TAO Nonlinear Conjugate Gradient and Quasi-Newton Methods: Accelerating Convergence for Large-Scale Optimization

Scientific Achievement

Improved performance of the Nonlinear Conjugate Gradient (NCG) and Quasi-Newton (QN) methods in the Toolkit for Advanced Optimization (TAO)

Significance and Impact

NCG and QN methods are key kernels used when solving large-scale PDE-constrained optimization problems; our unified NCG preconditioning and QN initialization framework allows us to both solve more problems **and** reduce the time to solution

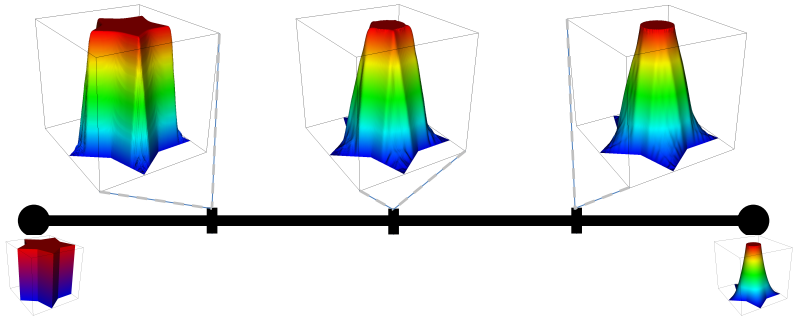
Research Details

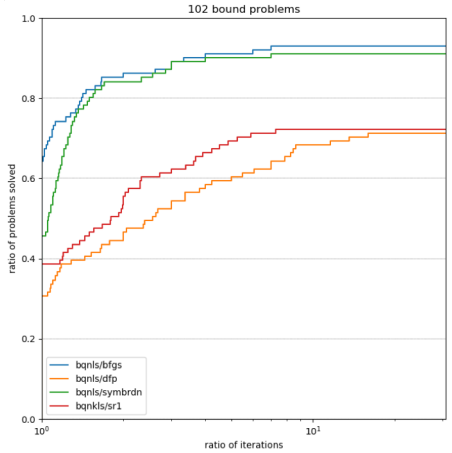
- Implemented range of NCG and Broyden-based self-scaling memoryless methods
- Developed diagonal Hessian approximations based on Broyden method for NCG preconditioning and QN initialization
- Performed computational study of wide range of NCG and QN methods on the standard CUTEst test problems
- Produced hands-on tutorial showcasing TAO/MFEM interoperability

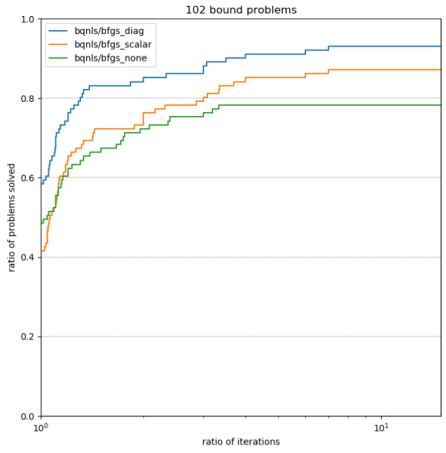
$$\min_u \quad \frac{1}{2}\int_\Omega \|\nabla u(x)\|^2 \, dx$$

$$s.t. \quad u(x) \geq \varphi(x)$$

Classical Obstacle Problem







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Work was performed at ANL.

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