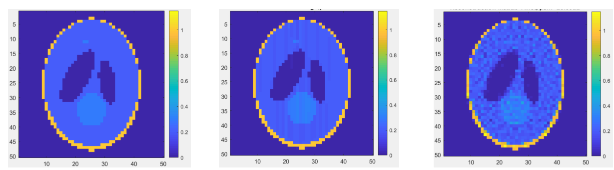
Inverted for 2.6M parameters

Sparse Regression

Goal: develop methods for composite optimization with a smooth term and a non-smooth sparse regularizer term

$$\min_{\mathbf{l} \leq \mathbf{x} \leq \mathbf{u}} \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \tau\|\mathbf{D}\mathbf{x}\|_1,$$

- Bound-constrained Regularized Gauss-Newton (BRGN) method available in PETSc/TAO 3.11 release
- Smooth approximation to the sparse regularizer
- Superior performance compared to widely-used TwIST solver
- Example: Tomography reconstruction



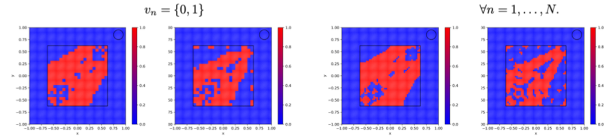
(a) Ground truth for comparison (b) Our solver, PSNR = 46.01 dB (c) TWIST solver, PSNR = 29.30 dB

Discrete Variables

Goal: produce numerical methods for solving mixed-integer PDE-constrained optimization (MIPDECO) problems

- Developed trust-region method to refine relaxed, rounded solutions obtained from TAO bound-constrained solvers
- Example: Design of electromagnetic scatterer (cloak) with robust model that considers multiple angles

$$\begin{aligned} P(\theta) = \underset{v}{\text{minimize}} \quad & J(u) = \frac{1}{2}\|u - u_0(\theta)\|^2_{2,D_0} & \\ \text{subject to} \quad & -\Delta u_{\text{Re}} - k_0^2(1+qw)u_{\text{Re}} = k_0^2 qw \cos(k_o(\cos(\theta)x + \sin(\theta)y)) & \text{in } D \\ & -\Delta u_{\text{Im}} - k_0^2(1+qw)u_{\text{Im}} = k_0^2 qw \sin(k_o(\cos(\theta)x + \sin(\theta)y)) & \text{in } D \\ & \frac{\partial u_{\text{Re}}}{\partial n} = -k_o u_{\text{Im}} \quad \text{and} \quad \frac{\partial u_{\text{Im}}}{\partial n} = k_o u_{\text{Re}} & \text{on } \partial D \\ & w = v_n & \text{in } \hat{\Omega}_n \ \forall n = 1, \dots, N \\ & w = 0 & \text{in } D \setminus \left(\cup_n \hat{\Omega}_n\right) \\ & v_n = \{0,1\} & \forall n = 1, \dots, N. \end{aligned}$$

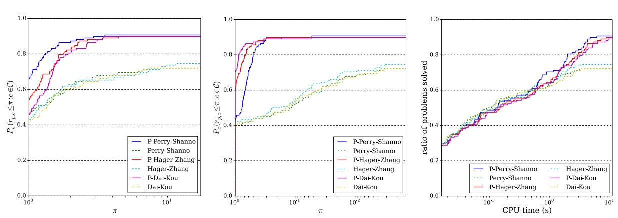


(a) Nominal and robust design for 20x20 control mesh (b) Nominal and robust design for 40x40 control mesh

Large-Scale Optimization

Goal: improve the conjugate gradient method for problems with expensive function/gradient evaluations

- Diagonalized quasi-Newton preconditioner for nonlinear conjugate gradient (NCG) methods
- Reduced reliance on specialized line searches
- Preconditioned NCG is competitive with limited-memory quasi-Newton methods at a smaller memory footprint
- Tested on 119 CUTEst problems with up to 100,000 free variables



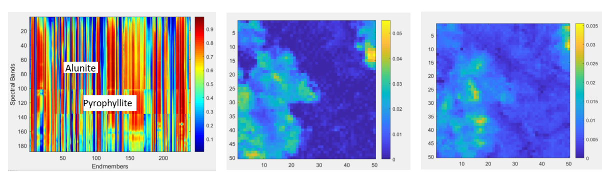
(a) Function/gradient evaluation comparison (b) Line search step length comparison (c) CPU time comparison

Joint-Sparsity Regularization

Goal: provide scalable support for joint-sparsity in sparse regression

$$\min_{\mathbf{L} \leq \mathbf{X} \leq \mathbf{U}} \frac{1}{2}\|\mathbf{A}\mathbf{X} - \mathbf{B}\|^2_F + \tau\|\mathbf{D}\mathbf{X}\|_{2,1},$$

- Extends BRGN for joint-sparsity applications with X defined as a matrix
- Example: Hyperspectral un-mixing



(a) Matrix A: 188 hyperspectral bands of 240 "minerals" (b) Alunite component (c) Pyrophyllite component

Applications

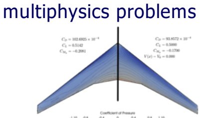
Goal: support numerical optimization needs of SciDAC applications

- **NP:** Nuclear Computational Low Energy Initiative – PI Carlson (LANL)
- **HEP:** Community Project for Accelerator Science and Simulation – PI Amundson (FNL)
- **HEP:** Accelerating HEP Science: Inference and Machine Learning at Extreme Scales – PI Habib (ANL)
- **HEP:** Data Analytics on HPC – PI Kowalkowski (FNL)
- **BER:** Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models – PI Price (LANL)

Future Plans

Goal: continue to develop numerical methods to meet application needs; expand to dynamic optimization and multiphysics problems

- Enhance optimization support for users
  - FEniCS, Firedrake, AMReX
- Support multiphysics problems
- Support data analytics and UQ needs



Multiphysics example

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