Numerical Optimization Activities

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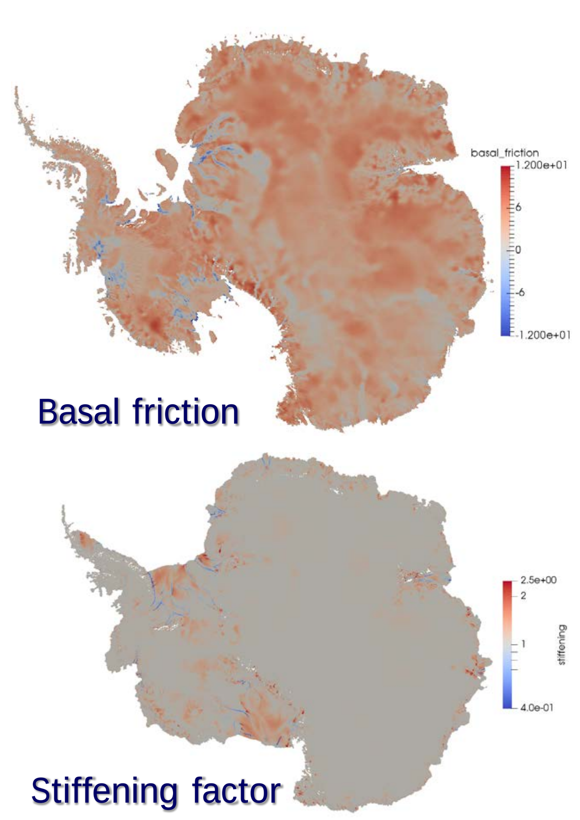
Numerical optimization is used in many applications to select parameters that minimize or maximize quantities of interest. Our focus is to develop methods for solving PDE-constrained optimization problems that may include state constraints, discrete variables, and multiple objectives, and for sensitivity analysis using surrogate models.

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
  - Parameter estimation
  - Design optimization
- Support several packages
  - Toolkit for Advanced Optimization
  - Rapid Optimization Library
- Enable dynamic optimization
  - Use adjoints to compute derivatives
  - Utilize second-order adjoints



Basal friction

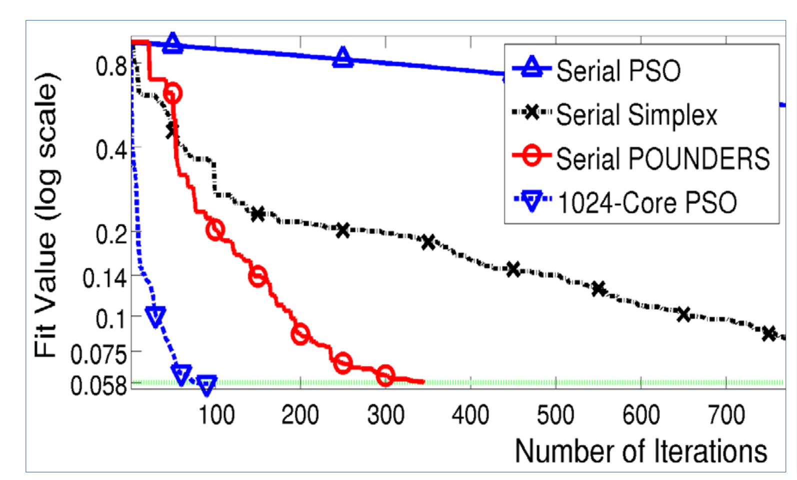
Stiffening factor

Inverted for 2.6M parameters

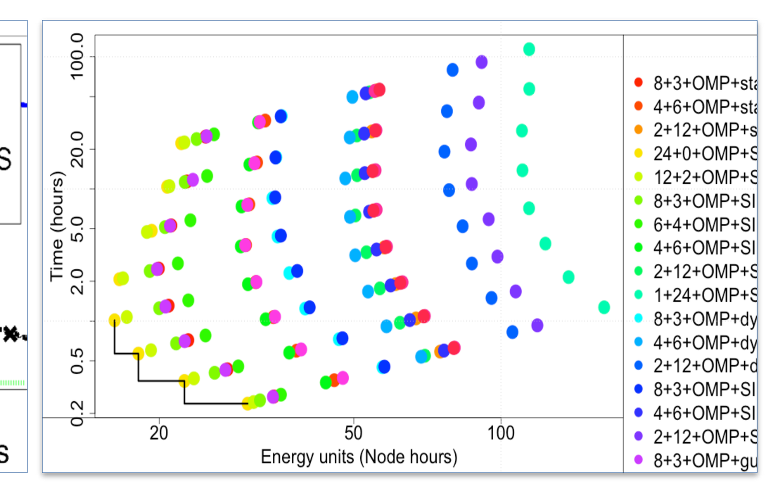
Multi-objective Optimization

Goal: develop methods for studying the tradeoffs between multiple competing metrics of interest when calculating an optimal design

- Exploit mathematical structure present in many optimization problems to reduce expense and improve solution quality
- Move beyond space-filling designs for multi-objective tradeoff studies and focus evaluations on regions satisfying approximate Pareto optimality
- Support concurrent simulation execution when possible



Exploiting structure in particle accelerator calibration

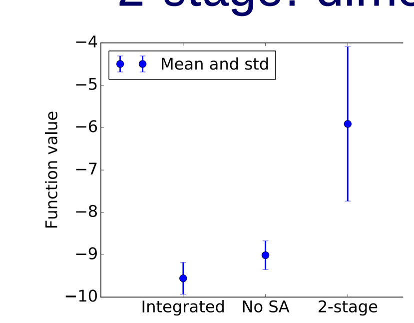


SciDAC3 SUPER + MPAS multi-objective optimization

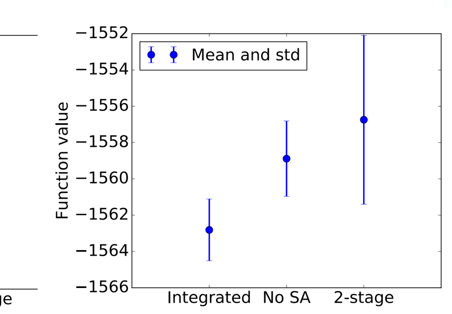
Sensitivity Analysis

Goal: devise an optimization algorithm that integrates sensitivity analysis to efficiently explore the parameter space

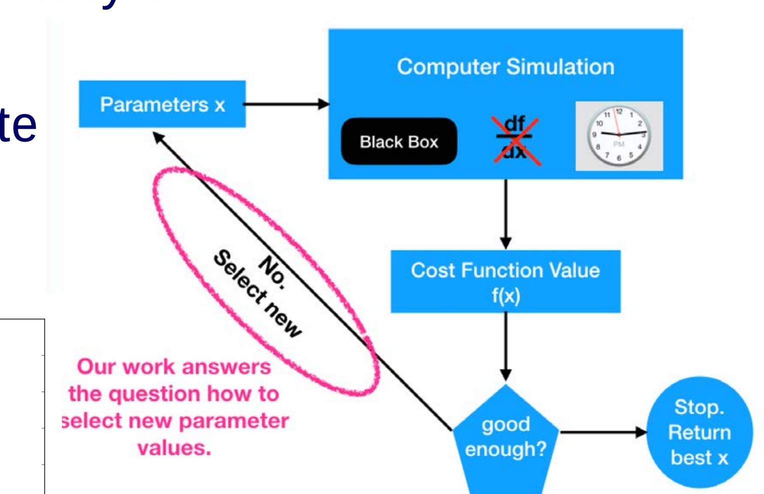
- Construct a computationally inexpensive radial basis function approximation to the functions
- Use the Morris elementary effects method to rank the parameters from most to least sensitive
- Produce a stepwise radial basis function surrogate using the rankings that is used for further analysis
- Example comparison:
  - Integrated: stepwise surrogate
  - No SA: standard surrogate
  - 2-stage: dimension reduction



9 variable problem



20 variable problem



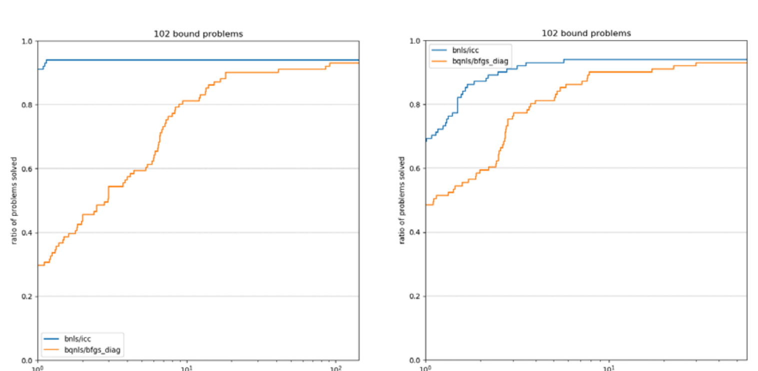
Surrogate-based optimization algorithm

Numerical Optimization Methods

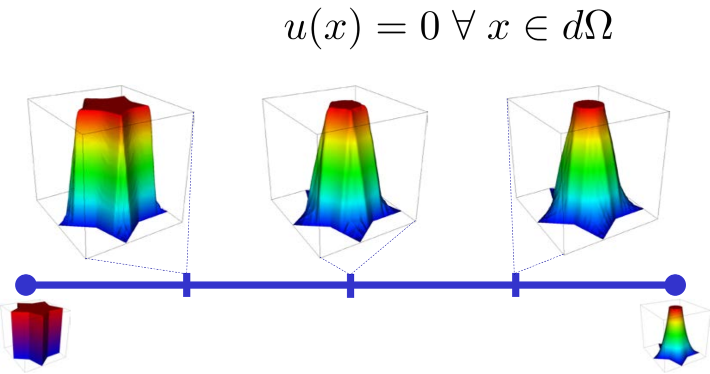
Goal: develop numerical methods for solving optimization problems with general nonlinear constraints

- Improved bound-constrained methods in the Toolkit for Advanced Optimization (TAO)
  - Nonlinear conjugate gradient methods with scaling
  - Quasi-Newton (QN) methods with scaling
  - Newton-Krylov (NK) methods
- Parametric study of methods
- Example: obstacle problem

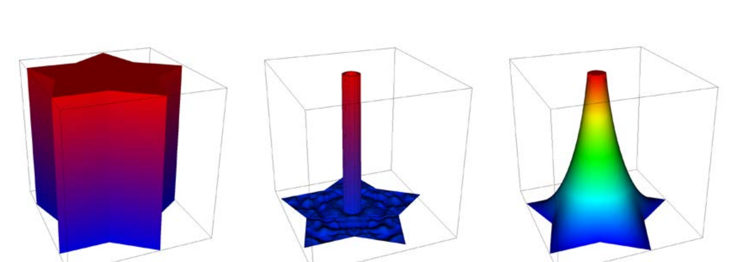
$$\begin{aligned} \underset{u}{\text{minimize}} \quad & \int_\Omega |\nabla u|^2 dx \\ \text{subject to} \quad & u(x) \geq \phi(x) \; \forall\, x \in \Omega \\ & u(x) = 0 \; \forall\, x \in d\Omega \end{aligned}$$



Comparison of NK and QN methods



Obstacle: QN converges in 292 iterations



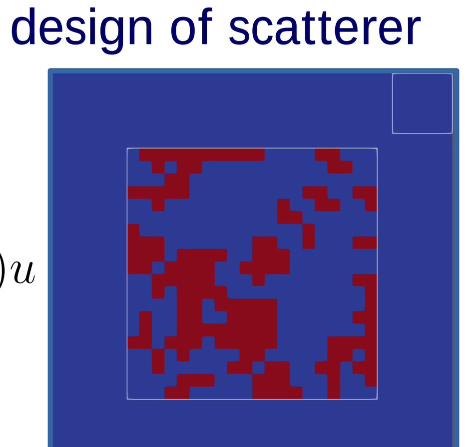
Obstacle: NK converges in 3 iterations

Discrete Variables

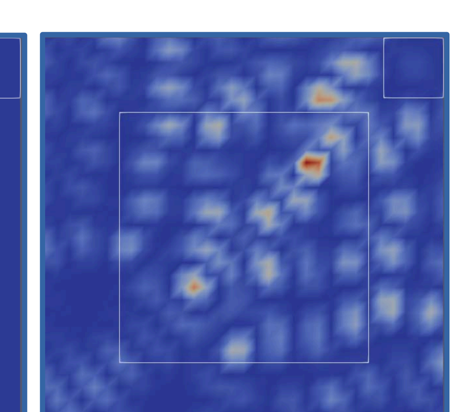
Goal: produce numerical methods for solving mixed-integer PDE-constrained optimization (MIPDECO) problems and apply them to optimal design problems

- Developed new set-based, steepest-descent, trust-region method with promising numerical results and theoretical foundations (stationary limits)
- Example: Design of electromagnetic scatterer (cloak)
  - Objective: Cloak the top-right region
  - PDE: 2D Helmholtz equation
  - Discrete variables: 0-1 design of scatterer

$$\begin{aligned} \min_{u,w} \quad & \|u + u_0\|^2_{2,\Omega_0} \\ \text{subject to} \quad & -\Delta u - k_0^2(1 + qw)u \\ & = k_0^2 q w u_0 \\ & w \in \{0,1\}^n \end{aligned}$$



Scatterer



Difference of waves

Applications

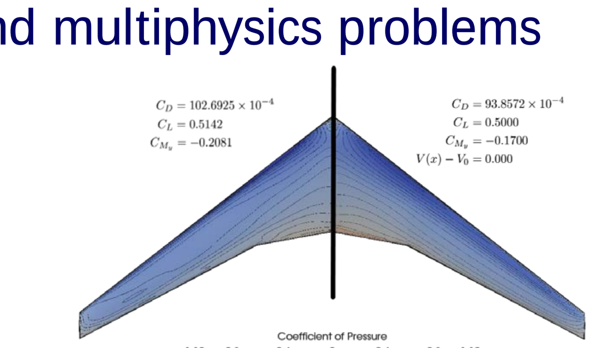
Goal: support numerical optimization needs of SciDAC applications

- **BER:** Probabilistic Sea-Level Projections from Ice Sheet and Earth System – PIs Ng (LBNL) and Price (LANL)
- **HEP:** Community Project for Accelerator Science and Simulation – PI Amundson (FNL)
- **HEP:** Data Analytics on HPC – PI Kowalkowski (FNL)
- **NP:** Nuclear Computational Low Energy Initiative – PI Carlson (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, MFEM
- Support multiphysics problems
  - Albany/Trilinos, PETSc/TAO
- Support data analytics and UQ needs



Multiphysics example

For more information: http://www.fastmath-scidac.org or contact: Todd Munson, ANL, tmunson@mcs.anl.gov, 630-252-4279

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