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Utilizing Adjoint-Based Techniques to Effectively Perform UQ on Discontinuous Responses

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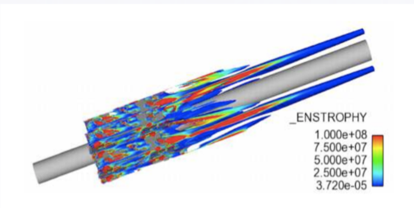
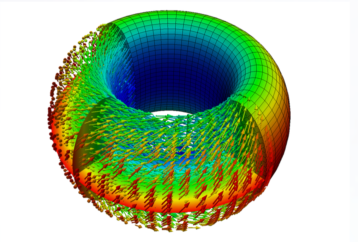
Motivation

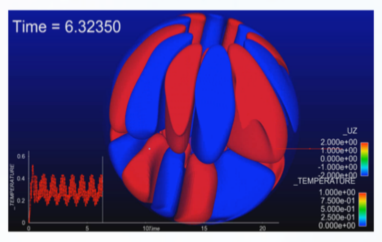
Trilinos Based, Adjoint Enabled, Multi-physics Simulator: Drekar



Flow in Nuclear Reactor (Turbulent CFD)

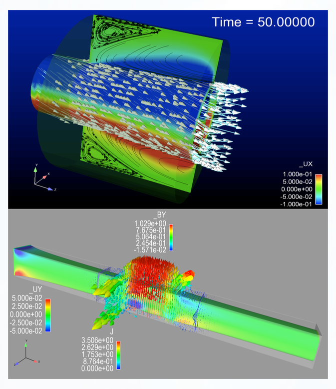


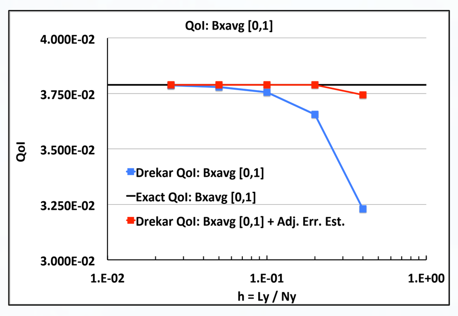
Tokamak Equilibrium (MHD)



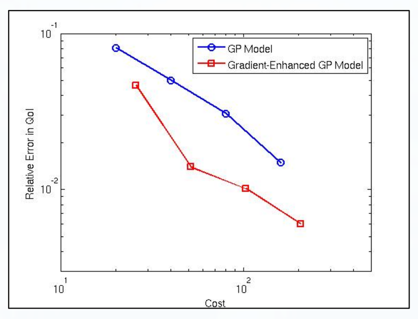
Geodynamo (MHD)

Excellent adjoint-based results for fully-implicit CFD and MHD:





Convergence of error estimate



Adjoint-enhanced UQ

Starting to investigate conservation laws with shocks

Can we compute adjoint-based error estimates?

Can we use adjoint information to enhance UQ?

Model Problem and Discretization

Consider the following system of conservation laws:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial}{\partial x}\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{0}, \quad \boldsymbol{u}(0) = \boldsymbol{u}_0.$$

Subject to appropriate boundary conditions

We focus on 1D for ease of notation, but everything carries over to 2D and 3D unless otherwise noted.

Partition the computation domain into a finite set of elements.

$$x_L = x_{1/2} < x_{3/2} < \cdots < x_{N+1/2} = x_R$$
$$E_i = \left[x_{i-1/2}, x_{i+1/2}\right], \quad 1 \le i \le N$$
$$\Delta x_i = x_{i+1/2} - x_{i-1/2}, \quad h = \max_i \Delta x_i.$$

Define a discontinuous finite element space:

$$V_h^k = \{v : v|_{E_i} \in P^k(E_i);\ 1 \le i \le N\}$$

Weak formulation:

$$\int_{E_i} \frac{\partial \boldsymbol{u}_h}{\partial t}\cdot \boldsymbol{v}\, dx - \int_{E_i} \boldsymbol{F}(\boldsymbol{u}_h)\cdot\frac{\partial \boldsymbol{v}}{\partial x}\, dx + \int_{\partial E_i} \hat{\boldsymbol{F}}(\boldsymbol{u}_h)\boldsymbol{n}\cdot \boldsymbol{v}\, dx = 0$$

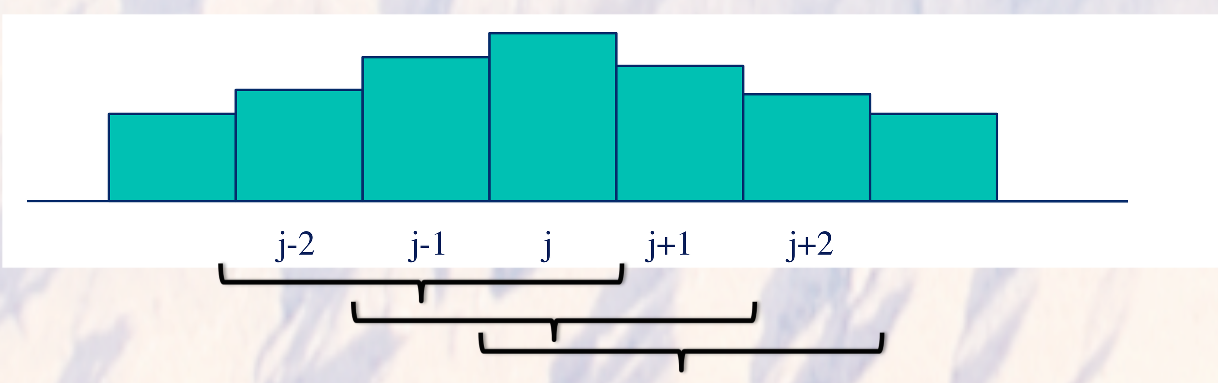
Compute finite volume (k=0) or discontinuous Galerkin approximation

All examples use Roe Riemann solver (HLLC gave similar results)

Higher-order DG requires slope limiting or artificial viscosity

All examples use explicit 2nd or 4th order Runga Kutta

Finite volume cases uses 5th order WENO to achieve high-order



Adjoint Based Error Estimates

Adjoint problem assuming continuous solutions:

$$-\frac{\partial \boldsymbol{\phi}}{\partial t} - \boldsymbol{J}^T \frac{\partial}{\partial x}\boldsymbol{\phi} = \boldsymbol{0}, \quad \boldsymbol{\phi}(T) = \psi. \quad \mathrm{J_{i,j}} = \frac{\partial \mathrm{F_i}}{\partial \mathrm{u_j}} \quad \psi = \frac{\partial \boldsymbol{G}(\boldsymbol{u})}{\partial \boldsymbol{u}}$$

Error representation:

$$\boldsymbol{G}(\boldsymbol{u}) - \boldsymbol{G}(\boldsymbol{u}_h) \approx \sum_i \int_{E_i} (\boldsymbol{u}_0 - \boldsymbol{u}_h(x,0))\cdot \boldsymbol{\phi}(x,0)\, dx - \sum_i \int_{E_i}\left(\frac{\partial \boldsymbol{u}_h}{\partial t}\cdot\boldsymbol{\phi} - \boldsymbol{F}(\boldsymbol{u}_h)\cdot\frac{\partial \boldsymbol{\phi}}{\partial x}\right) dx - \int_{\partial E_i} \boldsymbol{F}(\boldsymbol{u}_h)\boldsymbol{n}\cdot\boldsymbol{\phi}\, dx$$

For discontinuous solutions, the adjoint has an internal boundary condition at the shock:

$$\psi = \begin{cases} \frac{[G]}{[u]}, & \text{at the shock,} \\ \frac{\partial G}{\partial u}, & \text{elsewhere} \end{cases}$$

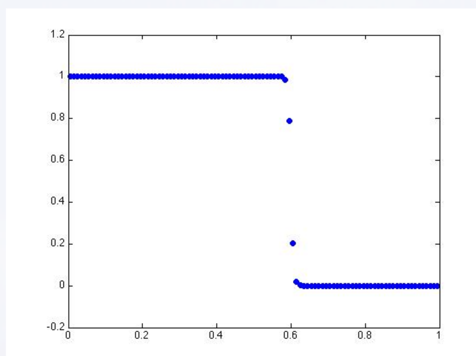
Requires precise knowledge of the location of the shock.

Recent work has shown that the discrete adjoint, *which does not have an interval BC*, converges to the continuous adjoint.

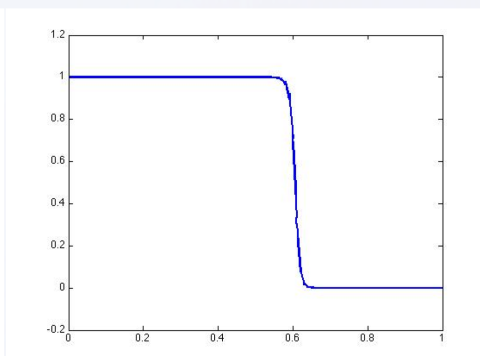
Can we discretize the continuous adjoint, *without the internal BC*, and obtain accurate error estimates and sensitivities?

Burgers equations with no viscosity:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right) = 0, \quad u_0 = \begin{cases} 1, & x \le 0.5 \\ 0, & x > 0.5 \end{cases}$$

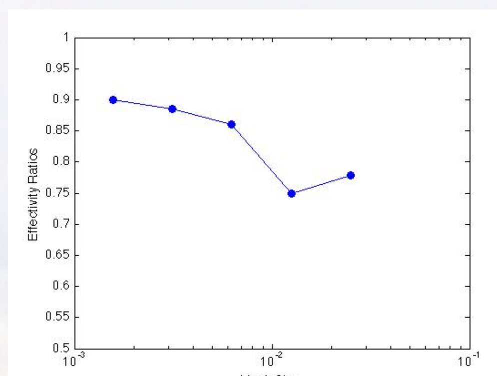


5th order WENO at T = 0.2 with 100 cells

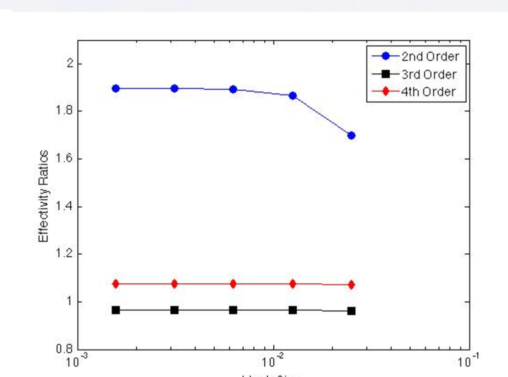


2nd order DG at T = 0.2 with 100 cells

Our quantity of interest is the average value of the solution over [0.5 0.65] at t = 0.3.



Effectivity for WENO

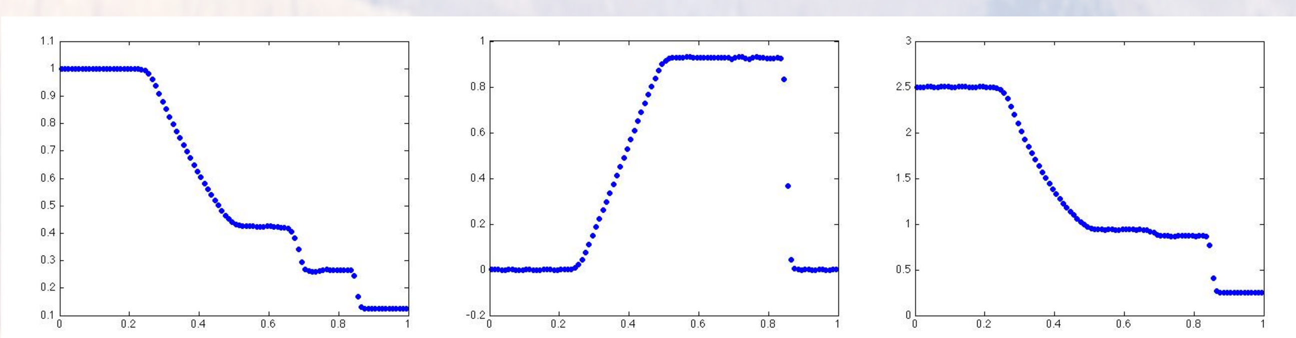


Effectivity for DG

Euler equations:

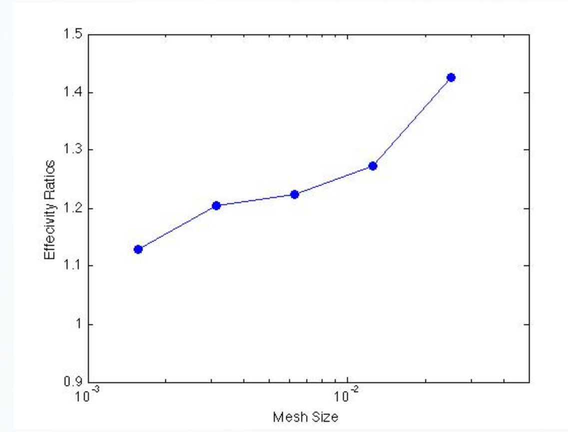
$$\boldsymbol{u} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} \quad \boldsymbol{F}(\boldsymbol{u}) = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ (E+p)u \end{bmatrix} \quad p = (\gamma - 1)(E - \frac{1}{2}\rho u^2), \quad \gamma = 1.4$$

Sod shock tube: $\rho = \begin{cases} 1, & x \le 0.5 \\ 1/8, & x > 0.5 \end{cases}, \quad \rho u = 0, \quad E = \begin{cases} 2.5, & x \le 0.5, \\ 0.25, & x > 0.5 \end{cases}$

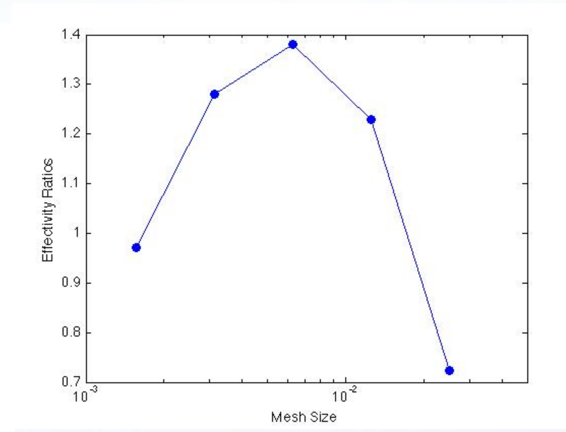


5th order WENO approximations using 100 cells. Density (left), velocity (middle), energy (right).

Quantity of interest is the average density over [0.85, 1] at t = 0.2

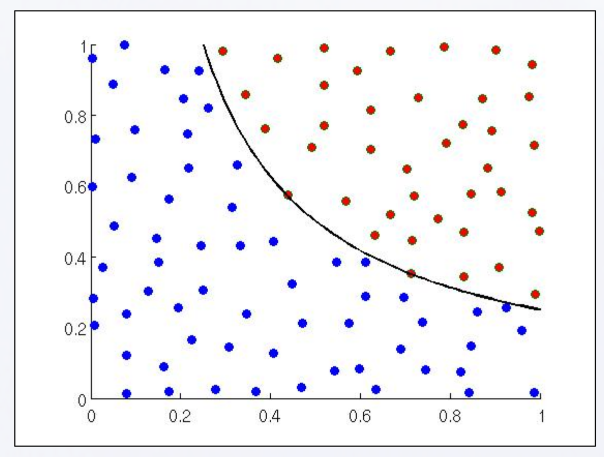


Effectivity for WENO



Effectivity for DG

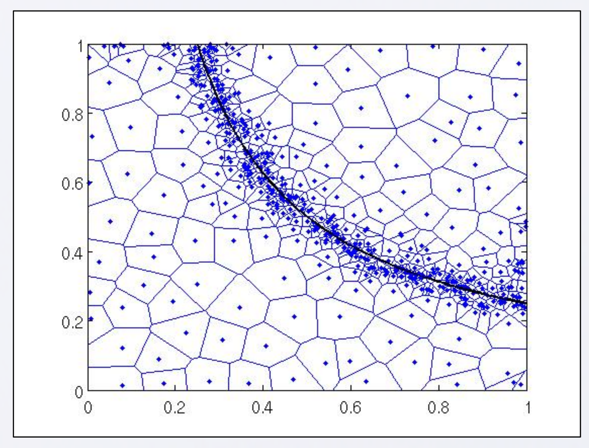
Adjoint Enabled UQ



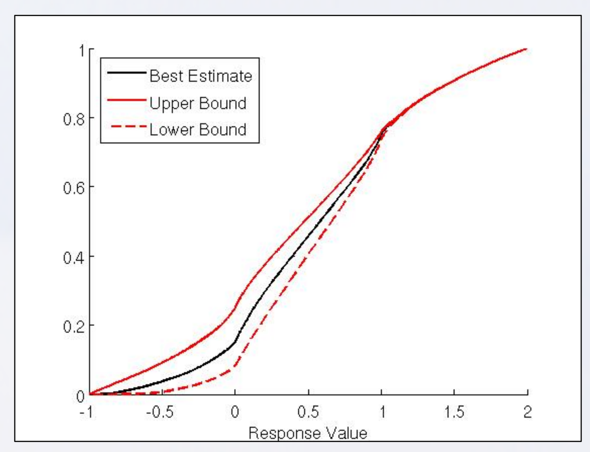
- Quantities of interest may have discontinuities
- Developed adjoint-enhanced discontinuity detection
  - Uses both point values and gradients
  - Leverages ENO/WENO smoothness indicators

$$\beta = \sum_{j=1}^{3} \Delta x^{2j-1} \int_{s=x_1}^{s=x_2} \left(\frac{\partial^j}{\partial s^j} p(s)\right)^2 ds,$$

- Enables clustering of samples
- Gradient-enhanced surrogates on each cluster



- Adaptive resolution of discontinuity is straightforward
  - Standard approach in literature
  - Typically very expensive
  - May not even be necessary depending on the QoI.



- We view the location of the discontinuity as an epistemic uncertainty
- We solve a discrete optimization problem to provide **robust bounds on probabilistic quantities given our lack of knowledge regarding the precise location of the discontinuity.**

Conclusions

- Adjoints provide additional information that may be used in optimization, error estimation, and/or uncertainty quantification.
- Defining an adjoint for problems for discontinuous solutions can be challenging.
- High-order numerical approximations can be used to approximate the continuous adjoint.
- Quantities of interest may be discontinuous
- We can account for the epistemic uncertainty regarding the location of the discontinuity.

References

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