Parametric Uncertainty Quantification in Nuclear Reactor Depletion Calculations: An Exercise in Computational Sciences

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Fred Howes Presentation
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Experiences and Learnings at DOE facilities

Knolls Atomic Power Laboratory (KAPL) – Summer 2008
- Go to graduate school
- Focus on “Computational Methods”

Sandia National Laboratory (CSRI) – Summer 2009
- Exposure to Applied Mathematics & Uncertainty Quantification

*Lawrence Livermore National Laboratory (Climate) – Summer 2010
- Statistics & Uncertainty Quantification
- Applications outside nuclear can also be interesting

*Argonne National Laboratory (MCS) – Summer 2011
- Zero-in on dissertation topic, light at end of tunnel
The DOE CESAR Exascale Co-Design Center

**Task:** Build and achieve scalability on exascale hardware for nuclear reactor calculations

- Hardware
- Software/Algorithms

Two physics of particular interest

1. Neutron transport
2. Fluid dynamics
I focused on scalable methods for uncertainty quantification (UQ) in neutron transport calculations.

Uncertainty quantification: estimate the sensitivity of and error in a design metric or quantity of interest (QOI)

- Sensitivity with respect to uncertain inputs and initial conditions
- Error due to discretization and inexact physics

The adjoint approach: efficient for computing UQ information in high-dimensional problems

- Multi-physics friendly approach: important for reactor calculations
- Error estimate is an original contribution to the NE community

CESAR hopes to leverage advancements in computing to achieve faster evaluation of licensing applications for nuclear power generating stations.

- The industry lags most others in commercial application of high-performance computing.
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Why higher-fidelity, and why uncertainty quantification?

1. Next-generation designs rely on complex processes for inherent safety and extended lifetimes.

2. Design certifications require quantified margins and confidence bounds.

For example: life extension via a careful balance of production and destruction of fuel:

- Highly localized variation requires fine-grained spatial resolution
- Miscalculation → early shutdown → ($$)
This research led to opportunities to explore and learn about many facets of computational science.

Physics
- Identify and formulate the problem to be solved
- Develop a mathematical description of the problem

Mathematics
- Formulate the adjoint problem
- Establish existence and uniqueness of solution for target problems

Computer Science
- Implement the mathematical formulation
- Focus on scalability to future architectures
Target Problem: Traveling Wave Reactor Benchmark

- 1D slab geometry
- 100 homogenous assemblies
- Prescribed power density
- Two prescribed shuffling patterns
- Each shuffle ejects two burnt assmb. and inserts two feed assmb.
- Eventually we reach an equilibrium cycle

Inward-Convergent:

Convergent-Divergent:
Example benchmark results – Neutron Flux & Fuel Burnup

Neutron Flux

Fuel Burnup

Equilibrium-cycle discharge burnup = 11.6%
Physics Model: The depletion equations model the coupling between the neutron flux and material density fields.

The depletion equations include:

- A material balance equation (Bateman equations):

\[
\frac{dN}{dt} = B(\psi, p)N
\]

- A neutron balance equation (Transport equation):

\[
\Omega \cdot \nabla \psi + \Sigma_t(N, p)\psi = S_S(N, \psi, p) + S_F(N, \psi, p) + S_0(p)
\]

The field variables are:

- \( N = N(r) \): the material densities, varying with space
- \( \psi = \psi(r, E, \Omega) \): the neutron flux, varying with space, angle, and energy
- \( p \): a vector of parameters (e.g. material properties)

This is a nonlinear system of differential-algebraic equations (DAEs).
Summary of Bateman Chain

Chosen actinide chain. **Red** lines indicate decay parent/children, **black** lines indicate reaction parent/children.
Our results are in the right ballpark (Fuel Burnup)

Equilibrium-cycle discharge burnup = 11.6%

Reference burnup profiles

PDT burnup profiles
Equilibrium cycle neutron reproduction factor
Our goal is to formulate a general Uncertainty Quantification formalism for multiphysics problems.

Remember: Uncertainty quantification means

- Sensitivity to uncertain parameters, \( \frac{dQ}{dp} \)
- Errors due to numerical discretization & inexact physics, \( \Delta Q \)

Our design problem with uncertainty quantification:

\[
\begin{align*}
\frac{dN}{dt} &= BN \\
\Omega \cdot \nabla \psi + \Sigma_t \psi &= S \\
N(t_0) &= N_0
\end{align*}
\]

\[\rightarrow\] compute QOI:

\[ Q = g(\psi, N, t) \]

estimate sensitivity:

\[ \frac{dQ}{dp} \]

estimate error:

\[ \Delta Q \equiv Q_{true} - Q_{predicted} \]

We target large systems, lots of p’s, and scalability on advanced architectures.
An adjoint approach is practical in the regime of lots of $p$’s and a few QOI’s.

Task: solve $A(p)x = b$ and compute: $Q = \langle g(x,p) \rangle$ and $\frac{dQ}{dp}$

- Operator $A$ has an adjoint operator $A^\dagger$ that satisfies $\langle x^\dagger, Ax \rangle = \langle x, A^\dagger x^\dagger \rangle$
- With some simple manipulations, we can show that if $A^\dagger x^\dagger = \frac{\partial g}{\partial x}$, then

$$\frac{dQ}{dp} = \frac{\partial \langle g \rangle}{\partial p} - \frac{\partial}{\partial p} \langle x^\dagger, Ax \rangle$$

Key Point: The cost to produce a full gradient

Via the adjoint approach:
1. 1 forward solve (invert $A$)
2. 1 adjoint solve (invert $A^\dagger$)
3. 1 inner product per $p$

Via brute-force finite difference:
1. $O(p)$ forward solves (inversions of $A$)
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We are focused on maintaining flexibility in our approach.

- Adjoint theory in NE tends to be overly-prescriptive.
- Our contribution is a layer of abstraction designed to provide flexibility in a multi-physics environment.
- We abstract to a general differential algebraic system:
  \[
  \begin{aligned}
  \left\{ \begin{array}{l}
  \frac{dN}{dt} - BN \\
  \Omega \cdot \nabla \psi + \Sigma_t \psi - S(\psi)
  \end{array} \right\} \equiv \left\{ \begin{array}{l}
  F^d(\dot{x}^d, x, p, t) \\
  F^a(x, p, t)
  \end{array} \right\} = 0
  \\
  N(t_0) = x^d(t_0) = x_0^d(p)
  \\
  t \in [t_0, t_f].
  \end{aligned}
  \]

- We also assume that any QOI can be written in the form
  \[
  Q = g(x(t_f), p, t_f) + \int_{t_0}^{t_f} R(x, p, t) dt.
  \]
The adjoint equations in terms of the abstract operators.

The equations for adjoint variable $\lambda$ are

$$
\begin{bmatrix} \lambda^d \\ 0 \end{bmatrix}' = \begin{bmatrix} (F_{x}^{d})^T & (F_{x}^{a})^T \\ (F_{x}^{d})^T & (F_{x}^{a})^T \end{bmatrix} \begin{bmatrix} \lambda^d \\ \lambda^a \end{bmatrix} - \begin{bmatrix} (R_{x}^{d})^T \\ (R_{x}^{a})^T \end{bmatrix}.
$$

Once we have $\lambda$, our sensitivity expression has the form

$$
d\frac{Q}{dp} = \lambda \chi_p \bigg|_{t=t_0} + \int_{t_0}^{t_f} \left\{ R_p - \lambda F_p \right\} dt.
$$

NOTE: We need access to forward solution in order to solve for $\lambda$.

This gives us the sensitivity part of our UQ task. Sensitivities are used for

- Calibration – finding the “true” value of uncertain inputs
- Optimization – finding the “best” value of design parameters
- Experimental design – isolating “important” variables
We now turn to quantification of error due to discretization.

Truncation error is unavoidable in numerical calculations. As a result, any predicted QOI will have some error: we want to estimate this.

Consider the exact and discrete systems and their QOIs:

\[
\begin{align*}
F(\dot{x}, x, p, t) &= 0 \\
\tilde{F}(\dot{\tilde{x}}, \tilde{x}, p, t) &= r_1(t) \\
\{ Q &= g(x(t_f), p, t_f) \quad \tilde{Q} = g(\tilde{x}(t_f), p, t_f) \} 
\end{align*}
\]

\[\Delta Q = Q - \tilde{Q} = ?\]

Here, \( r_1 \) is a local residual. It is the error made by solving the discrete system instead of the continuous system.

The residual is difficult to estimate.

- For truncation in time, we use embedded Runge-Kutta schemes.
- For space, we have error bounds from the finite-element community.
- Truncation in angle and energy is much less obvious... we didn’t address these estimates
We have shown that the same adjoint variable can be used to estimate discretization error.

We develop the estimate by linearizing $F$ about $\tilde{F}$ to write an equation that is satisfied by the solution error, $e \equiv x - \tilde{x}$:

\[
F - \tilde{F} = -r_1(t) \\
= \tilde{F}_x \dot{e} + \tilde{F}_x e + O(\|e^2\|) \\
\rightarrow \tilde{F}_x \dot{e} + \tilde{F}_x e = -r_1(t)
\]

Similarly, we linearize the exact QOI about the discrete QOI and subtract:

\[
\Delta Q = Q - \tilde{Q} = g_x(t_f) e(t_f) + O(\|e^2\|)
\]

A crucial point:

- If we knew $e(t_f)$, we'd know $\Delta Q$! Of course we don't know this.
- But, the adjoint system corresponding to the error equation:

\[
\dot{\lambda}^T \tilde{F}_x = \lambda^T \tilde{F}_x
\]

is exactly the adjoint system developed in the previous section!
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is exactly the adjoint system developed in the previous section!
The adjoint-based error estimate is an original contribution to the nuclear engineering community.

This is crucial because basic ODE theory gives an expression for \( e(t_f) \) in terms of \( \lambda \).

- The QOI error estimate has the form of
  \[
  \Delta Q = \int_{t_0}^{t_f} \lambda \left[ F_{xa}^d \left[ F_{xa}^a \right]^{-1} r_1^a(s) - r_1^d(s) \right] ds
  \]
  where \( r_1^d \) and \( r_1^a \) are the differential and algebraic portions of the residual, respectively.

- We are already solving for \( \lambda \) to compute sensitivities, so this estimate comes at the cost of just one extra integration!

Discretization error estimates can

1. Help determine if and where refinement is needed
2. Identify physics approximations that are driving inaccuracy
Finally, we needed some mathematics to prove that our adjoint system has a unique solution.

The concern:

- In one formulation, the neutron transport equation is an eigenvalue problem: \( H\psi - \lambda G\psi = 0 \).
- The adjoint equation has a non-zero RHS: \( H^\dagger \psi^\dagger - \lambda G^\dagger \psi^\dagger = S^\dagger \).
- It is straightforward to show there is a solution \( \nu^\dagger \) that satisfies \( H^\dagger \nu^\dagger - \lambda G^\dagger \nu^\dagger = 0 \).
- Thus, the solution \( \psi^\dagger \) must not have any contribution from \( \nu^\dagger \), otherwise it will not be unique.

It turns out we need to satisfy each of these conditions in order to have a unique solution:

1. \( \langle \psi^\dagger, G\psi \rangle = 0 \) (comes naturally from adjoint prescription)
2. \( \langle S^\dagger, \psi \rangle = 0 \) (Fredholm alternative theorem, known result)
3. The QOI cannot depend on only the flux or its magnitude.
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Back to the Traveling Wave Problem: Say we are interested in the total reaction rate in Plutonium-239

Sensitivity measure = \( \frac{1}{Q} \rho \frac{dQ}{dp} \)
We can compare QOI perturbations to finite difference estimates as a verification exercise.
Recall that we need access to the forward solution at each stage during the adjoint solve.

Adjoint equations:

\[
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0
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\]

Sensitivity equation:

\[
\frac{dQ}{dp} = \lambda_{xp} \bigg|_{t=t_0} + \int_{t_0}^{t_f} \left\{ R_p - \lambda F_p \right\} dt.
\]

Anything in red might require access to $\psi$ and/or $N$ at each timestep.
The general checkpointing strategy

Overall Idea:

1) Progress through forward problem, checkpointing snapshots of forward solution at intervals
2) Enter adjoint mode
3) Recompute “chunks” of forward solution as required
Managing access to the forward solution is a very interesting challenge at large cpu counts and large unknown counts.

Using DOE's Sequoia as a model: 100k nodes with 16 cores/node and 16 GB RAM/node. A high-fidelity reactor problem might have (per node)

- (200 energy groups) \times (500 angles) \times (1000 spatial cells) \times (4 elements per cell (linear FEM))

That's 400M unknowns, or about 3.0GB per snapshot of \( \psi \) per node!

Idea: only store the converged source moments (right-hand-side) of the transport equation:

\[
\Omega \cdot \nabla \psi + \Sigma_t \psi = S(\psi)
\]

\[
\begin{align*}
\text{LHS: angle dependent} & \\
\text{RHS: angle integrated} & \quad \rightarrow \quad \text{Trade the cost of 1 sweep for reduced I/O}
\end{align*}
\]

Typically, the ratio of angles:moments is \( O(100) \).
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Solve time, sweep counts, and memory load for different checkpointing strategies (8cpus, 275k unk/cpu, 20 cycles).
This dissertation work afforded opportunities to explore multiple areas of computational science.

- We added a forward depletion algorithm to a massively parallel deterministic transport solver with proven scalability.
- We thought hard about formulation and implementation.
  - General formulation is multi-physics friendly, which is important for the CESAR center
  - The code produces results that are consistent with a fast reactor benchmark problem
  - Current work involves prediction and calibration of thermal scattering properties in Texas A&M’s research reactor.
- We demonstrated a method for checkpointing transport solutions on memory-limited architectures.
Remarks about the impact of the CSGF Program

1. The importance and value of the practicum experience (and the POS!)
   - Directly affected the quality and breadth of my research
   - Diversification accelerated project pace

2. Independence in direction of research

3. Passion and resources in the administration of the program
   - Participate with enthusiasm
   - Champion the program
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