Numerical Optimization Using PETSc/TAO

Presented to
ATPESC 2020 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 $f\colon \mathbb{R}^n \to \mathbb{R}$
  - 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	• Lift • Drag • Stress • Temperature

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Inputs → **Simulation** → **Outputs**

Inputs:
- Boundary Conditions
- Parameters
- Geometry

Simulation:
- Fluid Dynamics
- Continuum Mechanics
- Heat Transfer

Outputs:
- Lift
- Drag
- Stress
- Temperature

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

…many scientific questions present as inverse problems!

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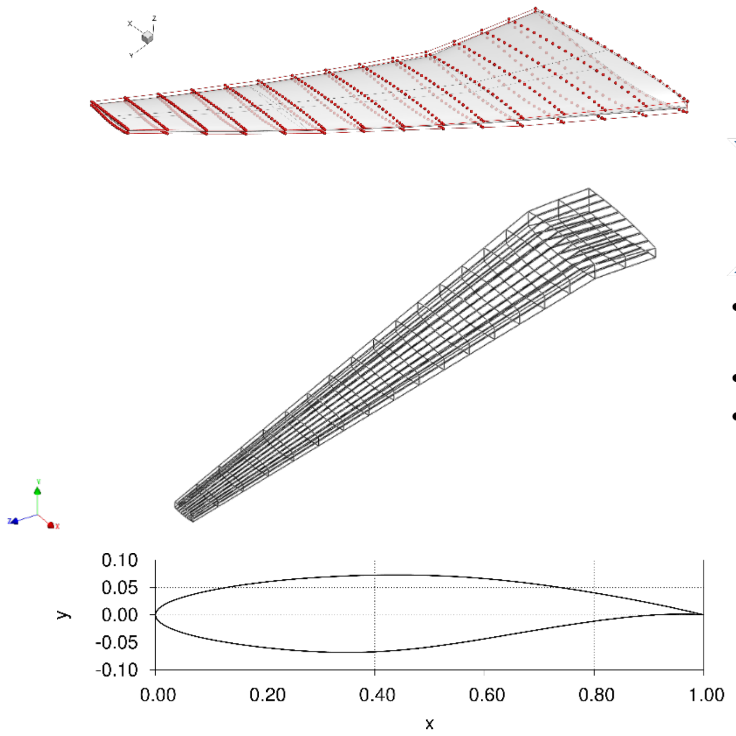

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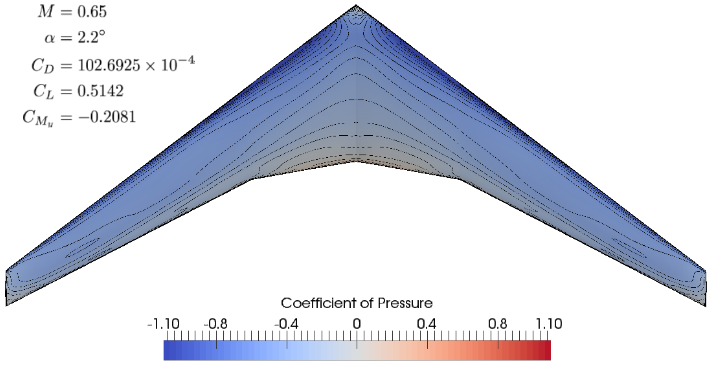
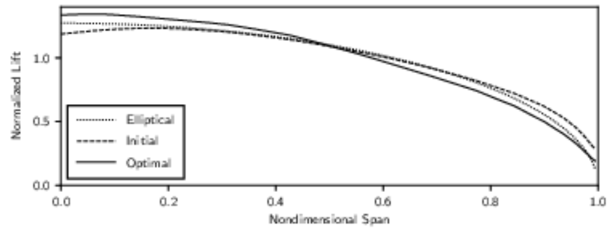




EXASCALE COMPUTING PROJECT

Outline

- Introduction to Gradient-Based Optimization
  - Sequential Quadratic Programming
  - Sensitivity Analysis
- Introduction to TAO
  - Sample main program
  - User/problem callback function
- Hands-on Examples: Multidimensional Rosenbrock

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., maxima) 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

$$
\begin{aligned}
&\textbf{for } k=0,1,2,\ldots \textbf{ do}\\
&\quad \min_d \quad f_k + d^T g_k + 0.5 d^T H_k d\\
&\quad \min_\alpha \quad \Phi(\alpha) = f(p_k + \alpha d)\\
&\quad p_{k+1} \leftarrow p_k + \alpha d\\
&\textbf{end for}
\end{aligned}
$$

- 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

- 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 a Secant approximation
  - **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

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

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

Full-Space Formulation

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

Reduced-Space Formulation

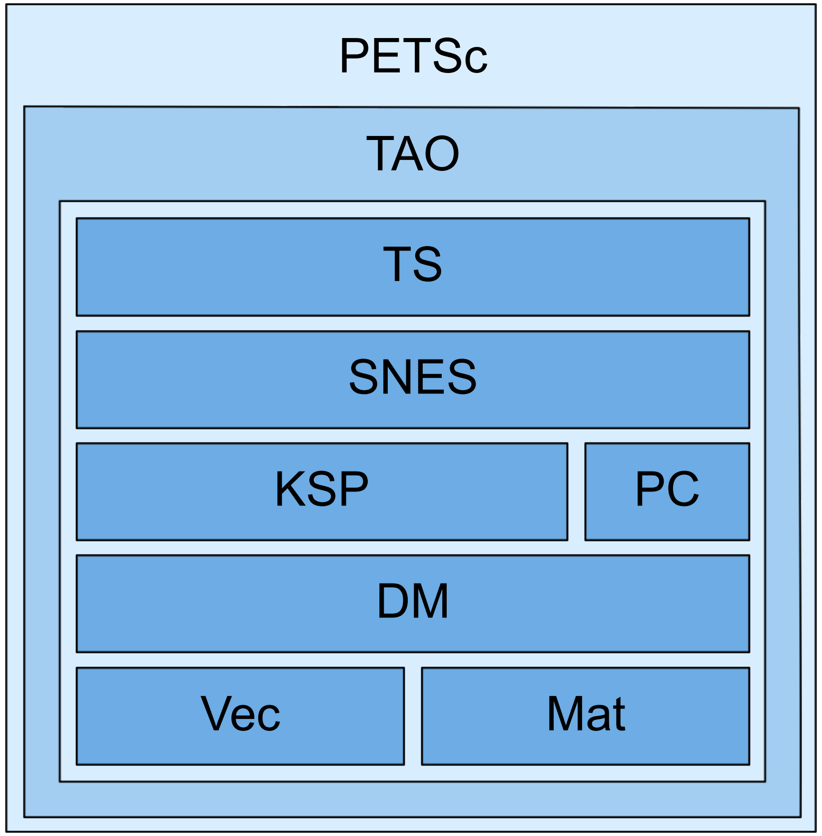
- State variables are implicit functions of parameters

- 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

PETSc TAO

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://www.mcs.anl.gov/petsc/)
- 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); /* BQNLS: quasi-Newton line search */
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

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

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VecCreateMPI(PETSC_COMM_WORLD, user.n, user.N, &P);
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TaoSetFromOptions(tao);
TaoSolve(tao);

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

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

TAO: User Function

- **Objective evaluation:**
  - Compute $f(p)$ at given p

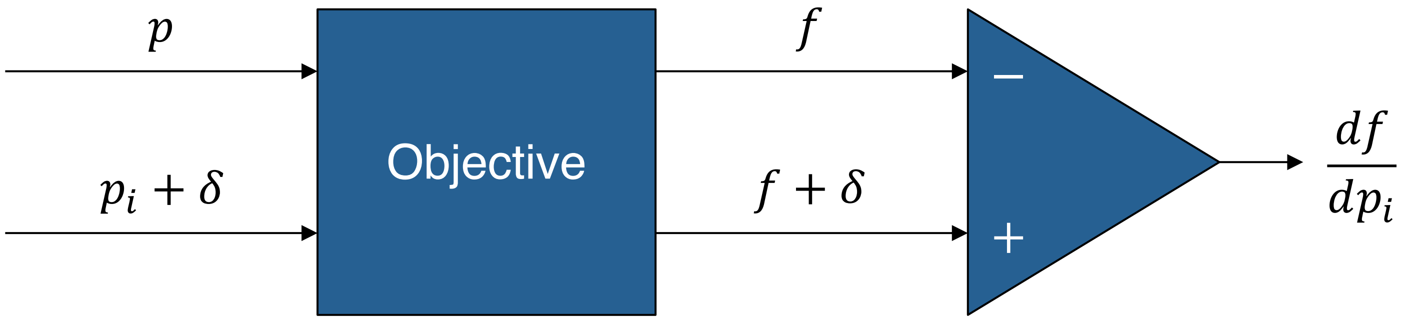
- **Sensitivity analysis:**
  - Compute $G = \nabla_p f$ at given p

→

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

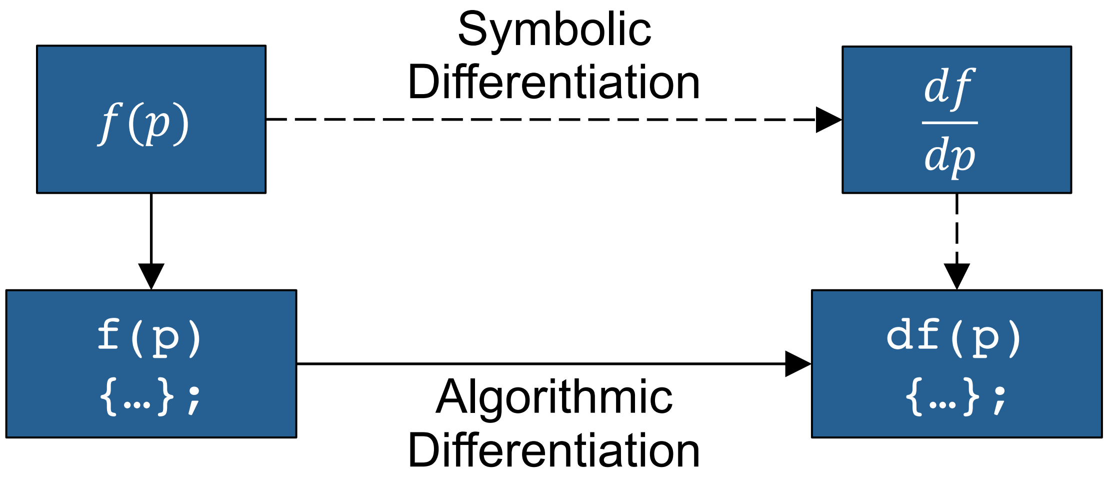
- **(ADVANCED) Second-order Methods:**
  - Compute $H = \nabla_p^2 f$ at given p
  - Use `TaoSetHessian()` interface

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

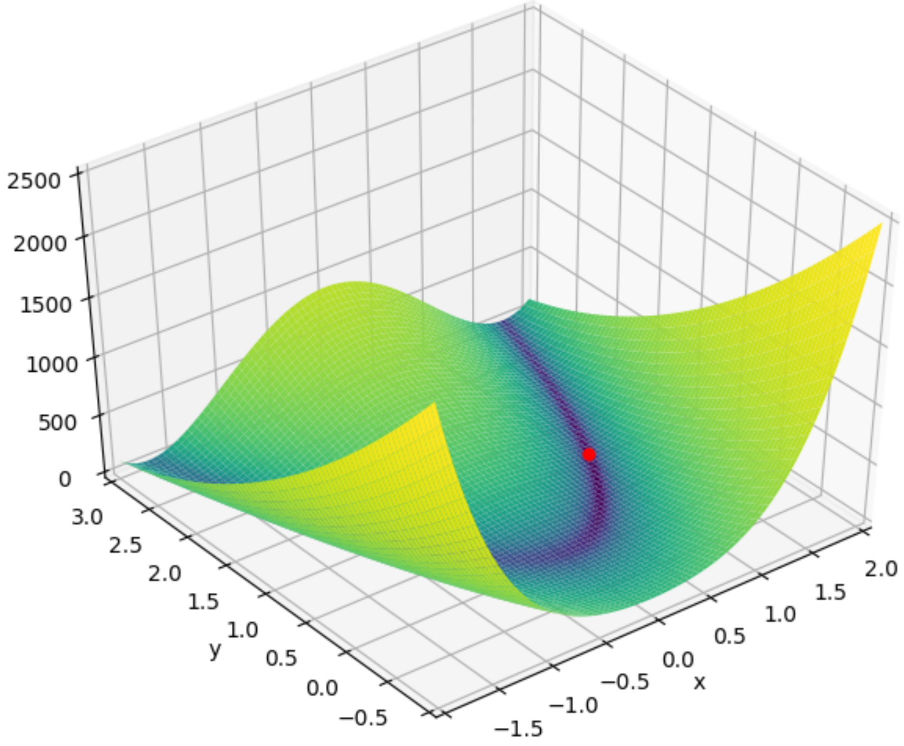


- **Symbolic** – manual hand-derived gradient, typically not applicable to simulation-based / HPC applications
- **Algorithmic** – source code transformation or operator overloading via AD tool/library (i.e., chain rule!)

- Computational cost is (mostly) independent of the number of optimization variables
- Implementation difficulty increases with function complexity
  – PDE-constrained problems need to implement the **adjoint method**
  – See ATPESC 2019 lesson for more details

Hands-on Example: Multidimensional Rosenbrock

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



- Original 2D version has a 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

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Hands-on Example: Multidimensional Rosenbrock

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

- 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/MathPackagesTraining2020/lessons/multidim_rosenbrock_tao/

Take Away Messages

- PETSc/TAO offers parallel optimization algorithms for large-scale problems.
- Efficient gradients are needed for best results (e.g., algorithmic differentiation).
- Second-order methods don't always achieve faster/better solutions.
- When apps can only provide function evaluations, PETSc/TAO can automatically compute gradients via finite differencing.
- PETSc/TAO can also use finite differencing to validate application-provided gradients and Hessians.

Acknowledgements

PETSc/TAO: https://www.mcs.anl.gov/petsc/

Offline Questions: adener@anl.gov

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