

Institute for Mathematics and its Applications
Workshop on Optimization in Simulation-Based Models
January 16, 2001

TAO: An Optimization Toolkit for Large-Scale
Applications

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Large-Scale Applications

- ◇ Containing features that may significantly enhance or restrict the performance of a solver.
 - ◇ Linear Solvers
 - ◇ Matrix structures
 - ◇ Preconditioners
- ◇ Could benefit from a parallel solver.
- ◇ Implemented using multiple software packages.

TAO Design Goals

- ◇ Offer algorithmic and computational flexibility.
 - ◇ Variety of data structures.
 - ◇ Multiple solvers.
- ◇ Provide parallel implementation of solvers, portable to serial and high-performance architectures.
- ◇ Leverage external toolkits.
 - ◇ Vector and Matrix classes.
 - ◇ Preconditioners.

Minimal Surface with Obstacles

Determine the surface of minimal area and given boundary data that lies above an obstacle.

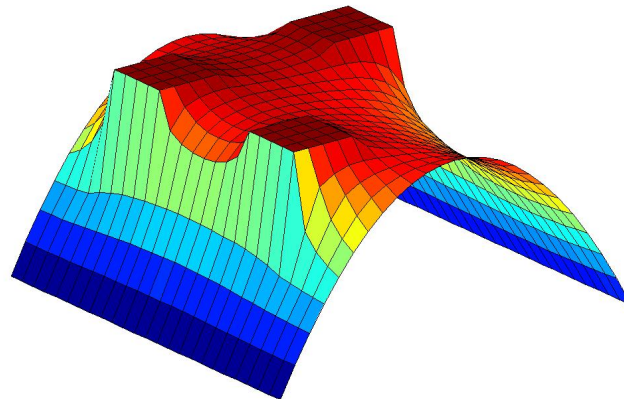
$$\min \{f(v) : v \in K\}$$

$$f(v) = \int_{\mathcal{D}} \sqrt{1 + \|\nabla v(x)\|^2} dx$$

$$K = \{v \in H^1 : v(x) = v_D(x), x \in \partial D, v(x) \geq v_L(x), x \in \mathcal{D}\}$$

Minimal Surface with Obstacles

Bound constrained problem. Number of active constraints depends on the height of the obstacle. Almost all multipliers are zero.



Computing a Solution

Tasks needed to compute a solution to this application include:

- ◇ Objective function and derivative information.
 - ◇ Mesh
 - ◇ Parallel Data Structures
- ◇ Optimization Solver.
 - ◇ Lower and upper bounds on variables.
 - ◇ Parallel implementation

The software packages needed to perform these tasks may differ.

Evaluate Objective using PETSc

PETSc offers:

- ◇ Parallel Vectors, with gathers and scatters.
- ◇ Parallel Matrices, with efficient assembly and several sparse storage formats
- ◇ Structured Mesh Object that manages parallel communications.

Plus:

- ◇ Krylov methods: GMRES, CG, ...
- ◇ Scalable Parallel Preconditioners – ILU, block Jacobi, overlapping additive Schartz methods.

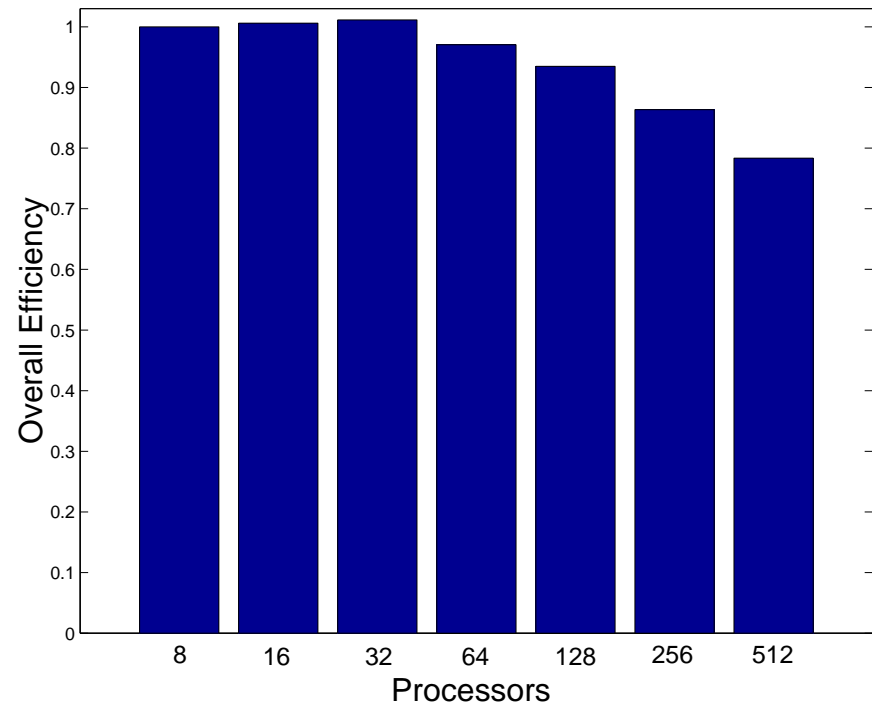
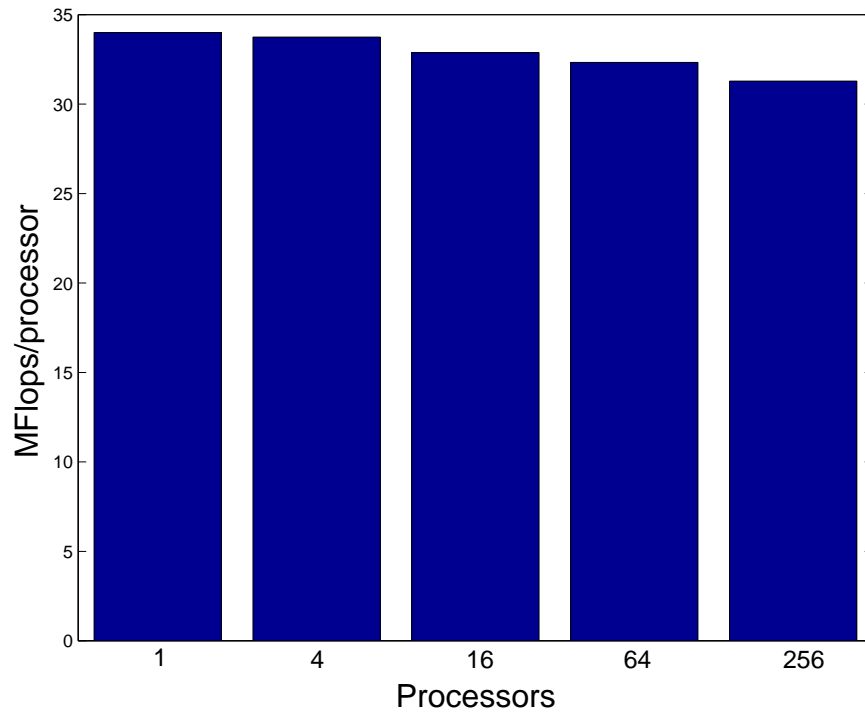
Optimization Using TAO

- ◇ Bound Constrained Solvers
 - ◇ Limited memory variable metric method.
 - ◇ Newton methods
- ◇ Well documented interface with PETSc.
- ◇ Mesh sequencing tools.

TAO Performance: Obstacle Problem

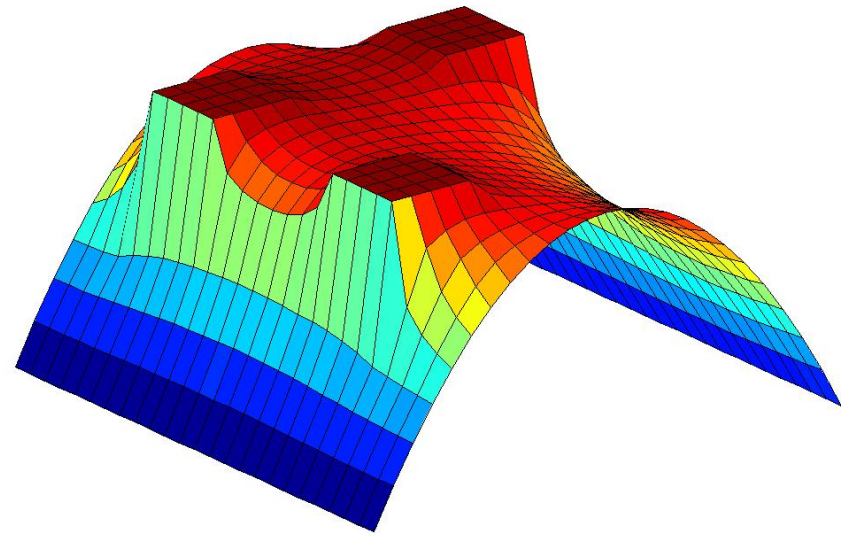
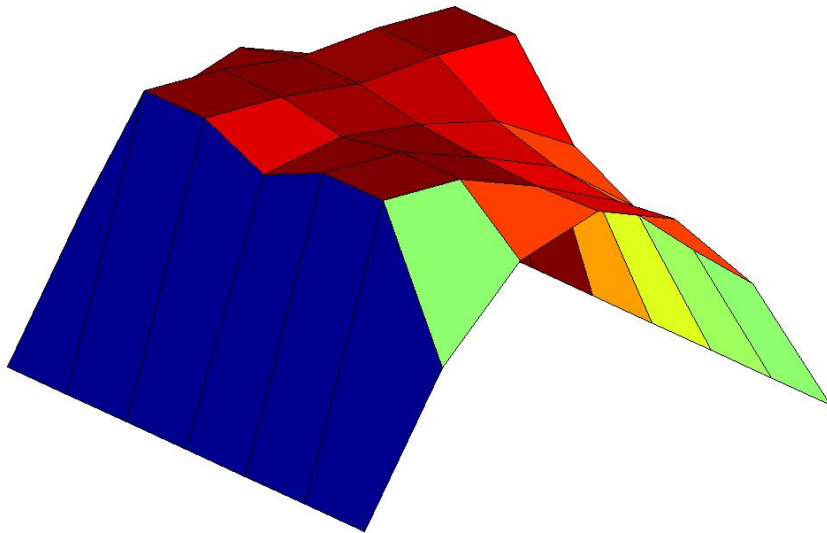
Cray T3E (NERSC)

$n = 2.56 \cdot 10^6$ variables



Mesh Sequencing

Use solutions on course mesh as initial guess on the fine mesh.



TAO Performance on 385 x 385 Mesh

Newton method, conjugate gradient linear solver with incomplete LU preconditioner:

	Iterations	Seconds
With Mesh Sequencing	4	21
Without Mesh Sequencing	18	120

Limited memory variable metric method:

	Iterations	Seconds
With Mesh Sequencing	197	31
Without Mesh Sequencing	2980	429

The Ginzburg-Landau Model for Superconductivity

Minimize the Gibbs free energy for a homogeneous superconductor with a vector potential perpendicular to the superconductor.

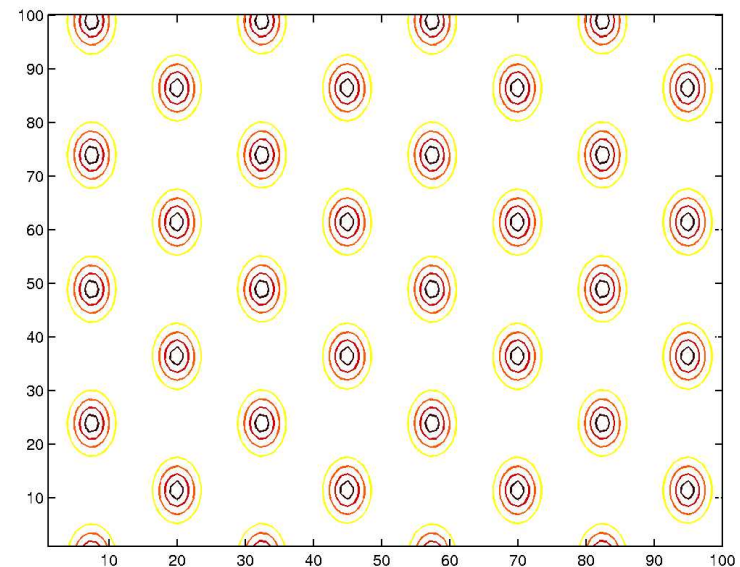
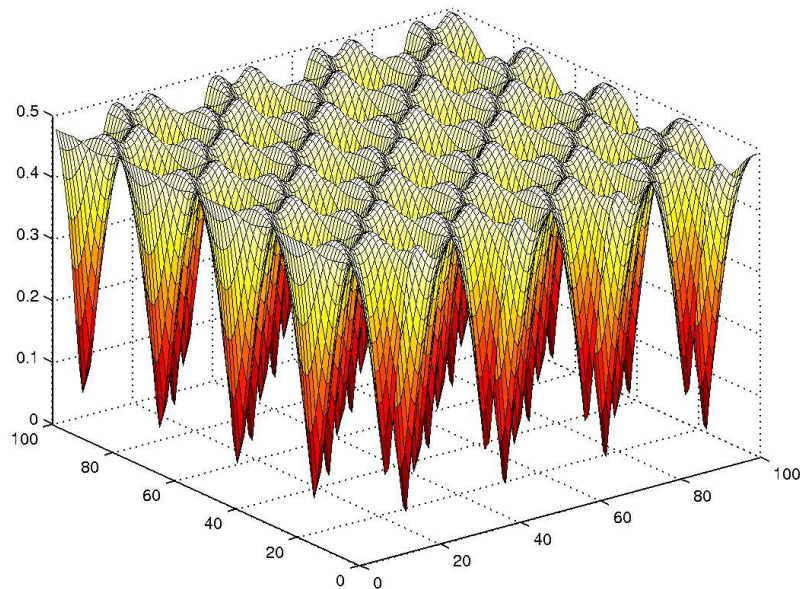
$$\int_{\mathcal{D}} \left\{ -|v(x)|^2 + \frac{1}{2}|v(x)|^4 + \|[\nabla - iA(x)]v(x)\|^2 + \kappa^2 \|(\nabla \times A)(x)\|^2 \right\} dx$$

$v : \mathbb{R}^2 \rightarrow \mathbb{C}$ is the order parameter

$A : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is the vector potential

The Ginzburg-Landau Model for Superconductivity

Unconstrained problem. Non-convex function. Hessian is singular.
Unique minimizer, but there is a saddle point.



Lennard-Jones Clusters

Given the positions p_1, p_2, \dots, p_n of n molecules (points) in \mathbb{R}^d , the energy potential function is defined as

$$V_d(p) = \sum_{j=2}^n \sum_{i=1}^{j-1} v(\|p_j - p_i\|_2),$$

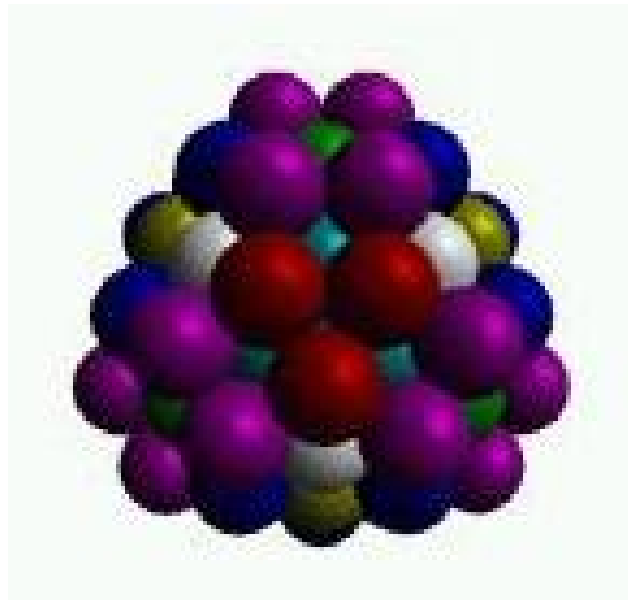
where $v : \mathbb{R} \rightarrow \mathbb{R}$ is the potential function between pairs of atoms.

We consider the Lennard-Jones potential function defined by

$$v(r) = r^{-12} - 2r^{-6}.$$

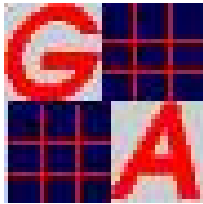
Lennard-Jones Clusters

The determination of the minimum energy configuration of a cluster of atoms or molecules is known as the molecular conformation problem. This is a central problem in the study of cluster statics.



Use of of Global Arrays

- ◇ Supports n -dimensional arrays using shared memory and distributed memory paradigms.
- ◇ Efficient support for dense matrices and direct parallel solver.
- ◇ Used in applications of chemistry and molecular dynamics.



TAO Provides

- ◇ Unconstrained Optimization Solvers
 - ◇ Limited memory variable metric method.
 - ◇ Newton methods
- ◇ Cubic line searches.
- ◇ Interface with Global Arrays.

Toolkit for Advanced Optimization

Goals include:

- ◇ Portability and an interface independent of architecture
- ◇ Performance and scalable parallelism



TAO Features

- ◇ Unconstrained and Bound Constrained solvers
- ◇ Extensible design allows for algorithmic and computational flexibility.
- ◇ Use with external toolkits.

TAO

www.mcs.anl.gov/tao

Version 1.4 (June 2002)

- ◇ Source Code
- ◇ Documentation
- ◇ Installation instructions
- ◇ Example problems
- ◇ Performance results
- ◇ Supported architectures