Workshop on the ACTS Toolkit
August 5–8, 2003
National Energy Research Scientific Computing Center

TAO – Toolkit for Advanced Optimization

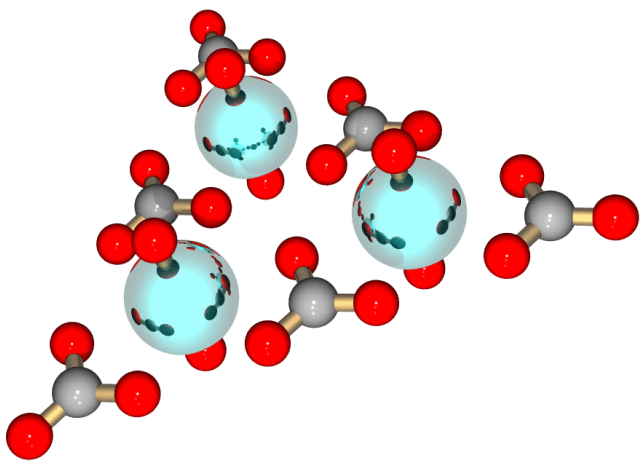
Steve Benson, Lois Curfman McInnes
Jorge J. Moré, and Jason Sarich

http://www.mcs.anl.gov/tao

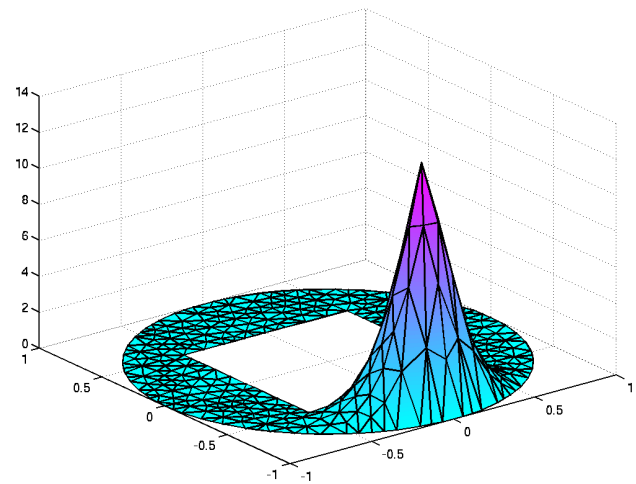
Mathematics and Computer Science Division
Argonne National Laboratory

Background: Nonlinearly Constrained Optimization

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



Electronic structure optimization



Mesh-based optimization

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

Outline

- TAO - Recent Developments
- Optimization applications
- TAO algorithms
- Performance for Grid Sequencing – Stalking optimality
- Using TAO

TAO: Toolkit for Advanced Optimization

The process of nature by which all things change and which is to be followed for a life of harmony.

- Object-oriented techniques
- Component-based interaction
- Leverage of existing parallel computing infrastructure
- Reuse of external toolkits (linear solvers, preconditioners, ...)

TAO: Recent Developments

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

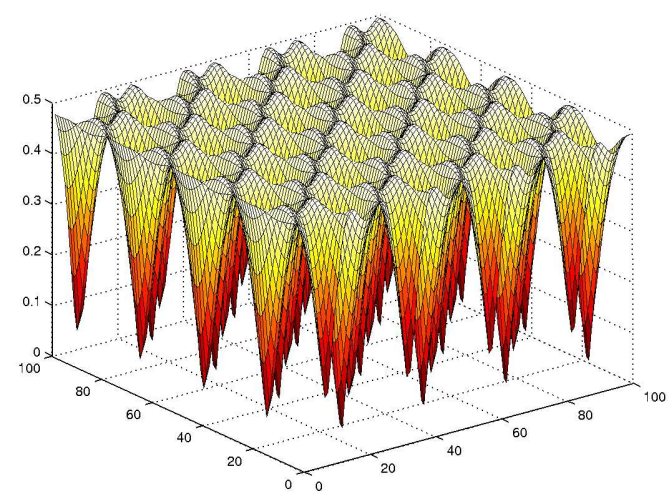
Powered by PETSc and ADIC!

The Ginzburg-Landau Model for Superconductivity

Minimize the Gibbs free energy

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

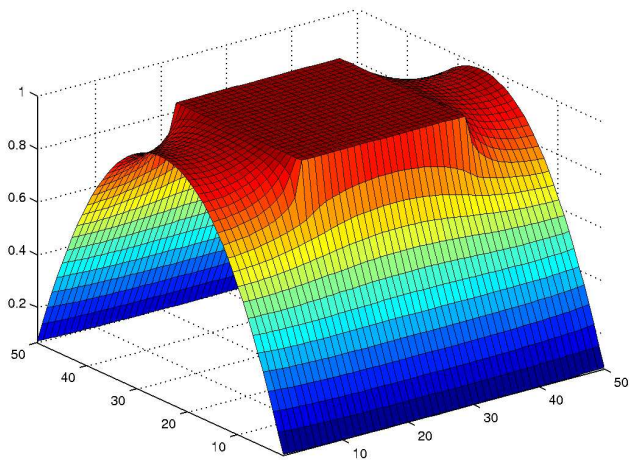
Order parameter $v : \mathbb{R}^2 \to \mathbb{C}$
Vector potential $A : \mathbb{R}^2 \to \mathbb{R}^2$

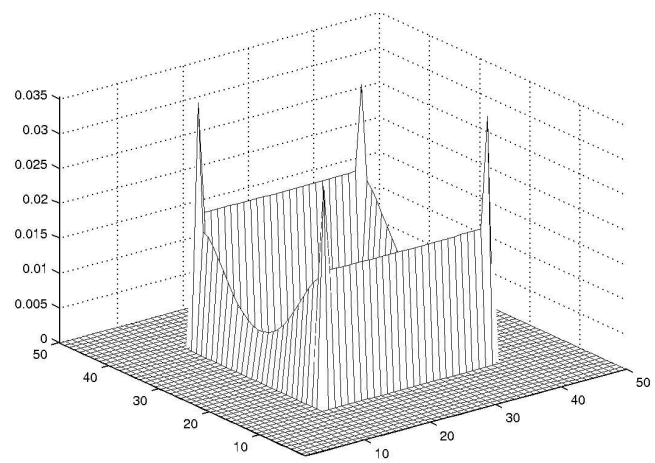


Non-convex function. Hessian is singular. Unique minimizer.

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.

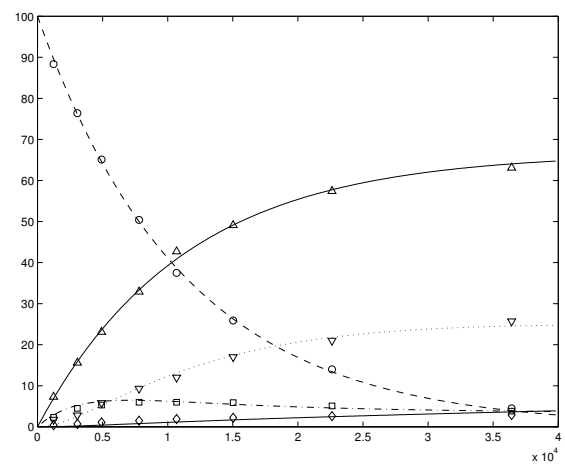
Isomerization of α-pinene

Determine the reaction coefficients by minimizing

$$\sum_{j=1}^{8} \|y(\tau_j;\theta) - z_j\|^2,$$

where z_j are the measurements and

$$\begin{aligned}
y_1' &= -(\theta_1+\theta_2)y_1 \\
y_2' &= \theta_1 y_1 \\
y_3' &= \theta_2 y_1 - (\theta_3+\theta_4)y_3 + \theta_5 y_5 \\
y_4' &= \theta_3 y_3 \\
y_5' &= \theta_4 y_3 - \theta_5 y_5
\end{aligned}$$



Hang Glider

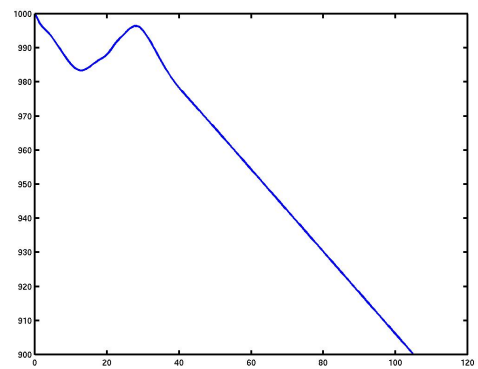
Maximize the final position of a glider whose flight has a thermal updraft at 250 meters. The equations of motion are

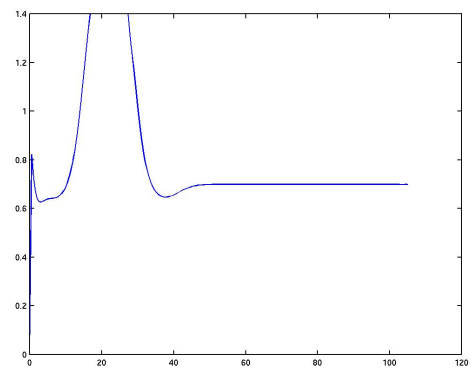
$$x'' = \frac{1}{m}(-L\sin(\eta) - D\cos(\eta)), \qquad y'' = \frac{1}{m}(L\cos(\eta) - D\sin(\eta)) - g,$$

where (x, y) is the position, m is the mass, and

$$\begin{aligned} \eta &= \eta(x, x', y') \\ L &= L(x, x', y', c_L) \\ D &= D(x, x', y,' c_L) \end{aligned}$$

$$0 \le c_L(t) \le c_M$$





The control (drag) c_L is not differentiable at the switching points.

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.

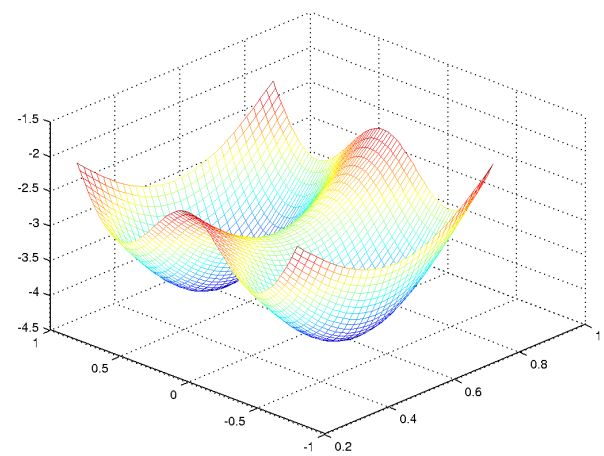
- A fundamental problem in biology, chemistry, and mathematics

A critical value of f is

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

when Γ is defined by

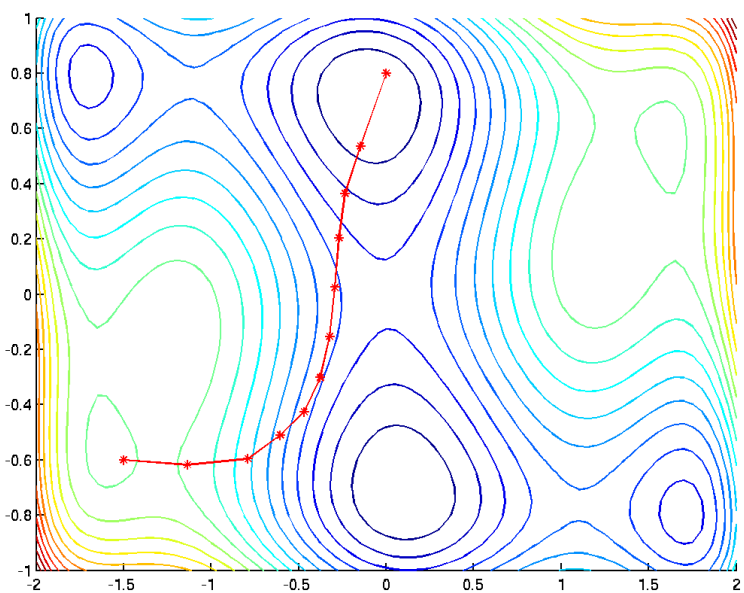
$$\Gamma = \{p \in C[0,1] : p(0) = x_a,\ p(1) = x_b\}\,.$$

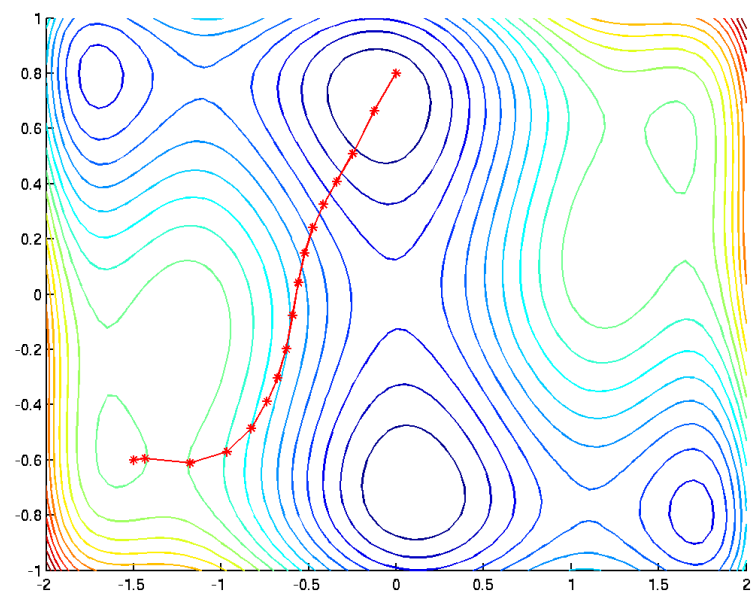


The Elastic String Algorithm

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

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





TAO Algorithms for Bound-Constrained Optimization

$$\min \{ f(x) : x_l \leq x \leq x_u \}$$

- ◇ Conjugate gradient algorithms
- ◇ Limited-memory variable-metric algorithms
- ◇ Newton algorithms

You must supply the function $f : \mathbb{R}^n \mapsto \mathbb{R}$ and the gradient

$$\nabla f(x) = (\partial_i f(x))$$

For Newton methods you also need to supply the Hessian matrix.

$$\nabla^2 f(x) = (\partial_{i,j} f(x))$$

Conjugate Gradient Algorithms

$$x_{k+1} = x_k + \alpha_k p_k$$

$$p_{k+1} = -\nabla f(x_k) + \beta_k p_k$$

where α_k is determined by a line search.

Three choices of β_k are possible ($g_k = \nabla f(x_k)$):

$$\beta_k^{FR} = \left(\frac{\|g_{k+1}\|}{\|g_k\|} \right)^2, \qquad \text{Fletcher-Reeves}$$

$$\beta_k^{PR} = \frac{\langle g_{k+1}, g_{k+1} - g_k \rangle}{\|g_k\|^2}, \qquad \text{Polak-Rivière}$$

$$\beta_k^{PR+} = \max\left\{ \beta_k^{PR}, 0 \right\}, \qquad \text{PR-plus}$$

Limited-Memory Variable-Metric Algorithms

$$x_{k+1} = x_k - \alpha_k H_k \nabla f(x_k)$$

where α_k is determined by a line search.

The matrix H_k is defined in terms of information gathered during the previous m iterations.

- H_k is positive definite.
- Storage of H_k requires $2mn$ locations.
- Computation of $H_k \nabla f(x_k)$ costs $(8m+1)n$ flops.

Trust Region Newton Algorithm

At each iteration the step s_k (approximately) minimizes

$$\min \{q_k(x_k + s) : s_i = 0,\ i \in \mathcal{A}_k,\ x_l \le x_k + s \le x_u,\ \|s\| \le \Delta_k\}$$

where q_k is the quadratic approximation,

$$q_k(w) = \langle \nabla f(x_k), w \rangle + \tfrac{1}{2} \langle w, \nabla^2 f(x_k) w \rangle,$$

to the function, and Δ_k is the trust region bound.

- Predict an active set $\mathcal{A}_k$.
- Compute a step s_k
- $x_{k+1} = x_k + s_k$ if $f(x_k + s_k) < f(x_k)$, otherwise $x_{k+1} = x_k$.
- Update Δ_k.

Mesh Sequencing Issues

- How much does mesh-sequencing save?
- Does mesh-sequencing resolve the convergence issue?
  - ◇ What is the order of convergence of $f(x_h^*)$?
  - ◇ What is the order of convergence of x_h^*?
  - ◇ How does the number of active constraints at x_h change?
  - ◇ What tolerance do we use to obtain x_h?
  - ◇ What is the impact on iterative methods on these results?

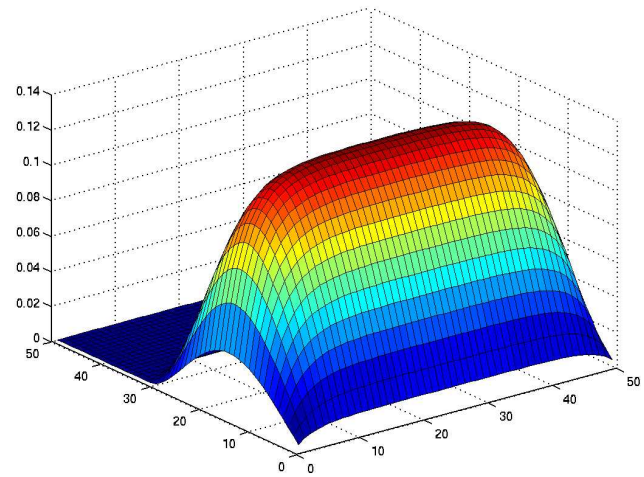
TAO Benchmark: Pressure in a Journal Bearing

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

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

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

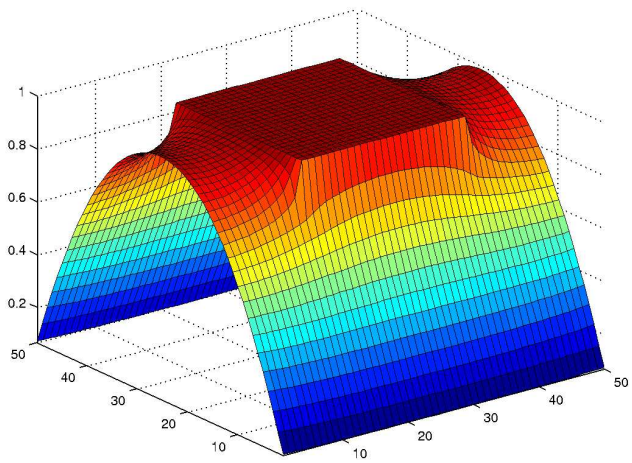
$$\mathcal{D} = (0, 2\pi) \times (0, 2b)$$

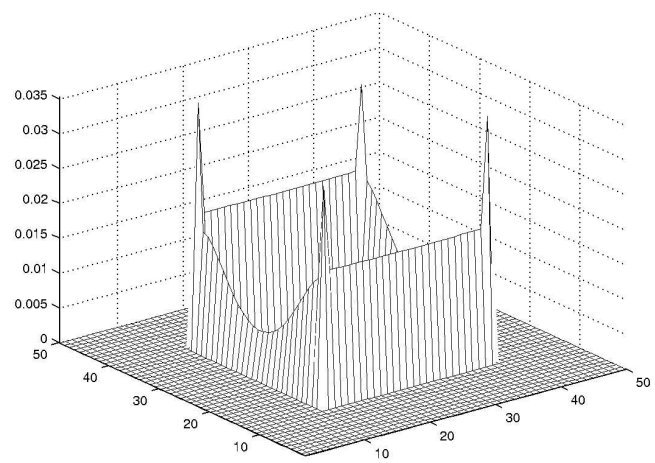


Number of active constraints depends on the choice of ϵ in $(0, 1)$.
Nearly degenerate problem. Solution $v \notin C^2$.

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	
Mesh	$\boxplus$	$\square$	$\boxplus$	$\square$	$\boxplus$	$\square$
769×769	17	283	10	142	7	86
1537×1537	73	3751	40	1861	22	938

Improvements

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

Mesh-Sequencing Performance: Obstacle Problem

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

† No convergence after 500 iterations!

Using TAO

There are three parts of a TAO application program:

- **Vector** and **matrix** objects from PETSc or other numerical packages.
- **Applications** contain routines that evaluate an objective function, define constraints on the variables, and provide derivative information.
- The **TAO solver** with desired algorithmic options and tolerances.

Using TAO with PETSc

```
TAO_SOLVER      tao;              /* TAO Optimization solver          */
TAO_APPLICATION app;              /* TAO Application using PETSc      */
AppCtx          user;             /* user-defined application context */
Vec             x;                /* solution vector                  */
Mat             H;                /* Hessian Matrix                   */

VecCreateSeq(PETSC_COMM_SELF,n,&x);
MatCreateSeqAIJ(PETSC_COMM_SELF,n,n,nz,PETSC_NULL,&H);
TaoCreate(PETSC_COMM_SELF,''tao_lmvm'',&tao);
TaoApplicationCreate(PETSC_COMM_SELF,&app);
TaoAppSetInitialSolutionVec(app,x);
TaoAppSetObjectiveRoutine(app, FormFunction,(void *)&user);
TaoAppSetGradientRoutine(app,FormGradient,(void *)&user);
TaoAppSetHessianMat(app,H,H);
TaoAppSetHessianRoutine(app,FormHessian,(void *)&user);
TaoSolveApplication(app,tao);
VecView(x,PETSC_VIEWER_STDOUT_SELF);
```

Objective Function and Gradient Evaluation

```
typedef struct {          /* Used in the minimum surface area problem */
  int         mx, my;            /* discretization in x, y directions */
  int         bmx, bmy, bheight;             /* The size of the plate */
  double      bheight;                     /* The height of the plate */
  double     *bottom, *top, *left, *right;         /* boundary values */
} AppCtx;

int FormFunction(TAO_APPLICATION app, Vec x, double *fcn, void *userCtx){
   AppCtx *user = (AppCtx *)userCtx;
   ...
}
int FormGradient(TAO_APPLICATION app, Vec x, Vec g, void *userCtx){
   AppCtx *user = (AppCtx *)userCtx;
   ...
}
int FormHessian(TAO_APPLICATION app, Vec x, Mat *H, Mat *H, int *flag, void *userCtx){
   AppCtx *user = (AppCtx *)userCtx;
   ...
}
```

Creating and Using a TAO Application

```
TAO_SOLVER      tao;              /* TAO Optimization solver          */
TAO_APPLICATION app;              /* TAO Application using PETSc      */
AppCtx          user;             /* user-defined application context */
Vec             x;                /* solution vector                  */
Mat             H;                /* Hessian Matrix                   */

VecCreateSeq(PETSC_COMM_SELF,n,&x);
MatCreateSeqAIJ(PETSC_COMM_SELF,n,n,nz,PETSC_NULL,&H);
TaoCreate(PETSC_COMM_SELF,"tao_lmvm",&tao);
TaoApplicationCreate(PETSC_COMM_SELF,&app);
TaoAppSetInitialSolutionVec(app,x);
TaoAppSetObjectiveRoutine(app,FormFunction,(void *)&user);
TaoAppSetGradientRoutine(app,FormGradient,(void *)&user);
TaoAppSetHessianMat(app,H,H);
TaoAppSetHessianRoutine(app,FormHessian,(void *)&user);
TaoSolveApplication(app,tao);
VecView(x,PETSC_VIEWER_STDOUT_SELF);
```

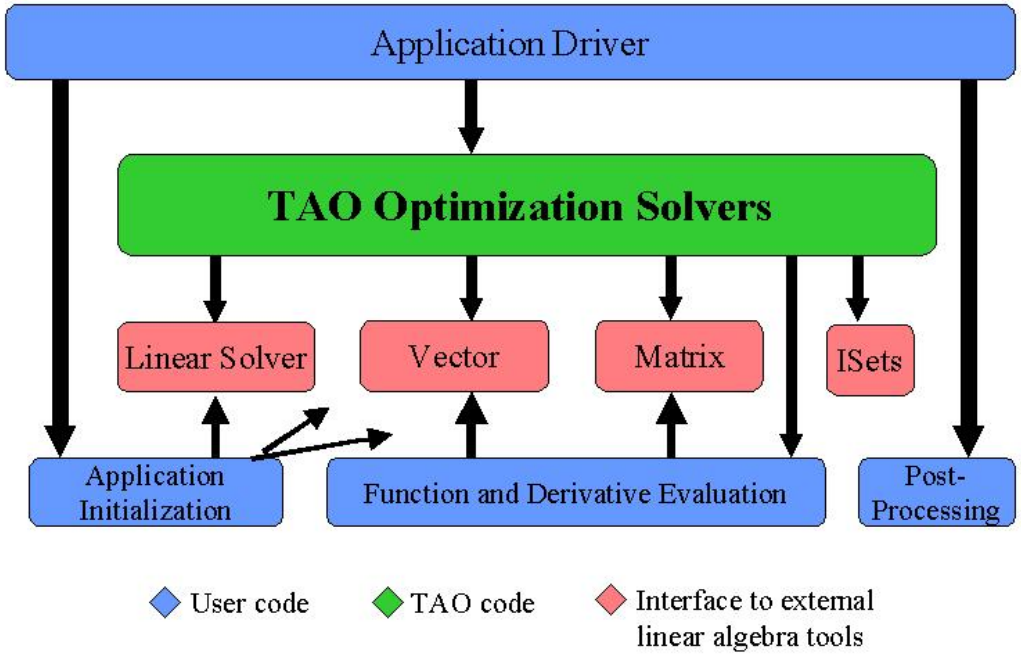
Creating and Using a TAO Solver

```
TAO_SOLVER      tao;              /* TAO Optimization solver          */
TAO_APPLICATION app;              /* TAO Application using PETSc      */
AppCtx          user;             /* user-defined application context */
Vec             x;                /* solution vector                  */
Mat             H;                /* Hessian Matrix                   */

VecCreateSeq(PETSC_COMM_SELF,n,&x);
MatCreateSeqAIJ(PETSC_COMM_SELF,n,n,nz,PETSC_NULL,&H);
TaoCreate(PETSC_COMM_SELF,"tao_lmvm",&tao);
TaoApplicationCreate(PETSC_COMM_SELF,&app);
TaoAppSetInitialSolutionVec(app,x);
TaoAppSetObjectiveRoutine(app,FormFunction,(void *)&user);
TaoAppSetGradientRoutine(app,FormGradient,(void *)&user);
TaoAppSetHessianMat(app,H,H);
TaoAppSetHessianRoutine(app,FormHessian,(void *)&user);
TaoSolveApplication(app,tao);
VecView(x,PETSC_VIEWER_STDOUT_SELF);
```

A TAO Program Outline

```
TAO_SOLVER      tao;              /* TAO Optimization solver          */
TAO_APPLICATION app;              /* TAO Application using PETSc      */
AppCtx          user;             /* user-defined application context */
Vec             x;                /* solution vector                  */
Mat             H;                /* Hessian Matrix                   */

VecCreateSeq(PETSC_COMM_SELF,n,&x);
MatCreateSeqAIJ(PETSC_COMM_SELF,n,n,nz,PETSC_NULL,&H);
TaoCreate(PETSC_COMM_SELF,"tao_lmvm",&tao);
TaoApplicationCreate(PETSC_COMM_SELF,&app);
TaoAppSetInitialSolutionVec(app,x);
TaoAppSetObjectiveRoutine(app,FormFunction,(void *)&user);
TaoAppSetGradientRoutine(app,FormGradient,(void *)&user);
TaoAppSetHessianMat(app,H,H);
TaoAppSetHessianRoutine(app,FormHessian,(void *)&user);
TaoSolveApplication(app,tao);
VecView(x,PETSC_VIEWER_STDOUT_SELF);
```

TAO Application Programs



Using PETSc Objects on Multiple Processors

```
TAO_SOLVER      tao;              /* TAO Optimization solver          */
TAO_APPLICATION app;              /* TAO Application using PETSc      */
AppCtx          user;             /* user-defined application context */
Vec             x;               /* solution vector                  */
Mat             H;                /* Hessian Matrix                   */

VecCreateMPI(PETSC_COMM_WORLD,n,&x);
MatCreateMPIAIJ(PETSC_COMM_WORLD,nlocal,nlocal,n,n,d_nz,d_nnz,o_nz,o_nnz,&H);
TaoCreate(PETSC_COMM_WORLD,"tao_lmvm",&tao);
TaoApplicationCreate(PETSC_COMM_WORLD,&app);
TaoAppSetInitialSolutionVec(app,x);
TaoAppSetObjectiveRoutine(app,FormFunction,(void *)&user);
TaoAppSetGradientRoutine(app,FormGradient,(void *)&user);
TaoAppSetHessianMat(app,H,H);
TaoAppSetHessianRoutine(app,FormHessian,(void *)&user);
TaoSolveApplication(app,tao);
VecView(x,PETSC_VIEWER_STDOUT_WORLD);
```

Convergence

Absolute tolerances specify acceptable errors in the optimality of the function and the constraints.

$$f(x) \leq f(x^*) + \epsilon_{fatol}$$

Relative tolerances specify the number of significant digits required in the solution and the constraints.

$$f(x) \leq f(x^*) + \epsilon_{frtol}|f(x^*)|$$

These tolerance can be changed

```
int TaoSetTolerances(TAO_SOLVER solver,double fatol,double frtol,
                                          double catol,double crtol)
```

TAO Basic Facilities

- TaoAppSetInitialSolutionVec
- TaoAppSetVariableBounds
- TaoGetLinearSolver
- TaoFromOptions
- TaoAppSetMonitor
- TaoView
- ...