TOPS: ISIC Review
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TOPS – Selected Optimization Developments

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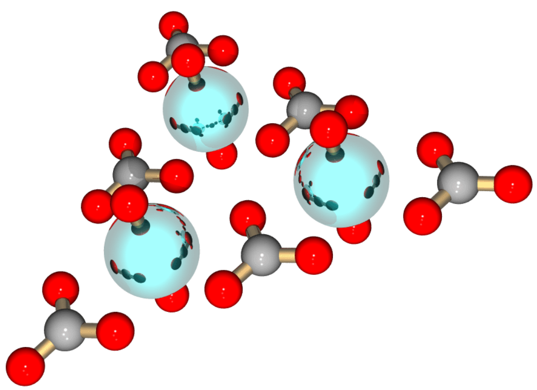
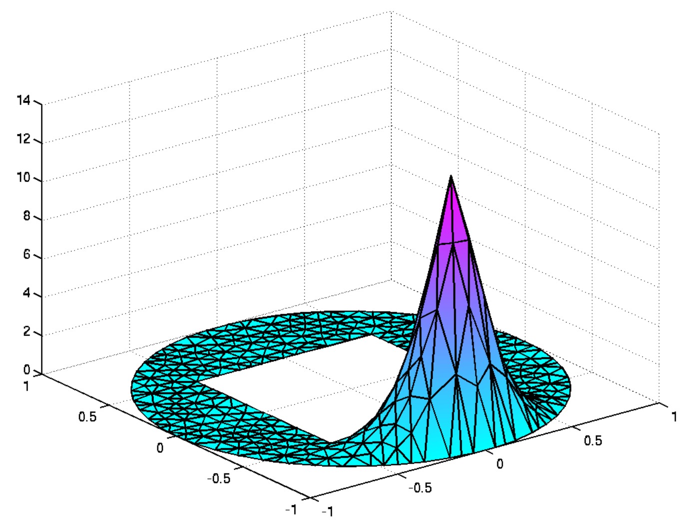
Background: Nonlinearly Constrained Optimization

$$\min\{f(x) : x_l \le x \le x_u,\ c_l \le c(x) \le c_u\}$$

- The constraints are defined by $c : \mathbb{R}^n \mapsto \mathbb{R}^m$
- The bounds on the variables $x \in \mathbb{R}^n$ are $x_l \le x \le x_u$





Note. Image of $(UO_2)_3(CO_3)_6$ courtesy of Wibe deJong (PNNL)

Outline

- ◇ TAO - Recent Developments
- ◇ GA and TaoSolve Components
- ◇ Performance for Grid Sequencing – Stalking optimality
- ◇ Future Developments
  - Optimization of simulations with minimal quadratic models
  - Constrained optimization with augmented Lagrangians
  - Transition states

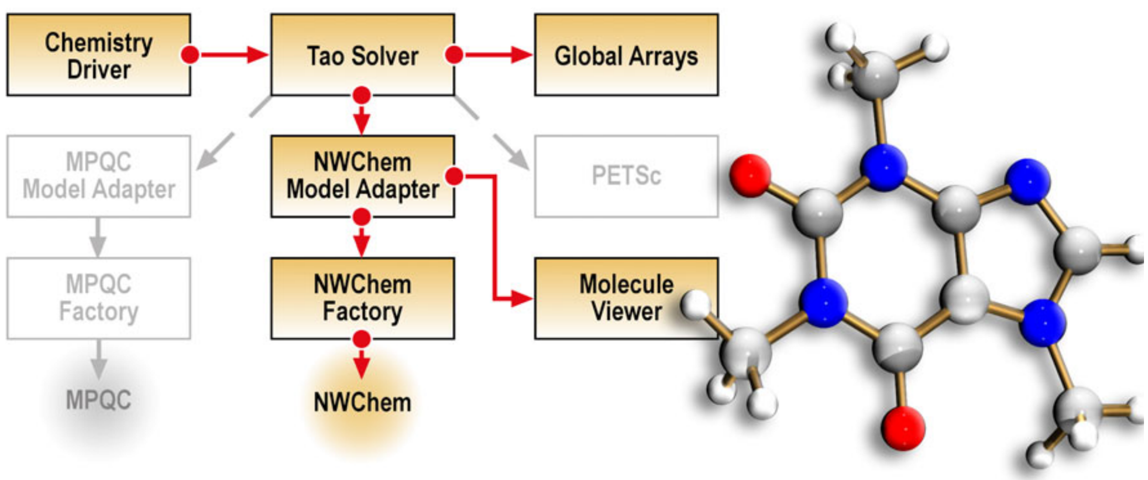
TAO: Recent Developments

- Version 1.5 (January 2003)
- TAO integration: MPQC (Sandia) and NWChem (PNNL)
- GA and TaoSolver Components
- Grid sequencing via Distributed Arrays (PETSc)
- Gradients of grid functions via ADIC
- Development of BLMVM
- Source code, documentation, tutorials, example problems, . . .

Powered by PETSc and ADIC!

GA and TaoSolver Components

- NWChem (PNNL) and MPQC (SNL) electronic structure components for energy, gradient, and Hessian computations
- TAO (ANL) optimization components
- GA (PNNL) and PETSc (ANL) linear algebra components



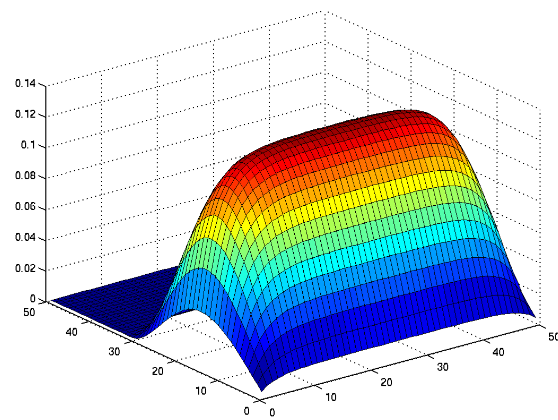
TAO Benchmark: Pressure in a Journal Bearing

$$\min \left\{ \int_{\mathcal{D}} \left\{ \tfrac{1}{2} w_q(x) \|\nabla v(x)\|^2 - w_l(x) v(x) \right\} \, dx : v \geq 0 \right\}$$

$$w_q(\xi_1, \xi_2) = (1 + \epsilon \cos \xi_1)^3$$

$$w_l(\xi_1, \xi_2) = \epsilon \sin \xi_1$$

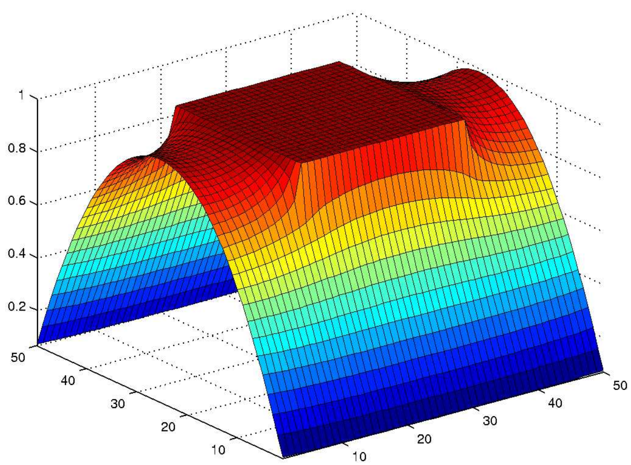
$$\mathcal{D} = (0, 2\pi) \times (0, 2b)$$

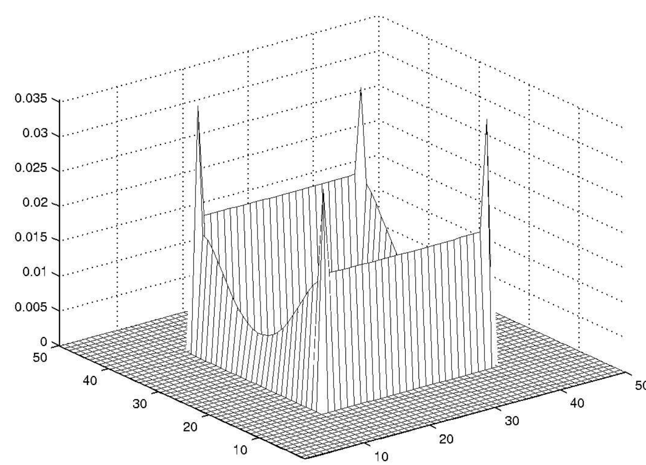


Number of active constraints depends on the choice of ϵ in $(0, 1)$.
Nearly degenerate problem. Solution $v \notin C^2$.

TAO Benchmark: Minimal Surface with Obstacles

$$\min \left\{ \int_{\mathcal{D}} \sqrt{1 + \|\nabla v(x)\|^2} \, dx : v \geq v_L \right\}$$





Number of active constraints depends on the height of the obstacle. The solution $v \notin C^1$. Almost all multipliers are zero.

Mesh-Sequencing Performance: Journal Bearing Problem

	Number of processors					
	16		32		64	
Grid	$\boxplus$	$\square$	$\boxplus$	$\square$	$\boxplus$	$\square$
769×769	17	283	10	142	7	86
1537×1537	73	3751	40	1861	22	938

Improvements

Grid	16	32	64
769×769	16	14	12
1537×1537	51	46	42

Mesh-Sequencing Performance: Obstacle Problem

	Number of processors					
	16		32		64	
Grid	$\boxplus$	$\square$	$\boxplus$	$\square$	$\boxplus$	$\square$
769×769	69	†	37	†	24	†
1537×1537	444	†	235	†	121	†

† No convergence after 500 iterations!

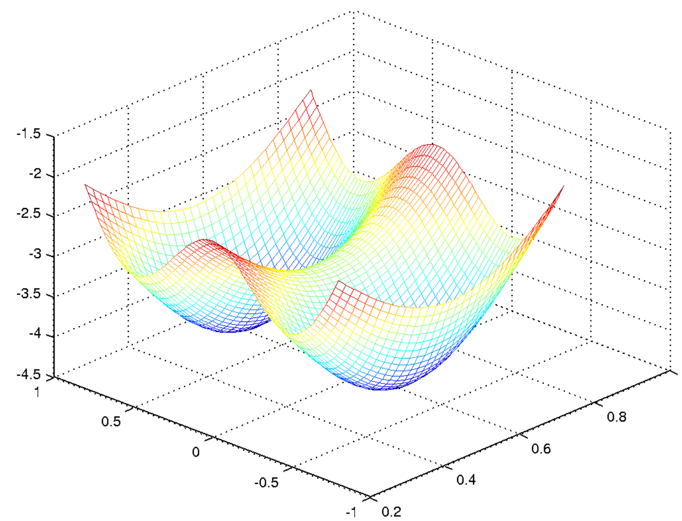
Transition States

Given a continuously differentiable function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and two points x_a and x_b, determine a critical point x^* on a minimal energy path between x_a and x_b.

- ◇ A fundamental problem in biology, chemistry, and mathematics

$$\gamma = \inf_{p \in \Gamma} \{ \max \{ f[p(t)] : t \in [0,1] \} \}$$

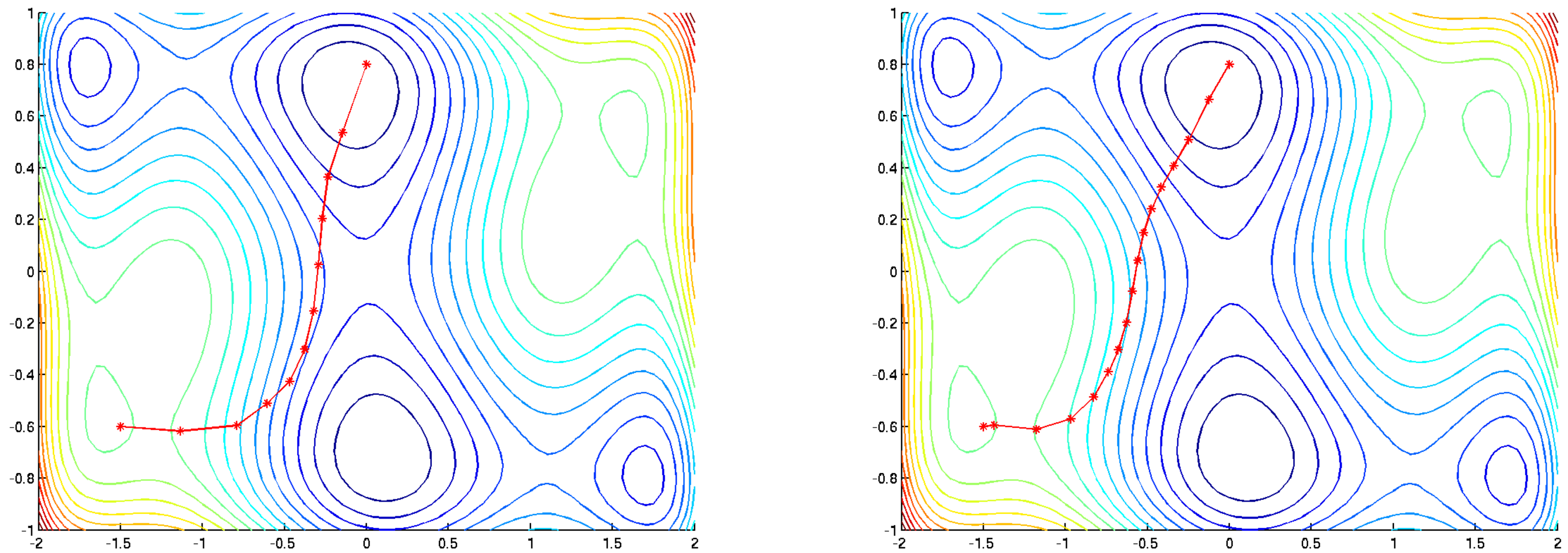
$$\Gamma = \{ p \in C[0,1] : p(0) = x_a,\ p(1) = x_b \}$$



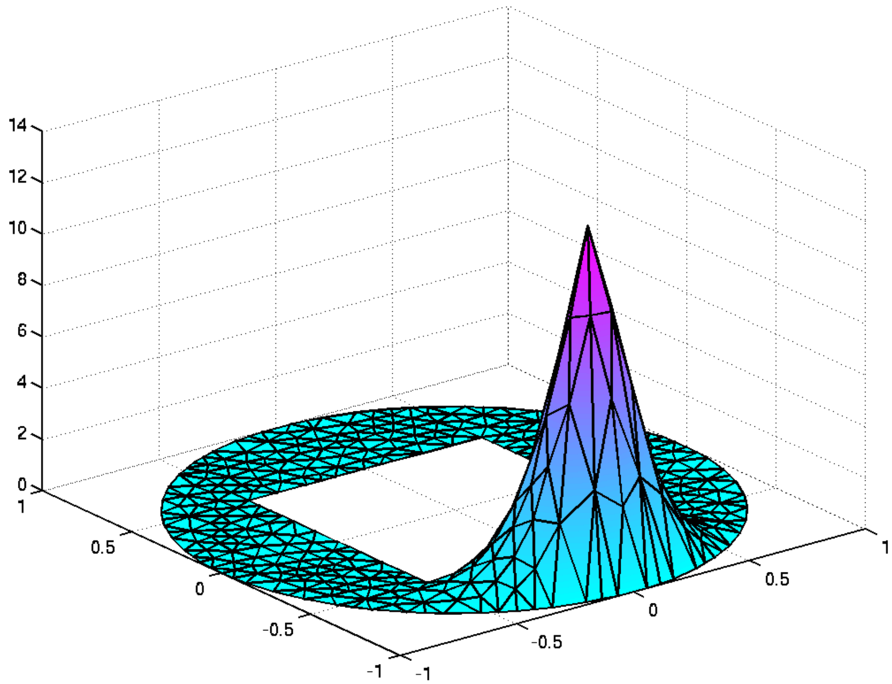
The Elastic String Algorithm

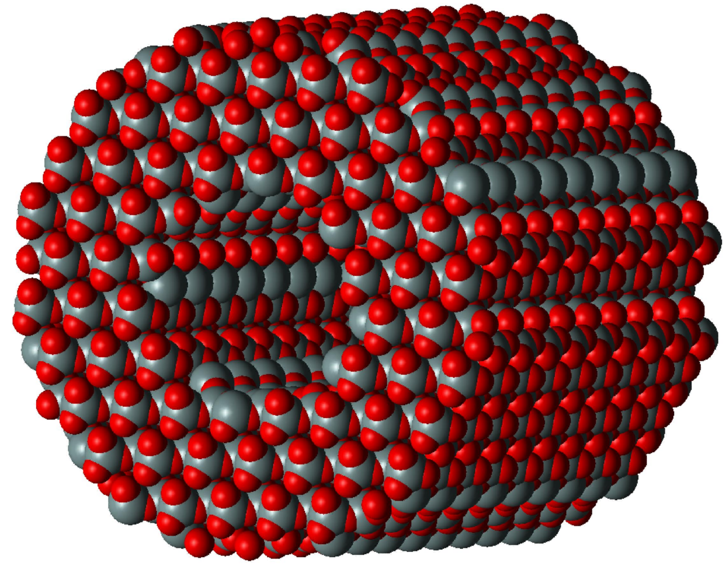
Compute breakpoints $x_k \in \mathbb{R}^n$ for a piecewise linear path such that

$$\min \left\{ \max \left\{ f(x_1), \ldots, f(x_m) \right\} : \| x_{k+1} - x_k \| \leq h_k, \ 0 \leq k \leq m \right\}.$$



Transitions States





Henon ground-state (left) and structure of SiO_2 pore (right)

Note. SiO_2 image courtesy of L. Curtiss and P. Zapol (ANL)