PDE-constrained Optimization Using PETSc/TAO

Presented to
ATPESC 2019 Participants

Alp Dener
Postdoctoral Appointee, MCS, ANL

Q Center, St. Charles, IL (USA)
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ATPESC Numerical Software Track

EXASCALE COMPUTING PROJECT

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, pressure, temperature, stress, strain

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
- Gradient-based: Find search directions based on $\nabla_p f$

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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

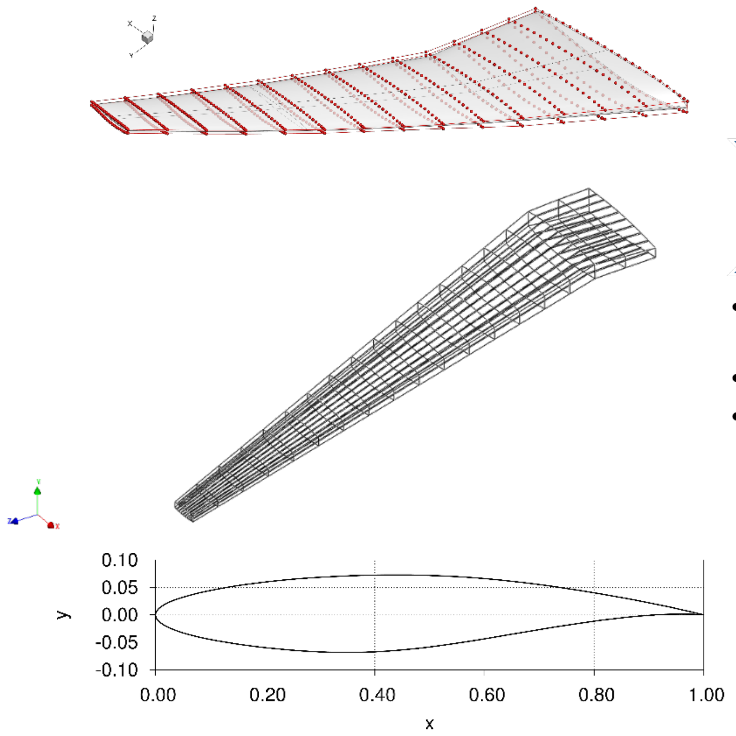
Simulation
- Fluid Dynamics
- Continuum Mechanics
- Heat Transfer

Outputs
- Lift
- Drag
- Stress
- Temperature

Control Decision Design ← Optimization ← Objective

…many scientific questions present as inverse problems!

Why do we care?



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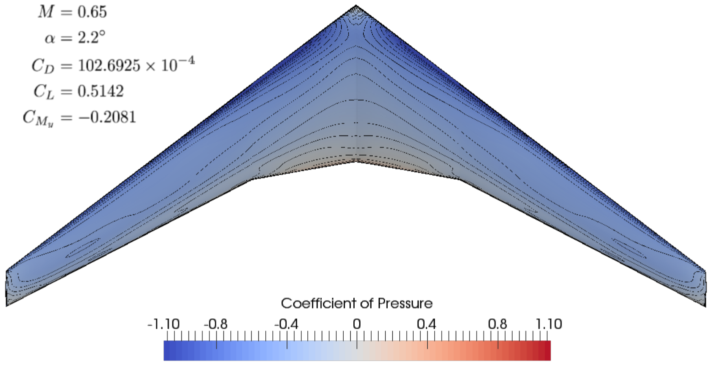

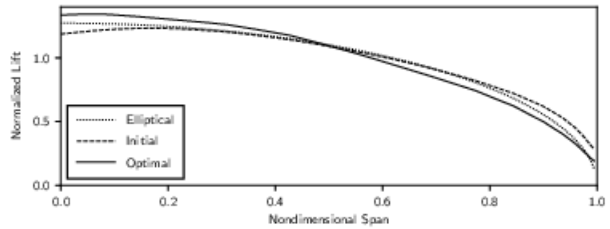

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Outline

- Intro to PDE-constrained Optimization
  - Full-space formulation
  - Reduced-space formulation
- Introduction to TAO
  - Sample main program
  - User/problem function callback
- Sensitivity Analysis
  - Finite difference method
  - Adjoint method
- Hands-on Example: Boundary Control w/ 2D Laplace Equation

PDE-constrained Optimization

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

- Optimization variables $p \in \mathbb{R}^n$
- State variables $u \in \mathbb{R}^m$
- State equations R: $\mathbb{R}^{n+m} \rightarrow \mathbb{R}^m$
- “Full-space” formulation – optimization includes both optimization and state variables

First-order Optimality Conditions

- Construct the Lagrangian where $\lambda \in \mathbb{R}^m$

$$\mathcal{L}(p, u, \lambda) = f(p, u) + \lambda^T R(p, u)$$

- Differentiate w.r.t. every input for first-order optimality

$$\begin{aligned}
\nabla_p \mathcal{L} &= \frac{\partial f}{\partial p} + \lambda^T \frac{\partial R}{\partial p} &= 0 \\
\nabla_u \mathcal{L} &= \frac{\partial f}{\partial u} + \lambda^T \frac{\partial R}{\partial u} &= 0 \\
\nabla_\lambda \mathcal{L} &= R(u, p) &= 0
\end{aligned}$$

- Also known as the Karush-Kuhn-Tucker (KKT) conditions

Solving the Problem

- Apply Newton's method to the KKT conditions

For k = 0, 1, 2, …

Convergence check (i.e., $\|\nabla_p \mathcal{L}\| \leq \varepsilon_p$ and $\|R\| \leq \varepsilon_u$)

Solve $$\begin{bmatrix} \nabla^2_{pp}\mathcal{L} & \nabla^2_{up}\mathcal{L} & \frac{\partial R}{\partial p}^T \\ \nabla^2_{pu}\mathcal{L} & \nabla^2_{uu}\mathcal{L} & \frac{\partial R}{\partial u}^T \\ \frac{\partial R}{\partial p} & \frac{\partial R}{\partial u} & 0 \end{bmatrix}_k \begin{pmatrix} \Delta p \\ \Delta u \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_p \mathcal{L} \\ -\nabla_u \mathcal{L} \\ -R(p,u) \end{pmatrix}_k$$

Step acceptance with globalization (e.g., line search)

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Solving the Problem

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Conjugate Gradient
Quasi-Newton
Newton-Krylov
…

Step acceptance with globalization (e.g., line search)

Solving the Problem

$$\begin{bmatrix} \nabla^2_{pp}\mathcal{L} & \nabla^2_{up}\mathcal{L} & \frac{\partial R}{\partial p}^T \\ \nabla^2_{pu}\mathcal{L} & \nabla^2_{uu}\mathcal{L} & \frac{\partial R}{\partial u}^T \\ \frac{\partial R}{\partial p} & \frac{\partial R}{\partial u} & 0 \end{bmatrix}_k \begin{pmatrix} \Delta p \\ \Delta u \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_p \mathcal{L} \\ -\nabla_u \mathcal{L} \\ -R(p,u) \end{pmatrix}_k$$

- **Full-space** formulation
  - PDE solution tightly coupled with optimization
  - Avoid the cost of a complete PDE solution at every optimization iteration
  - Large saddle-point problem – difficult to solve

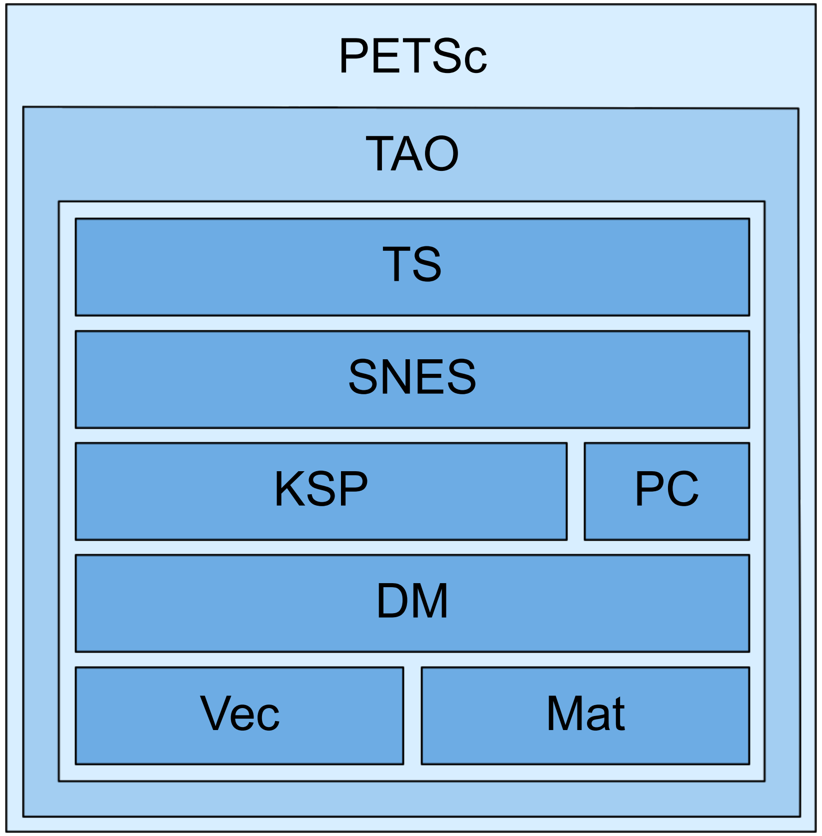
An Alternative Approach

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

- **Reduced-space** formulation
  - PDE-constraint is eliminated via implicit function theorem
  - Optimization algorithm and PDE solver are independent
  - Each objective evaluation requires a full PDE solution

Toolkit for Advanced Optimization (TAO)

- General-purpose continuous optimization toolbox for large-scale problems
  - Parallel (via PETSc data structures)
  - Gradient-based
  - Bound-constrained
  - Nonlinear constraint support under development
- **Support for reduced-space PDE-constrained optimization**
- 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);
TaoSetObjectiveAndGradientRoutine(tao, FormFunctionGradient, (void*) &user);
TaoSetFromOptions(tao);
TaoSolve(tao);

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

TAO: The Basics

- User provides function for problem implementation

```
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Tao tao;
Vec P;

PetscInitialize( &argc, &argv,(char *)0,help );
VecCreateMPI(PETSC_COMM_WORLD, user.n, user.N, &P);
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VecDestroy(&P);
TaoDestroy(&tao);
PetscFinalize();
```

TAO: User Function

- User function computes objective and gradient

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

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

   VecGetArrayRead(P, &pp);
   VecGetArray(G, &gg);
   /* USER TASK: Compute objective function and store in fcn */
   /* USER TASK: Compute compute gradient and store in gg */
   VecRestoreArrayRead(P, &pp);
   VecRestoreArray(G, &gg);

   return 0;
}
```


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TAO: User Function

- **State/PDE solution:**

  Solve $R(p, u) = 0$ for $u(p)$ at new p

- **Objective evaluation:**

  Compute $f(p, u(p))$

- **Sensitivity analysis:**

  Compute $\mathrm{G} = \nabla_p f$ at p and $u(p)$

TAO: User Function

- **State/PDE solution:**
  Solve $R(p,u) = 0$ for $u(p)$ at new p

- **Objective evaluation:**
  Compute $f(p, u(p))$

- **Sensitivity analysis:**
  Compute $G = \nabla_p f$ at p and $u(p)$

- Necessary for gradient-based optimization
- Converges to the local optimum faster than gradient-free methods (i.e., fewer PDE solutions)
- Types:
  - Finite difference
  - Discrete adjoint method

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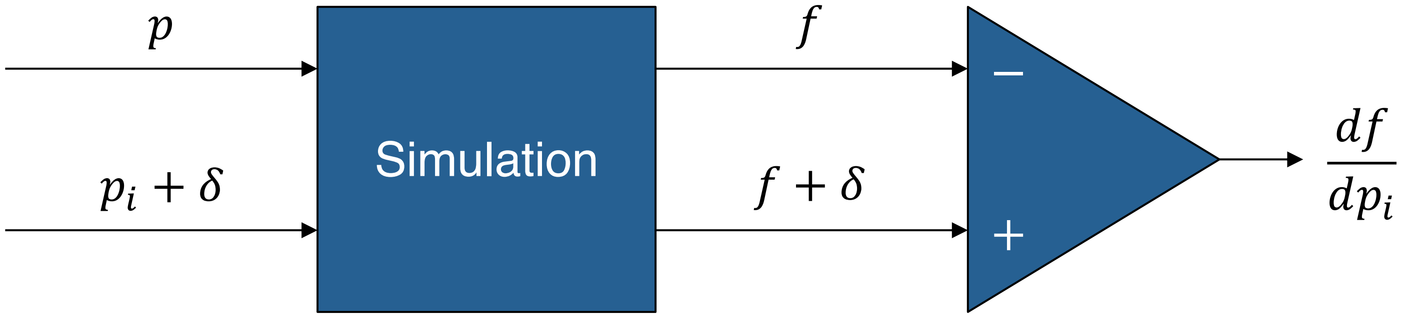
Sensitivity Analysis: Finite Difference



- Easy to implement
  - Only requires function evaluations
- Inefficient for large numbers of optimization variables
- Step-size dilemma – truncation error vs. subtractive cancellation

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Sensitivity Analysis: Discrete Adjoint Method

- Recall the first-order optimality conditions for PDE-constrained optimization

$$
\begin{aligned}
\nabla_p \mathcal{L} &= \frac{\partial f}{\partial p} + \lambda^T \frac{\partial R}{\partial p} &= 0 \quad (1)\\
\nabla_u \mathcal{L} &= \frac{\partial f}{\partial u} + \lambda^T \frac{\partial R}{\partial u} &= 0 \quad (2)\\
\nabla_\lambda \mathcal{L} &= R(u, p) &= 0 \quad (3)
\end{aligned}
$$

- Reduced-space formulation solves equations (2) and (3) fully at each optimization iteration and substitutes into equation (1)

Sensitivity Analysis: Discrete Adjoint Method

1. **State/PDE Solution:**

   Solve $R(p,u) = 0$ for u at new p

2. **Adjoint Solution:**

   Solve $\left(\frac{\partial R}{\partial u}\right)^T \lambda = -\frac{\partial f}{\partial u}$ for λ at new p and $\mathrm{u}(p)$

3. **Gradient Assembly:**

   Compute $\mathrm{G} = \nabla_p f = \frac{\partial f}{\partial p} + \lambda^T \frac{\partial R}{\partial p}$

Sensitivity Analysis: Discrete Adjoint Method

1. **State/PDE Solution:**

   Solve $R(p,u) = 0$ for u at new p ⟵ Solve $\nabla_\lambda \mathcal{L} = 0$ (eqn. 3)

2. **Adjoint Solution:**

   Solve $\left(\frac{\partial R}{\partial u}\right)^T \lambda = -\frac{\partial f}{\partial u}$ for λ at new p and $\mathrm{u}(p)$ ⟵ Solve $\nabla_u \mathcal{L} = 0$ (eqn. 2)

3. **Gradient Assembly:**

   Compute $\mathrm{G} = \nabla_p f = \frac{\partial f}{\partial p} + \lambda^T \frac{\partial R}{\partial p}$ ⟵ Evaluate $\nabla_p \mathcal{L}$ (eqn. 1)

Sensitivity Analysis: Discrete Adjoint Method

- Computational cost is independent of the number of optimization variables
  - One linear system solution for each scalar function

- Requires transpose operators for the PDE Jacobians (w.r.t. both state and optimization variables)

- PETSc/TS (Time Steppers) package implements checkpointing for backwards-in-time adjoint solutions
  - Not covered in this tutorial

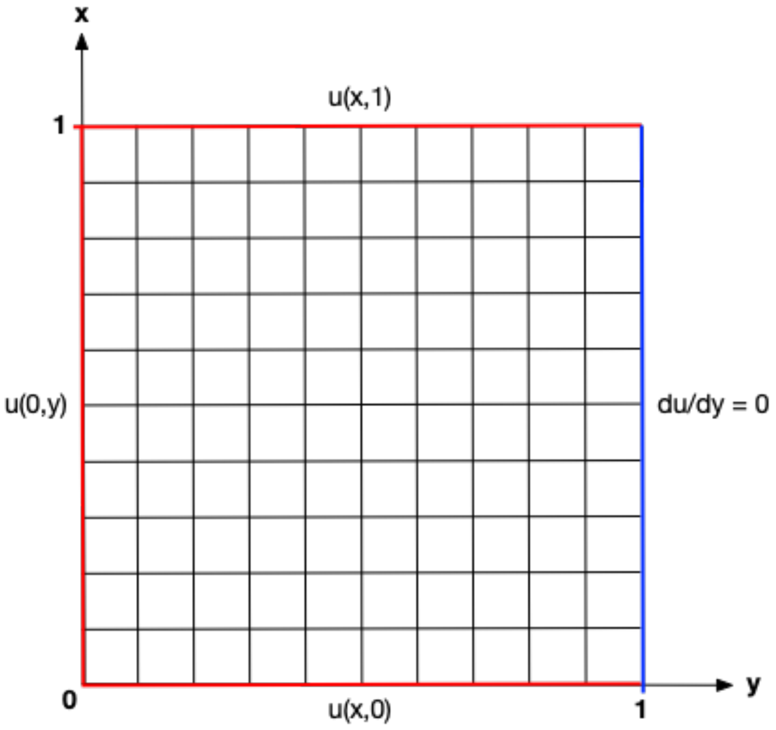
Hands-on Example: Boundary Control w/ 2D Laplace Eqn

$$\underset{p}{\text{minimize}} \quad \frac{1}{2}\int_0^1 (u(1,y) - u_{target})^2 dy$$

$$\text{governed by} \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \quad \forall\, x, y \in (0,1)$$

$$\left.\frac{\partial u}{\partial x}\right|_{u(1,y)} = 0, \quad \forall\, y \in (0,1)$$

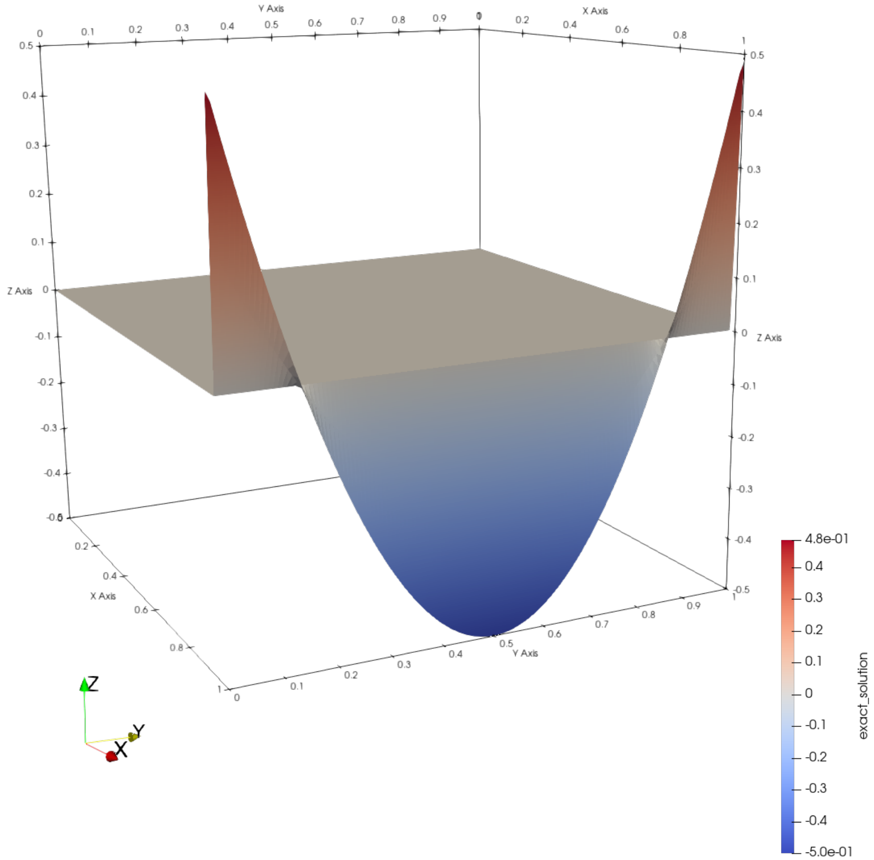
$$p = \begin{bmatrix} u(x,0) & u(x,1) & u(0,y) \end{bmatrix}^T$$



- Control left, top and bottom Dirichlet bounds to recover target solution at the right boundary

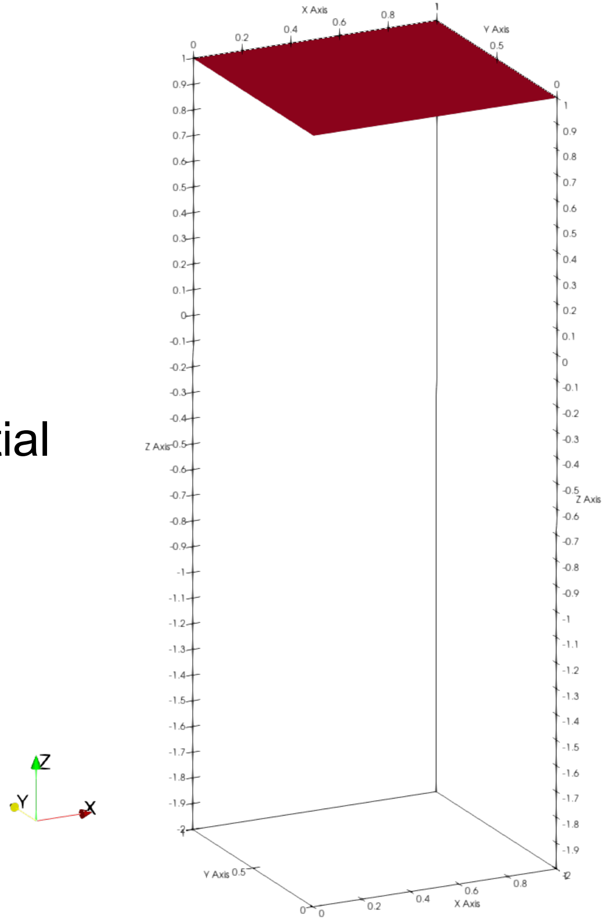
Hands-on Example: Boundary Control w/ 2D Laplace Eqn

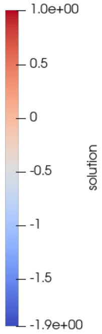
- PDE solution, objective function and gradient evaluations implemented with AMReX (https://amrex-codes.github.io/amrex/)
- Target solution set to $u_{target} = 4(y - 0.5)^2 - 0.5$
- Lapace equation is self-adjoint
  - PDE Jacobian is symmetric
- Command line options:
  - Problem size: `-nx 128`
  - Switch on finite difference gradient: `-fd`

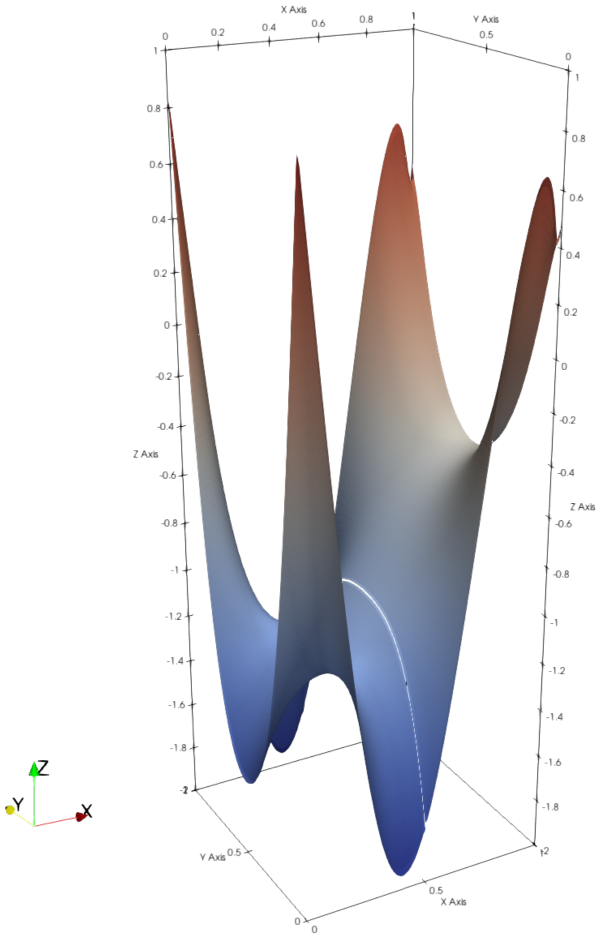


Hands-on Example: Boundary Control w/ 2D Laplace Eqn

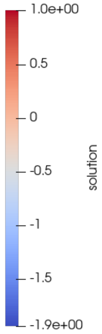
Initial







Final



Hands-on Example: Boundary Control w/ 2D Laplace Eqn

```
$ ./main2d.gnu.MPI.ex inputs -tao_monitor -tao_ls_type armijo -tao_fmin 1e-6 -tao_gatol 1e-12
```

```
AMReX (19.08) initialized
  0 TAO,  Function value: 0.00564792,  Residual: 4.57574e-08
  1 TAO,  Function value: 0.00564792,  Residual: 4.57574e-08
  2 TAO,  Function value: 0.000351831,  Residual: 6.72001e-09
  3 TAO,  Function value: 0.000104118,  Residual: 4.5399e-09
  4 TAO,  Function value: 4.39909e-06,  Residual: 5.62804e-10
  5 TAO,  Function value: 3.20011e-06,  Residual: 3.18434e-10
  6 TAO,  Function value: 2.90562e-06,  Residual: 3.67294e-10
  7 TAO,  Function value: 2.82687e-06,  Residual: 3.54986e-10
  8 TAO,  Function value: 2.74912e-06,  Residual: 3.45265e-10
  9 TAO,  Function value: 2.74912e-06,  Residual: 3.45265e-10
 10 TAO,  Function value: 2.5271e-06,  Residual: 1.99102e-10
 11 TAO,  Function value: 2.41122e-06,  Residual: 1.43435e-10
 12 TAO,  Function value: 2.10344e-06,  Residual: 8.34685e-11
 13 TAO,  Function value: 1.78759e-06,  Residual: 1.11393e-10
 14 TAO,  Function value: 1.30814e-06,  Residual: 8.4585e-11
 15 TAO,  Function value: 1.10837e-06,  Residual: 9.14759e-11
 16 TAO,  Function value: 1.08865e-06,  Residual: 9.52258e-11
 17 TAO,  Function value: 8.87623e-07,  Residual: 1.29118e-10
TaoSolve() duration: 1316289 microseconds
[The  Pinned Arena] space (MB) used spread across MPI: [8 ... 8]
AMReX (19.08) finalized
```

Hands-on Example: Boundary Control w/ 2D Laplace Eqn

- **Tutorial goals:**
  - Compare computational cost of finite difference gradient to the adjoint method
  - Verify that the cost of the adjoint method is (mostly) independent of the number of optimization variables
  - Solve the problem with different TAO algorithms
  - Interpret the TAO monitor output and assess convergence

Take Away Messages

- **PDE-constrained optimization does not need to be intimidating!**
  - PETSc/TAO provides interfaces and algorithms that work with reduced-space formulations
  - PETSc/TAO can compute gradients and Hessians automatically with finite differencing
  - PETSc data structures are easy to couple with most PDE solvers (e.g., AMReX)
- **The adjoint method is ideal for sensitivity analysis**
  - Some PDE solvers already have necessary building blocks
  - Possible to take implementation shortcuts in self-adjoint problems
- **PETSc/TAO offers parallel optimization algorithms for large-scale problems**
  - Optimization data structures are duplicated from user-generated PETSc vectors
  - User has full control over parallel distribution and vector type

Acknowledgements

AMReX: https://amrex-codes.github.io/amrex/

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

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