PETSc Adjoint Solvers for PDE-constrained Optimization

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PDEs, Optimization, and Eigenproblems with PETSc/TAO and SLEPc
Adjoints are key ingredients in PDE-constrained optimization

Research interests have been shifting beyond modelling and simulation of a physical system to outer-loop applications such as PDE-constrained optimization, optimal design and control, uncertainty quantification etc.

Solving optimization problems often requires to compute derivatives of a functional, which can be computed efficiently with adjoints.
What is PDE-constrained optimization?

Goal
Solve the discrete optimization problem

$$\minimize_{p, u} \mathcal{J}(u, p)$$

subject to

- $c(u, p, t) = 0$ (PDE constraint)
- $g(u, p) = 0$ (equality constraints)
- $h(u, p) \leq 0$ (inequality constraints)

where

- $\mathcal{J}$ is the objective functional
- $c$ represents the discretized PDE equation
- $u \in \mathbb{R}^n$ is the PDE solution state
- $p \in \mathbb{R}^m$ is the parameters

Because the dimension of $u$ can be really high, a reduced formulation is often used.

$$\mathcal{J}(p) = \mathcal{J}(u(p), p)$$
An example: data assimilation

The objective function of data assimilation is

\[
J(u(u_0), u_0^a) = \frac{1}{2} \| Qu - d \|^2 + \frac{\alpha}{2} \| L(u_0^a - u_0^b) \|^2
\]

- \( u \) is state variable
- \( d \) is data
- \( Q \) is observation operator
- \( L \) is cost functional for design
- \( \alpha \) is tradeoff between cost of design and fitting data

Physical interpretation: Determine the optimal initial conditions for a numerical model that minimizes the difference between the forecast and the observations

- A regularization term is often added to the cost functional to ensure existence and uniqueness
- Gradient-based optimization algorithms require local derivatives (sensitivities)
Computing sensitivities: finite differences

- Easy to implement
- Inefficient for many parameter case, due to one-at-a-time
- Possible to perturb multiple parameters simultaneously by using graph coloring
- Error depends on the perturbation value $\Delta p$
Computing sensitivities: automatic differentiation

- AD can evaluate the sensitivities for an arbitrary sequence of computer codes

- **Difficulties of low-level AD**
  - pointers
  - dynamic memory
  - directives
  - function calls from external libraries
  - iterative processes (e.g. Newton iteration)
  - non-smooth problems
Forward and adjoint sensitivity analysis (SA) approaches

We compute the gradients by differentiating the time stepping algorithm, e.g. backward Euler:

\[ y_{n+1} = y_n + h f(t_{n+1}, y_{n+1}) \]

**Forward SA**

\[
S_{\ell,n+1} = S_{\ell,n} + h f_y(t_{n+1}, y_{n+1}) S_{\ell,n+1}
\]

**Adjoint SA**

\[
\lambda_n = \lambda_{n+1} + h f_y(t_{n+1}, y_{n+1})^T \lambda_n
\]

<table>
<thead>
<tr>
<th></th>
<th>Forward</th>
<th>Adjoint</th>
</tr>
</thead>
<tbody>
<tr>
<td>Best to use when</td>
<td># of parameters &lt;&lt; # functionals</td>
<td># of parameters &gt;&gt; # of functionals</td>
</tr>
<tr>
<td>Complexity</td>
<td>( \mathcal{O} (# \text{ of parameters}) )</td>
<td>( \mathcal{O} (# \text{ of functionals}) )</td>
</tr>
<tr>
<td>Checkpointing</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Implementation</td>
<td>Medium</td>
<td>High</td>
</tr>
<tr>
<td>Accuracy</td>
<td>High</td>
<td>High</td>
</tr>
</tbody>
</table>
Interpretation of adjoint in a nutshell

Given a vector valued function \( y = F(x) \), the gradient of \( y \) with respect to \( x \) is a transposed Jacobian matrix (of the function \( F \)):

\[
J^T = \begin{pmatrix} 
\frac{\partial y_1}{\partial x_1} & \ldots & \frac{\partial y_m}{\partial x_1} \\
\vdots & \ddots & \vdots \\
\frac{\partial y_1}{\partial x_m} & \ldots & \frac{\partial y_m}{\partial x_m} 
\end{pmatrix}
\]

The adjoint solver is an engine for computing the transposed Jacobian-vector product. Given any vector \( v \), compute \( J^T \cdot v \). If \( v \) is the gradient of a scalar function \( l = g(y) \), that is \( v = \left( \frac{\partial l}{\partial y_1}, \ldots, \frac{\partial l}{\partial y_m} \right)^T \), then by the chain rule

\[
J^T \cdot v = \begin{pmatrix} 
\frac{\partial y_1}{\partial x_1} & \ldots & \frac{\partial y_m}{\partial x_1} \\
\vdots & \ddots & \vdots \\
\frac{\partial y_1}{\partial x_m} & \ldots & \frac{\partial y_m}{\partial x_m} 
\end{pmatrix}
\begin{pmatrix} 
\frac{\partial l}{\partial y_1} \\
\vdots \\
\frac{\partial l}{\partial y_m} 
\end{pmatrix}
= \begin{pmatrix} 
\frac{\partial l}{\partial x_1} \\
\vdots \\
\frac{\partial l}{\partial x_m} 
\end{pmatrix}
\]

Input
\( \begin{pmatrix} 
\frac{\partial l}{\partial y_1} \\
\vdots \\
\frac{\partial l}{\partial y_m} 
\end{pmatrix} \)

Output
\( \begin{pmatrix} 
\frac{\partial l}{\partial x_1} \\
\vdots \\
\frac{\partial l}{\partial x_m} 
\end{pmatrix} \)
Adjoint integration with PETSc

- PETSc: open-source numerical library for large-scale parallel computation
  [https://www.mcs.anl.gov/petsc/](https://www.mcs.anl.gov/petsc/)
  ~ 200,000 yearly downloads

- Portability
  - 32/64 bit, real/complex
  - single/double/quad precision
  - tightly/loosely coupled architectures
  - Unix, Linux, MacOS, Windows
  - C, C++, Fortran, Python, MATLAB
  - GPGPUs and support for threads

- Extensibility
  - ParMetis, SuperLU, SuperLU_Dist, MUMPS, HYPRE, UMFPACK, Sundials, Elemental, Scalapack, UMFPack...

- Toolkit
  - sequential and parallel vectors
  - sequential and parallel matrices (AIJ, BAIJ...)
  - iterative solvers and preconditioners
  - parallel nonlinear solvers
  - adaptive time stepping (ODE and DAE) solvers

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Full software stack

- Optimization
- Model equations
- Time stepping solves
- Nonlinear solves
- Linear solves
- Parallel Infrastructure (MPI, Vectors...)

New feature

Discrete Adjoint
Other software for adjoints and related functionality

Also available in:
- SUNDIALS
- Trilinos

This presentation focuses on experiences in PETSc.
TSAdjoint Interfaces are similar to TS interfaces

- Designed to reuse functionalities (implemented in PETSc or provided by users)
- Aim for general-purpose solutions
- Support both explicit and implicit methods and timestep adaptivity
- Allow multiple cost functionals

![Diagram of TS and TSAdjoint interfaces]

- **RHS Jacobian**
  - Input
  - TSSolve
  - TSTrajectorySet
  - TSEvent
  - TSSStep
  - TSMonitor
  - TSAAdapt
  - Solution

- **Jacobian w.r.t. parameters**
  - Input
  - TSAdjointSolve
  - TSAdjointEvent
  - TSAdjointStep
  - TSAdjointMonitor
  - Sensitivities
Optimal checkpointing for given storage allocation

- Minimize the number of recomputations and the number of reads/writes by using the **revolve** library of Griewank and Walther
  - **Revolve** is designed as a top-level controller for time stepping
  - TSTrajectory consults **revolve** about when to store/restore/recompute
- Incorporate a variety of single-level and two-level schemes for offline and online checkpointing
  - existing algorithms work great for RAM only checkpointing
  - optimal extension for RAM+disk

An optimal schedule given 3 allowable checkpoints in RAM:

- blue arrow: store a checkpoint
- red arrow: restore a checkpoint
- black arrow: a step
- circle: solution
Validating Jacobian and sensitivity is critical for optimization

- PETSc and TAO (optimization component in PETSc) can test hand-coded Jacobian and gradients against finite difference approximations on the fly

- **Jacobian test:** \(-\text{snes\_test\_jacobian}\)

<table>
<thead>
<tr>
<th>Norm of matrix ratio</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.83894e-08</td>
<td>1.08067e-05 (user-defined state)</td>
</tr>
<tr>
<td>3.36163e-08</td>
<td>1.31068e-05 (constant state -1.0)</td>
</tr>
<tr>
<td>3.33553e-08</td>
<td>1.3005e-05 (constant state 1.0)</td>
</tr>
</tbody>
</table>

- **Gradient test:** \(-\text{tao\_test\_gradient}\)

  - \(||fd|| = 0.16843, ||hc|| = 1.18456, \) angle cosine = \((fd'hc)/||fd||||hc|| = 0.987391\)
  - 2-norm \(||fd-hc||/\max(||hc||,||fd||) = 0.859896, difference ||fd-hc|| = 1.01859\)
  - max-norm \(||fd-hc||/\max(||hc||,||fd||) = 0.853218, difference ||fd-hc|| = 0.311475\)

- \(-\text{snes\_test\_jacobian\_view}\) and \(-\text{tao\_test\_gradient\_view}\) can show the differences element-wisely

- Nonlinear solve is not very sensitive to the accuracy of Jacobian, but adjoint solve needs accurate Jacobian
Solving dynamic constrained optimization

Set up TAO:
- Initial values for the variable vector
- Variable bounds for bounded optimization
- Objective function
- Gradient function
- Hessian matrix for Newton methods (optional)

Set up ODE solver and adjoint solver:
- ODE right-hand-side function and Jacobian
- Additional Jacobian w.r.t parameters if gradients to the parameters are desired.
- ODE Initial condition
- Terminal conditions (initial values for adjoint variables) for the adjoint variables
Example: an inverse initial value problem

\[ \begin{align*}
\text{minimize} & \quad \| U(t_f) - U^{ob}(t_f) \|_2 \\
\text{subject to} & \quad \frac{du}{dt} = D_1 \nabla^2 u - uv^2 + \gamma(1 - u) \\
& \quad \frac{dv}{dt} = D_2 \nabla^2 v + uv^2 - (\gamma + \kappa)v
\end{align*} \]

where \( U = [u; v] \) is the PDE solution vector, \( U_0 \) is the initial condition. The reaction and diffusion of two interacting species can produce spatial patterns over time.

Interpretation
Given the pattern at the final time, can we find the initial pattern?

Link to the hands-on example

Providing an objective function and gradient evaluation routine to TAO

```c
PetscErrorCode FormFunctionAndGradient(Tao tao, Vec P, PetscReal *f, Vec G, void *appctx)
{
  ...
  VecDuplicate(P, &SDiff)
  VecCopy(P, appctx->U);
  TSSGetDM(appctx->ts, &da);
  *f = 0;
  TSSolve(appctx->ts, appctx->U);
  PetscSNPrintf(filename, sizeof filename, "ex5opt.ob");
  PetscViewerBinaryOpen(PETSC_COMM_WORLD, filename, FILE_MODE_READ, &viewer);
  VecLoad(SDiff, viewer);
  PetscViewerDestroy(&viewer);
  VecAYPX(SDiff, -1., appctx->U);
  VecDot(SDiff, SDiff, &soberr);
  *f += soberr;
  TSGetCostGradients(appctx->ts, NULL, &lambda, NULL);
  VecSet(lambda[0], 0.0);
  InitializeLambda(da, lambda[0], appctx->U, appctx);
  TSAdjointSolve(appctx->ts);
  VecCopy(lambda[0], G);
  ...
}
```
Tips and advice

- Jacobian can be efficiently approximated using finite difference with coloring (-snes_fd_coloring); particularly convenient via DMDA
- Most of the difficulties stem from mistakes in the hand-coded Jacobian function; make sure to validate it carefully
- Use direct solvers such as SuperLU and MUMPS for best accuracy (but not scalability) of the gradients
- Use -tao_monitor -ts_monitor -ts_adjoint_monitor -snes_monitor -log_view for monitoring the solver behavior and profiling the performance
- -malloc_hbw allows us to do the computation using MCDRAM and checkpointing using DRAM on Intel’s Knights Landing processors (Argonne’s Theta, NERSC’s Cori)
- Check the user manual and the website for more information, and ask questions on the mailing lists
Takeaways

- PETSc and TAO help you rapidly develop parallel code for dynamic constrained optimization
- Adjoint as an enabling technology for optimization
- PETSc offers discrete adjoint solvers that take advantage of highly developed PETSc infrastructure: MPI, parallel vectors, domain decomposition, linear/nonlinear solvers
- Requires minimal user input, and reuses information provided for the forward simulation
- Advanced checkpointing, transparent to the user
- Validation for Jacobian and gradients using finite differences
Thank you!