Numerical Optimization Using PETSc/TAO

Presented to
ATPESC 2021 Participants

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ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

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What is optimization?

$$\underset{p}{\text{minimize}} \quad f(p)$$

- Optimization variables $p \in \mathbb{R}^n$
  - e.g.: boundary conditions, parameters, geometry
- Objective function $f: \mathbb{R}^n \to \mathbb{R}$
  - e.g.: lift, drag, max stress, total energy, error norms, etc.

What is optimization?

$$\underset{p}{\text{minimize}} \quad f(p)$$

- Simplification: $f(p)$ is minimized where $\nabla_p f(p) = 0$

- **Gradient-free:** Heuristic search through p space
  - Easy to use, no sensitivity analysis required

- **Gradient-based:** Find search directions based on $\nabla_p f$
  - Converges to local minima with significantly fewer function evaluations than gradient-free methods

Why do we care?

We know a lot about how to solve the forward problem…

Inputs	Simulation	Outputs
• Boundary Conditions • Parameters • Geometry	• Fluid Dynamics • Continuum Mechanics • Heat Transfer	• Density • Pressure • Temperature • Deformation

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- Parameters
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Simulation

- Fluid Dynamics
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Outputs

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Control Decision Design ← **Optimization** ← **Objective**

…many scientific questions present as inverse problems!

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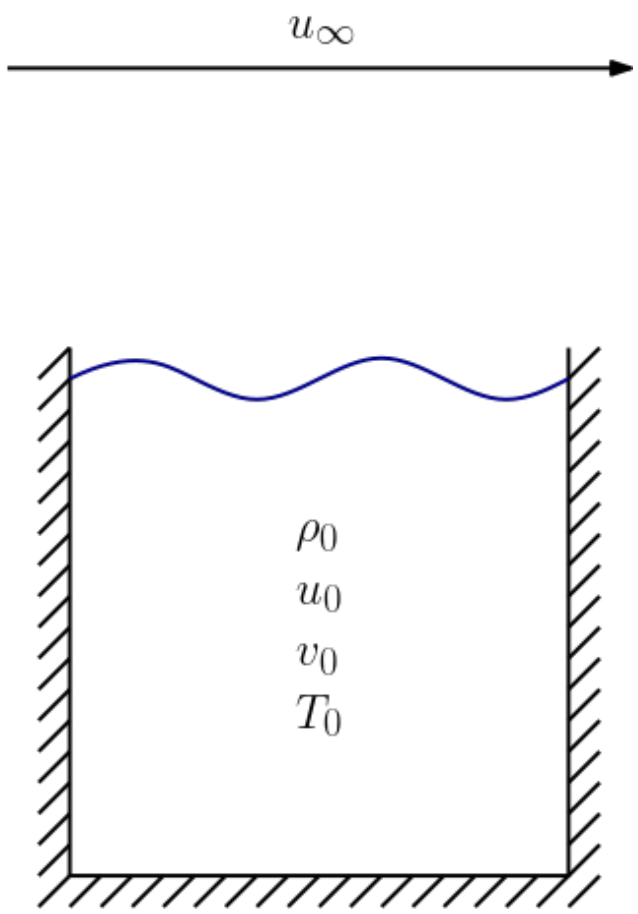

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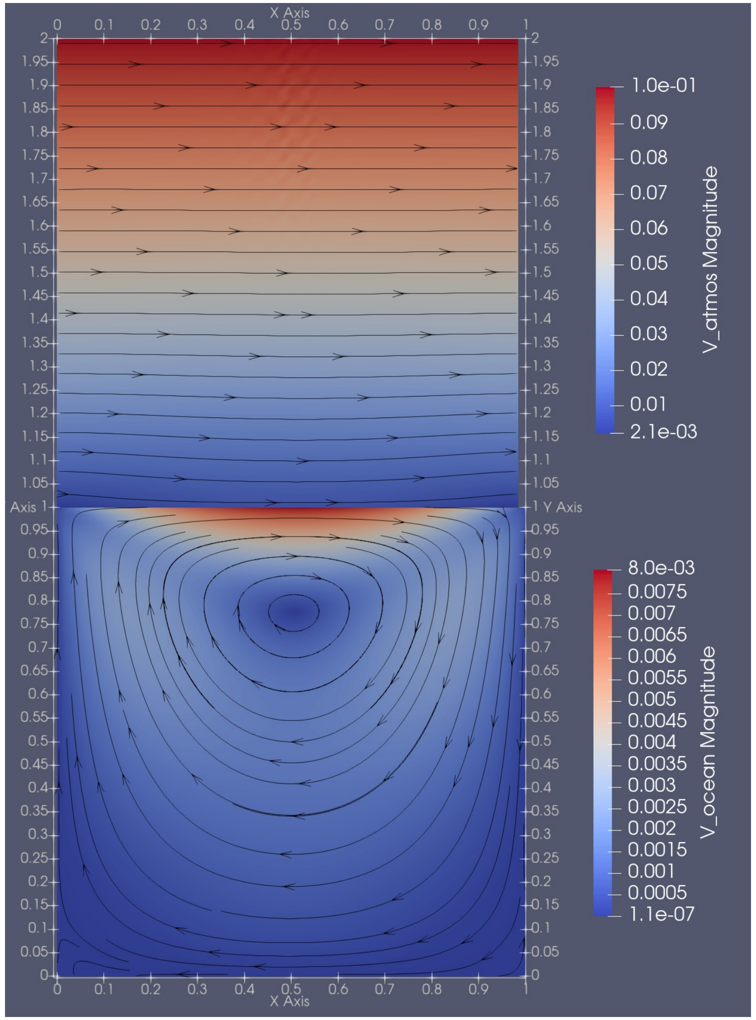

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Outline

- Introduction to Gradient-Based Optimization
  - Sequential Quadratic Programming
  - Sensitivity Analysis

- Introduction to TAO
  - Sample main program
  - User/problem callback function

- Hands-on Examples: Rosenbrock Equation
  - 2-dimensional unconstrained
  - Multidimensional unconstrained
  - 2-dimensional with general constraints

Intro to Numerical Optimization

$$\underset{p}{\text{minimize}} \quad f(p)$$

- Optimization variables $p \in \mathbb{R}^n$
- Objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$
- Local minima where gradient is zero (optimality condition)
- Optimality condition is **necessary** but not sufficient
  - Other stationary points (e.g., maximums) also satisfy $\nabla_p f(p) = 0$

Sequential Quadratic Programming

for k=0,1,2,... **do**

$$\min_d \quad f_k + d^T g_k + 0.5 d^T H_k d$$

$$\min_\alpha \quad \Phi(\alpha) = f(p_k + \alpha d)$$

$$p_{k+1} \leftarrow p_k + \alpha d$$

end for

- Solution at k^{th} iteration p_k
- Gradient $g_k = \nabla_p f(p_k)$
- Hessian $H_k = \nabla^2_{pp} f(p_k)$
- Search direction $d \in \mathbb{R}^n$
- Step length α

- Replace original problem with a sequence of quadratic subproblems
  - Solution given by $d = -H_k^{-1} g\_k$
- Line search maintains consistency between local quadratic model and global nonlinear function (globalization)
  - Avoids undesirable stationary points

Sequential Quadratic Programming

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- Different approximations to search direction yield different algorithms
  - **Newton's method:** $d = -H_k^{-1} g_k$, no approximation
  - **Quasi-Newton:** $d = -B_k g_k$ with $B_k \approx H_k^{-1}$ based on the secant condition
  - **Conjugate Gradient:** $d_k = -g_k + \beta_k d_{k-1}$ with β defining different CG updates
  - **Gradient Descent:** $d = -g_k$, replace Hessian with identity

PDE-Constrained Optimization

$$\underset{p,u}{\text{minimize}} \quad f(p,u) \qquad\qquad \underset{p}{\text{minimize}} \quad f(p, u(p))$$
$$\text{subject to} \quad R(p,u) = 0$$

Full-Space Formulation

- State variables $u \in \mathbb{R}^m$
- State equations $R: \mathbb{R}^{n+m} \rightarrow \mathbb{R}^m$

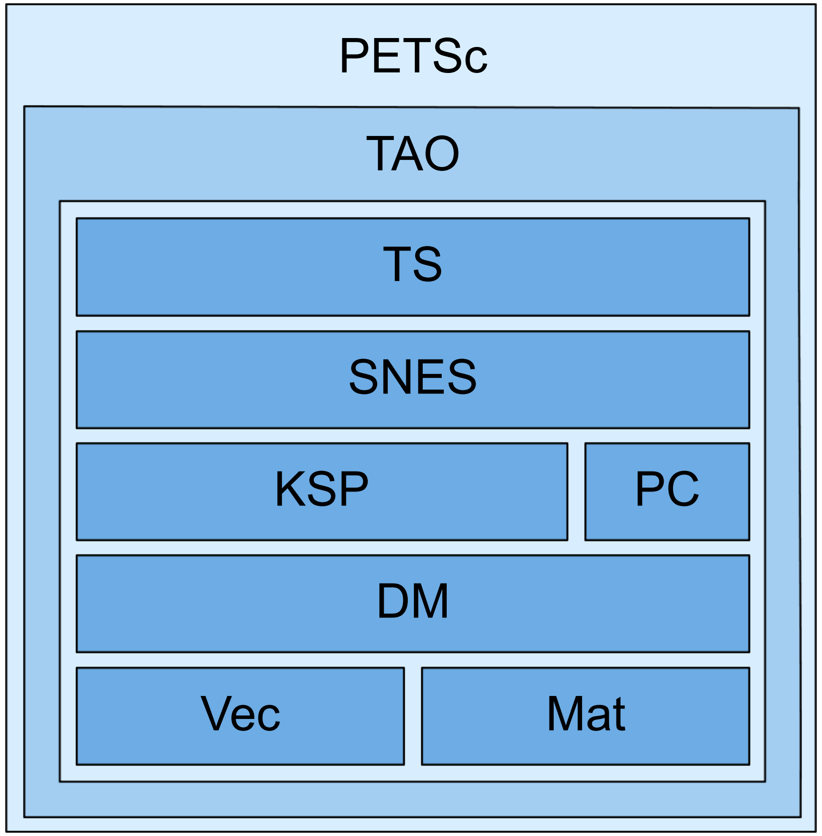
Reduced-Space Formulation

- State variables are implicit functions of parameters

- Reduced-space formulation enables use of conventional unconstrained optimization algorithms to solve PDE-constrained problems
- Each reduced-space function evaluation requires a full PDE solution
- See ATPESC 2019 lesson for more details

Toolkit for Advanced Optimization

- General-purpose continuous optimization toolbox for large-scale problems
  – Parallel (via PETSc data structures)
  – Gradient-based
  – Bound-constrained
  – Nonlinear/general constraint support under development
  – PDE-constrained problems w/ reduced-space formulation
- Distributed with PETSc (https://petsc.org)
- Similar packages:
  – Rapid Optimization Library (https://trilinos.github.io/rol.html)
  – HiOP (https://github.com/LLNL/hiop)



TAO: The Basics

- Sample main program

```
AppCtx user;
Tao tao;
Vec P;

PetscInitialize( &argc, &argv,(char *)0,help );
VecCreateMPI(PETSC_COMM_WORLD, user.n, user.N, &P);
VecSet(P, 0.0);

TaoCreate(PETSC_COMM_WORLD, &tao);
TaoSetType(tao, TAOBQNLS);        /* bound-constrained quasi-Newton */
TaoSetInitialVector(tao, P);
TaoSetObjectiveRoutine(tao, FormFunction, &user);
TaoSetGradientRoutine(tao, FormGradient, &user);
TaoSetFromOptions(tao);
TaoSolve(tao);

VecDestroy(&P);
TaoDestroy(&tao);
PetscFinalize();
```

TAO: The Basics

- User provides function for problem implementation

```
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PetscFinalize();
```

TAO: User Function

- User functions compute objective and gradient

```
typedef struct {
    /* user-created context for storing application data */
} AppCtx;
```

```
PetscErrorCode FormFunction (Tao tao, Vec P, PetscReal *fcn, void *ptr)
{
    AppCtx *user = (AppCtx*) ptr;
    const PetscScalar *pp;

    VecGetArrayRead(P, &pp);

    /* USER TASK: Compute objective function and store in fcn */

    VecRestoreArrayRead(P, &pp);

    return 0;
}
```

```
PetscErrorCode FormGradient(Tao tao, Vec P, Vec G, void *ptr)
{
    AppCtx *user = (AppCtx*) ptr;
    const PetscScalar *pp;
    PetscScalar *gg;

    VecGetArrayRead(P, &pp);
    VecGetArray(G, &gg);

    /* USER TASK: Compute compute gradient and store in gg */

    VecRestoreArrayRead(P, &pp);
    VecRestoreArray(G, &gg);

    return 0;
}
```


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TAO: User Function

- **Objective evaluation:**
  - Compute $f(p)$ at given p
- **Sensitivity analysis:**
  - Compute $\mathrm{G} = \nabla_p f$ at given p
- **(ADVANCED) Second-order Methods:**
  - Compute $H = \nabla_p^2 f$ at given p
  - Use `TaoSetHessian()` interface
- **(ADVANCED) Constraints:**
  - Set bound constraints $\mathrm{p_l} \leq p \leq p_u$
  - Define nonlinear constraints $c_e(p) = 0,\ c_i(p) \geq 0$

TAO: User Function

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- Necessary for gradient-based optimization algorithms
- Types:
  - Numerical
  - Analytical

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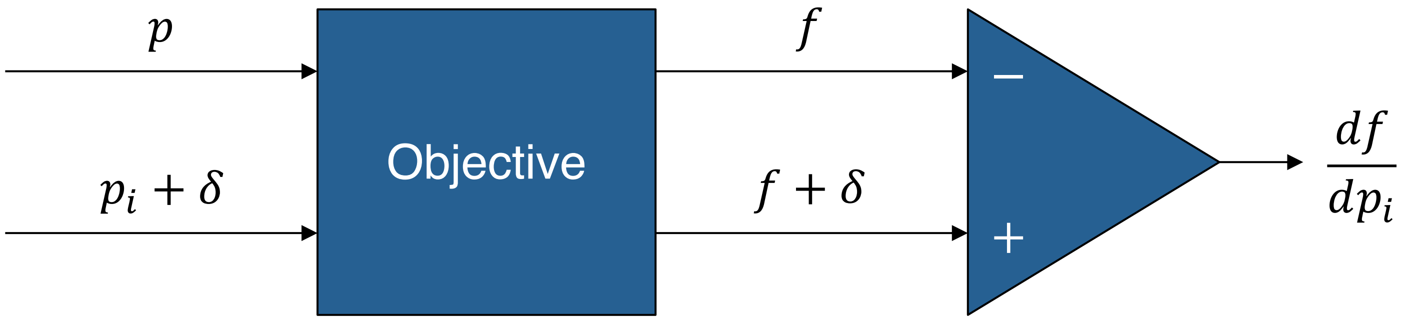
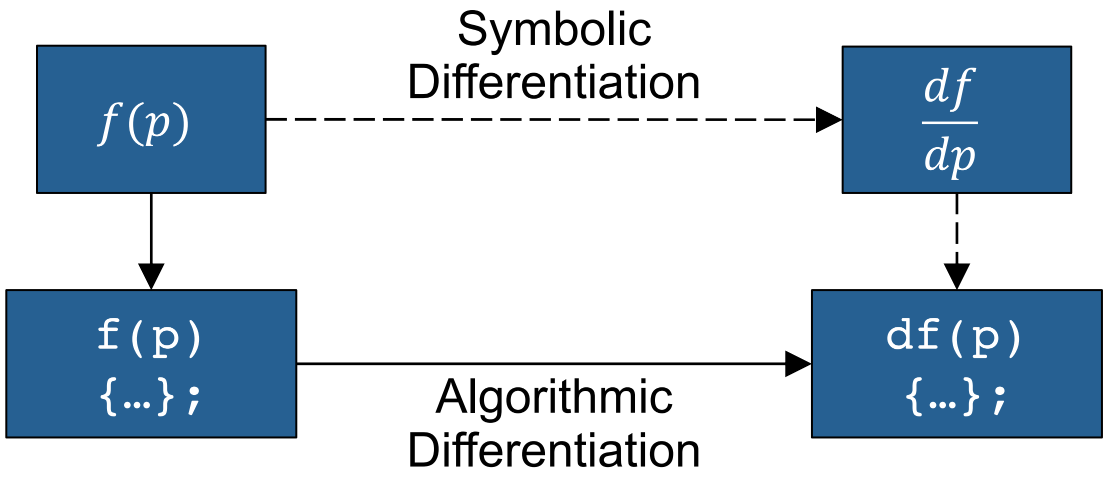
Sensitivity Analysis: Numerical Differentiation



- Finite-difference method is easy to implement
  - Only requires function evaluations
- Inefficient for large numbers of optimization variables
- Step-size dilemma – truncation error vs. subtractive cancellation
- TAO provides automatic FD gradient and Hessian evaluations

Sensitivity Analysis: Analytical Differentiation



- **Symbolic** –hand-derived gradient with direct code implementation
- **Algorithmic** – source code transformation or operator overloading via AD tool/library (i.e., chain rule!)

- Computational cost is (mostly) independent of the number of optimization variables
- Some popular AD tools:
  - ADIC (ANSI C)
  - ADIFOR (Fortran77/Fortran95)
  - OpenAD (Fortran77/Fortran95/C/C++)
  - Sacado (C/C++)
  - ForwardDiff.jl (Julia)
  - JAX (Python)

TAO: Bound Constraints

- What if we wanted to restrict the solution variables?

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & x_l \leq x \leq x_u \end{aligned}$$

```
VecDuplicate(X, &XL);
VecSet(XL, PETSC_NINFINITY);
VecDuplicate(X, &XU);
VecSet(XU, 0.0);
TaoSetVariableBounds(tao, XL, XU);
```

- Must use bound-constrained TAO algorithms
  - `TAOBNLS`: Bounded Newton Line-Search
  - `TAOBNTR`: Bounded Newton Trust Region
  - `TAOBQNLS`: Bounded quasi-Newton Line-Search
  - `TAOBNCG`: Bounded Nonlinear Conjugate Gradient

TAO: General Nonlinear Constraints

- Incorporate all constraint types

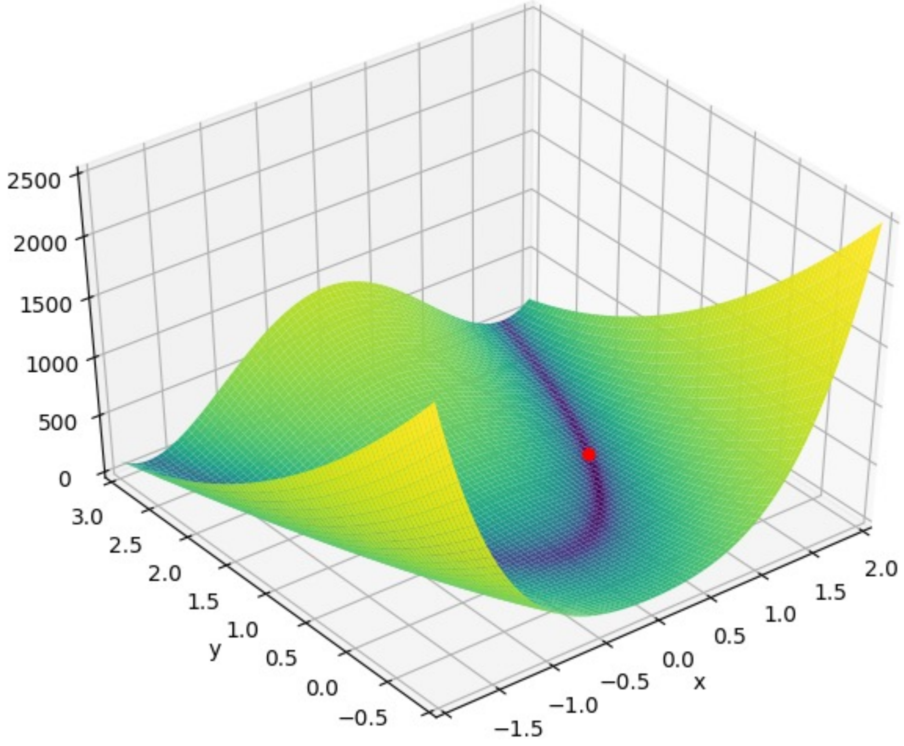
$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(x) \\
\text{subject to} \quad & c_e(x) = 0 \\
& c_i(x) \geq 0 \\
& x_l \leq x \leq x_u
\end{aligned}
$$

- Must use `TAOALMM` solver
  - Augmented Lagrangian method w/ interior-point formulation for inequality constraints
- Define constraints with user call-backs
  - `FormEqualityConstraints(Tao,Vec,Vec,void*)` → `TaoSetEqualityConstraintsRoutine()`
  - `FormEqualityJacobian(Tao,Vec,Mat,Mat,void*)` → `TaoSetJacobianEqualityRoutine()`
  - `FormInequalityConstraints(Tao,Vec,Vec,void*)` → `TaoSetInequalityConstraintsRoutine()`
  - `FormInequalityJacobian(Tao,Vec,Mat,Mat,void*)` → `TaoSetJacobianInequalityRoutine()`

Hands-on Example: 2-dimensional Rosenbrock

$$\underset{p}{\text{minimize}} \quad f(p) = (1 - p_1)^2 + 100(p_2 - p_1^2)^2$$

- Global minimum at $p = (1, 1)$
- Also called the “banana function”
- Canonical test problem for optimization algorithms
- Easy to find the valley, difficult to traverse it towards the solution



Hands-on Example: Multidimensional Rosenbrock

$$\underset{p}{\text{minimize}} \quad f(p) = \sum_{i=1}^{N-1} (1 - p_i)^2 + 100(p_{i+1} - p_i^2)^2$$

- Global minimum at $p_i = 1, \forall\, i = 1,2, \ldots, N$

- Implementation supports parallel runs and provides analytical gradient and sparse Hessian
  - Simulation-based / HPC apps. would use algorithmic differentiation

- TAO can compute sensitivities via finite-differencing when analytical derivatives are not available
  - Convenient for prototyping or debugging
  - Computationally expensive for large optimization problems or expensive objectives

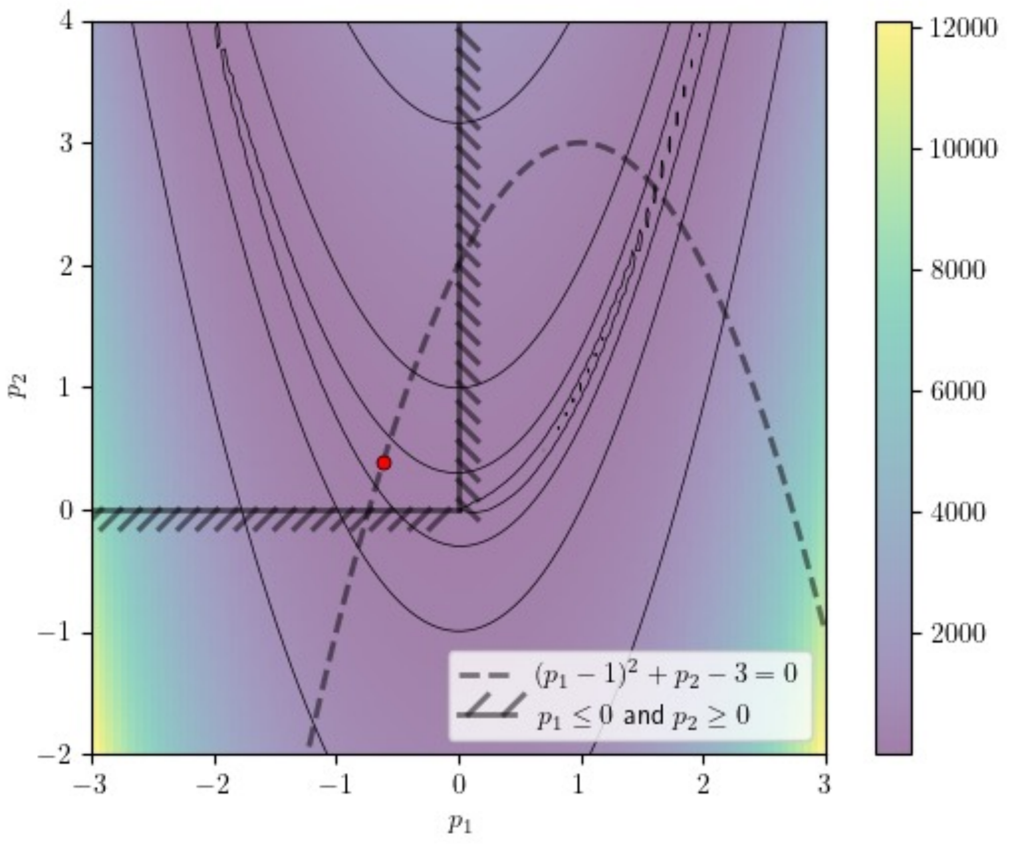
- Hands-on Activities:

  https://xsdk-project.github.io/MathPackagesTraining2021/lessons/numerical_optimization_tao/

Hands-on Example: 2D Rosenbrock w/ Constraints

$$\begin{aligned} \underset{p}{\text{minimize}} \quad & f(p) = (1 - p_1)^2 + 100(p_2 - p_1^2)^2 \\ \text{subject to} \quad & (p_1 - 1)^2 + p_2 - 3 = 0 \\ & p_1 \leq 0 \\ & p_2 \geq 0 \end{aligned}$$

- Bound-constrained global minimum at $f(0,0) = 1$
- Equality-constraints have two local minima
  - $f(-0.62, 0.38) = 2.62$
  - $f(1.62, 2.62) = 0.38$
- Combined constraints yield global minimum at $f(-0.62, 0.38) = 2.62$
- Constraints are not valid for the multidimensional Rosenbrock problem



Take Away Messages

- PETSc/TAO offers parallel optimization algorithms for large-scale problems.

- Efficient gradients are needed for best results (e.g., algorithmic differentiation), and second-order methods don’t always achieve faster/better solutions.

- PETSc/TAO can automatically compute gradients via finite differencing.

- PETSc/TAO can incorporate bound, equality and inequality constraints into the solution.

- Most scientific problems are nonlinear and nonconvex... starting point matters!

Acknowledgements

PETSc/TAO Documentation: https://petsc.org

GitLab Repo: https://gitlab.com/petsc/petsc

Offline questions: adener@anl.gov

Need help with your PETSc/TAO application? petsc-users@mcs.anl.gov

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