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Error Estimation with Adjoints in Drekar: Applications to Fluid Flow and Magnetohydrodynamics Models

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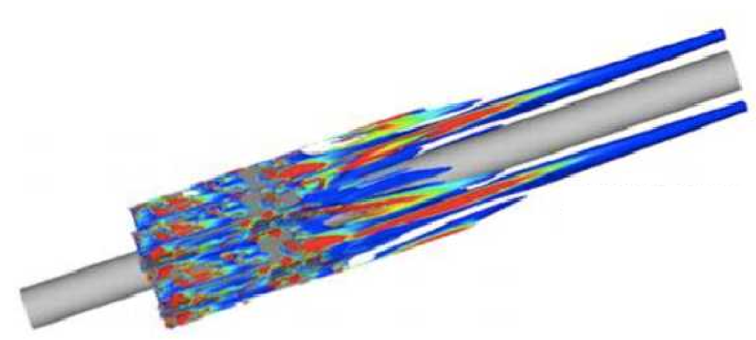
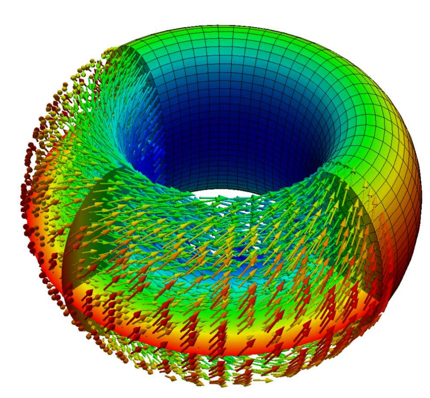
Problem

Multiphysics systems are critical to important DOE-mission science efforts (e.g. fluid-flow, transport/reaction, flow turbulence, magneto-hydrodynamics (MHD)).


Flow in Nuclear Reactor (Turbulent CFD)


Tokamak Equilibrium (MHD)

The path to predictive computational analysis and uncertainty quantification (UQ) for multiphysics has many open challenges:

- Uncertainties arise from: discretization errors, boundary and initial conditions, model parameters, and stochastic physical models.
- Extreme-scale computing required for accuracy of forward simulation.
- Analysis and design often focus on a set of quantities-of-interest (QoIs) rather than the partial differential equation (PDE) solution.
- The stability, error propagation and sensitivity characteristics for QoIs can be significantly different from the PDE solution itself.

Approach

We address these challenges using adjoint-based methods to accurately and efficiently compute numerical error estimates and to conduct sensitivity analysis for QoIs.

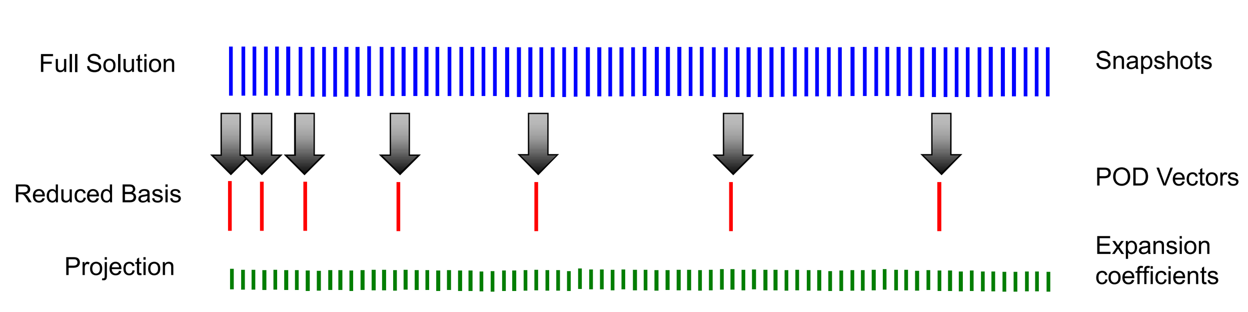
- These methods focus on specific QoIs (e.g. space/time averages of the solution or fluxes, current flow, total energy released, etc.)
- Adjoints provide local derivative/sensitivity information.

Forward Problem	Adjoint Problem
$\mathcal{L}(u) = f$	$\left(\mathcal{L}'(u)\right)^* \phi = \partial_u g$

Error Estimate: $g(u) - g(U) \approx (\phi, f - \mathcal{L}(U))$

QoI Derivative: $\partial_p g(U) = (\phi, \partial_p f - \partial_p \mathcal{L}(U))$

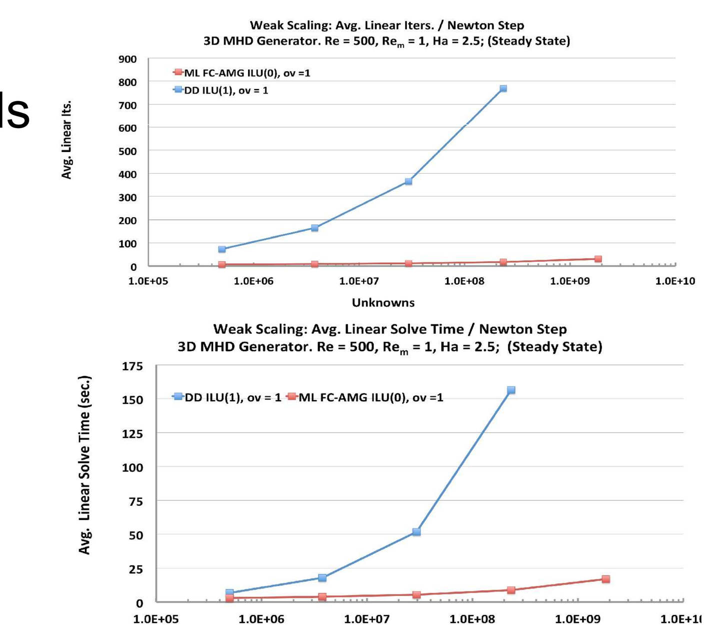
- There are practical limitations on the number of simulations (function evaluations) and adjoint-based methods allow greater utilization of each evaluation (e.g. building fast surrogate models).
- Transient problems require storage and backwards-in-time access of the full forward solution. We developed data compression techniques to help alleviate this burden.



Results

Drekar – A large-scale parallel implicit and steady-state CFD/MHD unstructured FE solver with adjoint capabilities

- 2D and 3D unstructured stabilized and mixed interpolation FE methods
- Robust and efficient Newton/Krylov iterative solvers
- Scalable approximate block factorization, physics-based, and AMG enabled preconditioners
- Built on Agile components concept utilizing many Trilinos packages



Initial Weak Scaling on Titan to 128K cores

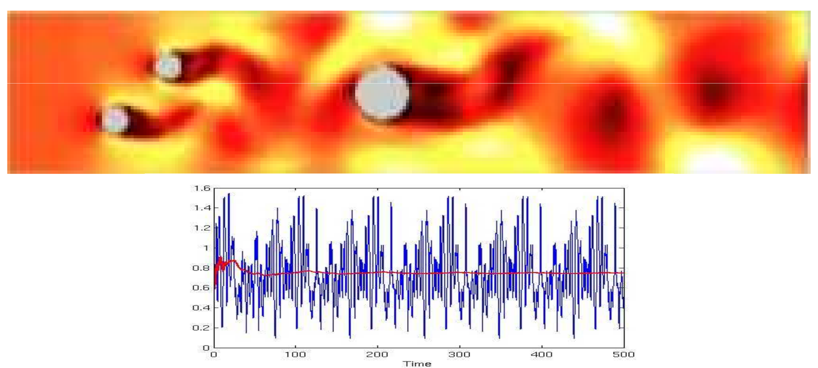
Fluid flow Examples

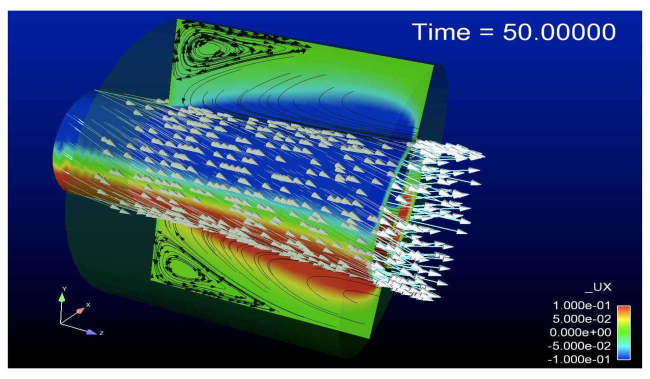
Transient Navier-Stokes

QoI: time avg point value Vx

QoI ~ 0.74565 – 0.10592;

Err. Est. = -14.2%





SA Steady RANS Turbulence Model

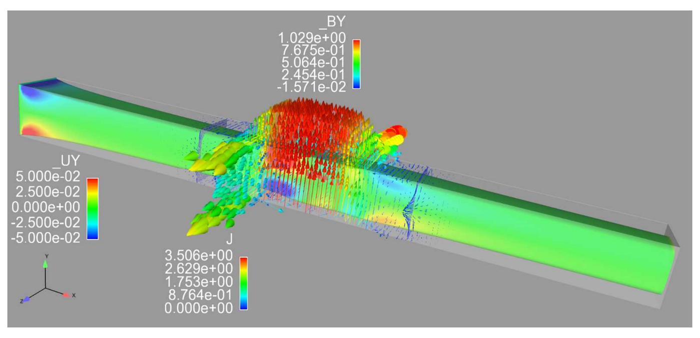
QoI: point value Vx

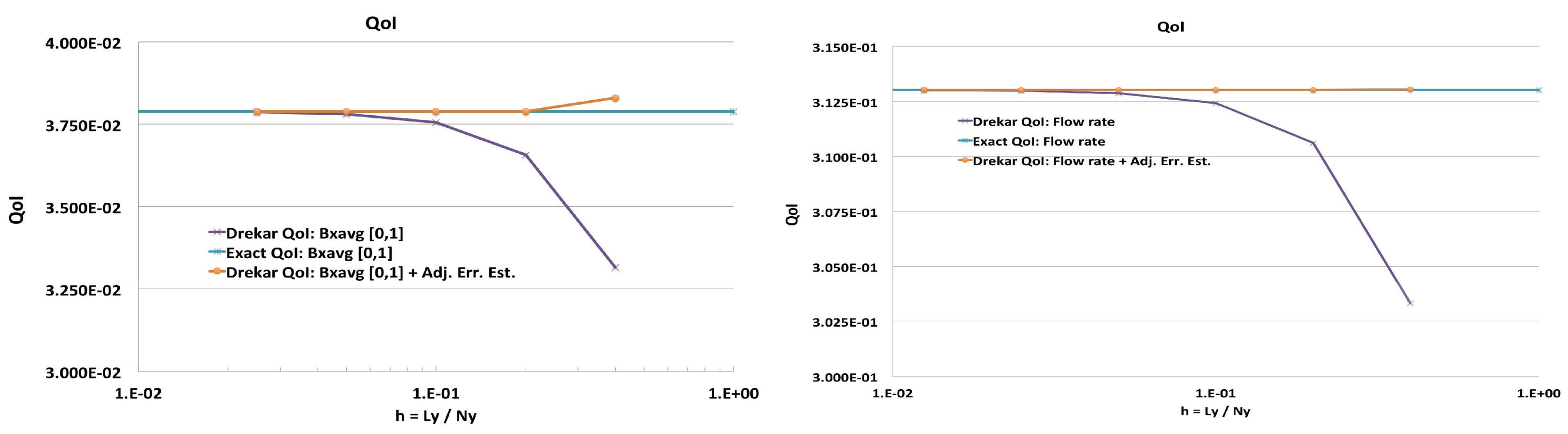
QoI ~ 1.96e-1 – 1.54e-4

Err. Est. = -.8%

Resistive MHD: 3D Generator

- QoI(1) Flow: Avg. Fluid velocity (**Vx**)
- QoI(2) Magnetics: Avg. of induced field in streamwise direction (**Bx**)
- Analytic asymptotic results shown (Hartmann problem)





Significance

This work demonstrates

- Adjoint-based methods can be used to provide accurate and efficient error estimates.
- A new unique large-scale parallel adjoint capability in Drekar.

These methods will play a critical role in developing future predictive computational analysis, inversion and optimization capabilities with UQ.

References

•Shadid, Pawlowski, et. al., "Towards a Scalable Fully-Implicit Fully-coupled Resistive MHD Formulation with Stabilized FE Methods", JCP, 229, 20, 7649 – 7671, 2010.
•Wildey, Cyr, Pawlowski, Shadid, Smith. *Adjoint Based a posteriori Error Estimation in Drekar::CFD*, October 2012, SAND2012-8910.
•Cyr, Shadid, Wildey, *Approaches for Adjoint-Based a Posteriori Analysis of Stabilized Finite Element Methods*, Submitted to SISC, 2012.
•Cyr, Shadid, Wildey, *Data Compression Techniques for Efficient Adjoint Computations*, in preparation.

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