Error and Uncertainty Quantification in the Numerical Simulation of Complex Fluid Flows

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The growth in computer hardware performance and capacity has enabled large scale computations of complex physical models.

These calculations raise several questions:

- How accurate is the simulation?
- Can predictions be trusted?
- Can differences between computation and experiment be rigorously reconciled?
Overview

- The main topic of discussion is error representation and error control of functional outputs via dual problems (Erickson et. al., 1995), (Becker and Rannacher, 1997).

- Particular attention is given to the time-dependent calculation of the compressible Navier-Stokes flow. Specifically, we examine the backwards-in-time dual problem and issues associated with
  - the deterioration (blowup) of dual problems with increasing Reynolds number,
  - the loss of sharpness in error bounds over long time integrations.

- In the remainder of the presentation, we briefly examine a novel uncertainty quantification technique proposed by Estep and Neckels (2006) for the quantification of uncertain functional outputs given aleatoric (statistical) random variable inputs.

- Surprisingly, the dual problems in the Estep and Neckels technique are identical to those arising in a posteriori error estimation (!!) but now the dual problem is used to construct a piecewise linear approximation of the random variable response surface.
Motivating Computational Challenge #1: Cylinder Flow

Cylinder flow at Mach = 0.10, logarithm of |vorticity| contours

- Quartic space-time elements
- 25K element mesh
- Viscous walls only imposed on cylinder surface
- Reynolds number based on cylinder diameter

**Question:** How is the ability to estimate and control numerical error effected by increasing Reynolds number?
Nonlinear Conservation Law Systems

Conservation law system in $\mathbb{R}^{d \times 1}$

$$u_t + \text{div} \, f = 0, \quad u, f_i \in \mathbb{R}^m \quad i = 1, \ldots, d$$

Convex entropy extension

$$U_t + \text{div} \, F \leq 0, \quad U, F_i \in \mathbb{R}$$
Space-Time Discontinuous Galerkin Formulation

Piecewise polynomial approximation space:

\[ \mathcal{V}^h = \left\{ \mathbf{v}_h \mid \mathbf{v}_h|_{K \times I^n} \in \left( \mathcal{P}_k(K \times I^n) \right)^m \right\} \]

Find \( \mathbf{v}_h \in \mathcal{V}^h \) such that for all \( \mathbf{w}_h \in \mathcal{V}^h \)

\[ B(\mathbf{v}_h, \mathbf{w}_h)_{DG} = \sum_{n=0}^{N-1} B^n(\mathbf{v}_h, \mathbf{w}_h)_{DG} = 0 , \]

\[ B^n(\mathbf{v}, \mathbf{w})_{DG} = \int_{I^n} \sum_{K \in \mathcal{T}} \int_K -(\mathbf{u}(\mathbf{v}) \cdot \mathbf{w}, t + f(\mathbf{v}) \cdot \mathbf{w}, x_i) \, dx \, dt \]

\[ + \int_{I^n} \sum_{K \in \mathcal{T}} \int_{\partial K} \mathbf{w}(x_\mp) \cdot \mathbf{h}(\mathbf{v}(x_\mp), \mathbf{v}(x_\pm); \mathbf{n}) \, ds \, dt \]

\[ + \int_{\Omega} \left( \mathbf{w}(t^n_{n+1}) \cdot \mathbf{u}(\mathbf{v}(t^n_{n+1})) - \mathbf{w}(t^n_{n-1}) \cdot \mathbf{u}(\mathbf{v}(t^n_{n-1})) \right) \, dx \]

- Proposed by Reed and Hill (1973), LeSaint and Raviart (1974) and further developed for conservation laws by Cockburn and Shu (1990)

- \( \mathbf{u} \) the conservation variables, \( \mathbf{v} \) the symmetrization variables

- \( \mathbf{h} \) a numerical flux function, \( \mathbf{h}(\mathbf{v}_-, \mathbf{v}_+; \mathbf{n}) = -\mathbf{h}(\mathbf{v}_+, \mathbf{v}_-; -\mathbf{n}), \mathbf{h}(\mathbf{v}, \mathbf{v}; \mathbf{n}) = f(\mathbf{v}) \cdot \mathbf{n} \)
The Discontinuous in Time Approximation Space

- Natural setting for the discontinuous Galerkin (DG) method for hyperbolic problems
- Utilized in the space continuous Galerkin least-squares method (Hughes and Shakib, 1988)
- Often used in the discretization of parabolic problems (Douglas and Dupont, 1976)
- Requires solving the implicit slab equations.

Discontinuous timeslab intervals

Space-time prism element
Theorem E: Global space-time entropy inequality (Cauchy IVP):

$$\int_{\Omega} U(u^*(t_0)) \, dx \leq \int_{\Omega} U(u(v_h(x, t^0))) \, dx \leq \int_{\Omega} U(u(v_h(x, t_0))) \, dx$$

$$u^*(t_0) = \frac{1}{\text{meas}(\Omega)} \int_{\Omega} u(v_h(x, t_0)) \, dx$$

whenever the numerical flux satisfies the system extension of Osher’s famous “E-flux” condition

$$[v]^{x+}_{x-} \cdot (h(v_-, v_+; n) - f(v(\theta)) \cdot n) \leq 0 \quad \forall \theta \in [0, 1] \quad v(\theta) = v_- + \theta[v]^+_1$$

Several flux functions satisfy this technical condition when recast in entropy variables, e.g. Lax-Friedrichs, HLLE, Roe with modifications, etc.
Nonlinear Stability of Space-Time DG Formulations

Suppose $\mathbf{u}, \mathbf{v}$ remains bounded in the sense

$$0 < c_0 \leq \frac{\mathbf{z} \cdot \mathbf{u}, \mathbf{v}(\mathbf{v}_h(x, t), \mathbf{z}}}{\|\mathbf{z}\|^2} \leq C_0, \quad \forall \mathbf{z} \neq 0$$

and Theorem E is satisfied for the Cauchy IVP, then following $L_2$ stability result is readily obtained

$L_2$ Stability:

$$\|\mathbf{u}(\mathbf{v}_h(\cdot, t^N) - \mathbf{u}^*(t^0)\|_{L_2(\Omega)} \leq (c_0^{-1} C_0)^{1/2} \|\mathbf{u}(\mathbf{v}_h(\cdot, t^0)) - \mathbf{u}^*(t^0)\|_{L_2(\Omega)}.$$
Space-Time Error Control

Given a system of PDEs with exact solution $u \in \mathbb{R}^m$ in a domain $\Omega$, the overall objective is to construct a locally adapted discretization with numerical solution $u_h$ that achieves

- Norm control [Babuska and Miller, 1984]
  \[ \|u - u_h\| < \text{tolerance} \]

- Functional output control [Erickson et. al. (1995), Becker and Rannacher, 1997]
  \[ |J(u) - J(u_h)| < \text{tolerance} , \quad J(u) : \mathbb{R}^m \mapsto \mathbb{R} \]

Example functional outputs:
- Time-averaged lift force, drag force, pitching moments
- Average flux rates through specified surfaces
- Weighted-average functionals of the form
  \[ J_\psi(u) = \int_{T_0}^{T_1} \int_{\Omega} \psi(x, t) \cdot N(u) dx \, dt \]
  for some user-specified weighting $\psi(x, t)$ and nonlinear function $N(u)$
Assume $\mathcal{B}(\cdot, \cdot)$ bilinear and $J(\cdot)$ linear.

**Primal Numerical Problem:** Find $u_h \in \mathcal{V}_h^B$ such that

$$B(u_h, w) = F(w) \quad \forall \ w \in \mathcal{V}_h^B.$$ 

**Auxiliary Dual Problem:** Find $\Phi \in \mathcal{V}^B$ such that

$$B(w, \Phi) = J(w) \quad \forall \ w \in \mathcal{V}^B.$$ 

\[
J(u) - J(u_h) = J(u - u_h) \\
= B(u - u_h, \Phi) \quad \text{(linearity of } J) \\
= B(u - u_h, \Phi - \pi_h \Phi) \quad \text{(dual problem)} \\
= B(u, \Phi - \pi_h \Phi) - B(u_h, \Phi - \pi_h \Phi) \quad \text{(Galerkin orthogonality)} \\
= F(\Phi - \pi_h \Phi) - B(u_h, \Phi - \pi_h \Phi) \quad \text{(linearity of } B) \\
= F(\Phi - \pi_h \Phi) - B(u_h, \Phi - \pi_h \Phi) \quad \text{(primal problem)}
\]

**Final error representation formula:**

$$J(u) - J(u_h) = F(\Phi - \pi_h \Phi) - B(u_h, \Phi - \pi_h \Phi)$$
Estimating $\Phi - \pi_h \Phi$:

Various techniques in use for estimating $\Phi - \pi_h \Phi$:

- Higher order solves [Becker and Rannacher, 1998], [B. and Larson, 1999], [Süli and Houston, 2002], [Houston and Hartman, 2002]

- Patch postprocessing techniques [Cockburn, Luskin, Shu, and Süli, 2003]

- Extrapolation from coarse grids
Mean-value linearized forms:

\[ B(u, v) = B(u_h, v) + \overline{B}(u - u_h, v) \quad \forall \ v \in V^B \]

\[ J(u) = J(u_h) + \overline{J}(u - u_h), \]

Example: \( B(u, v) = (L(u), v) \) with \( L(u) \) differentiable

\[ L(u_B) - L(u_A) = \int_{u_A}^{u_B} \frac{dL}{du} du = \int_{u_A}^{u_B} \frac{dL}{du} dL \cdot \frac{d\tilde{u}(\theta)}{d\theta} \cdot (u_B - u_A) = \overline{L}_u \cdot (u_B - u_A) \]

with \( \tilde{u}(\theta) \equiv u_A + (u_B - u_A) \theta \).

\[ B(u, w) = B(u_h, w) + (\overline{L}_u \cdot (u - u_h) \cdot w) \]

\[ = B(u_h, w) + \overline{B}(u - u_h, w) \quad \forall \ v \in V^B \]
Error Representation: Nonlinear Case

Semilinear form $\mathcal{B}(\cdot, \cdot)$ and nonlinear $J(\cdot)$.

**Primal numerical problem:** Find $u_h \in \mathcal{V}_h^\mathcal{B}$ such that

$$
\mathcal{B}(u_h, w) = F(w) \quad \forall \ w \in \mathcal{V}_h^\mathcal{B}.
$$

**Linearized auxiliary dual problem:** Find $\phi \in \mathcal{V}_h^\mathcal{B}$ such that

$$
\overline{\mathcal{B}}(w, \phi) = \overline{J}(w) \quad \forall \ w \in \mathcal{V}_h^\mathcal{B}.
$$

$$
J(u) - J(u_h) = \overline{J}(u - u_h) \quad \text{(mean value } J) \\
= \overline{\mathcal{B}}(u - u_h, \phi) \quad \text{(dual problem)} \\
= \overline{\mathcal{B}}(u - u_h, \phi - \pi_h \phi) \quad \text{(Galerkin orthogonality)} \\
= \mathcal{B}(u, \phi - \pi_h \phi) - \mathcal{B}(u_h, \phi - \pi_h \phi) \quad \text{(mean value } \mathcal{B}) \\
= F(\phi - \pi_h \phi) - \mathcal{B}(u_h, \phi - \pi_h \phi), \quad \text{(primal problem)}
$$

**Final error representation formula:**

$$
J(u) - J(u_h) = F(\phi - \pi_h \phi) - \mathcal{B}(u_h, \phi - \pi_h \phi)
$$
Refinement Indicators

Space-time error representation formula

\[ B_{DG}(v_h, w) - F_{DG}(\Phi - \pi_h \Phi) = \sum_{n=0}^{N-1} \sum_{Q^n} B_{DG, Q^n}(v_h, \Phi - \pi_h \Phi) - F_{DG, Q^n}(\Phi - \pi_h \Phi) \]

Stopping Criteria:

\[ |J(u) - J(u_h)| = \left| \sum_{n=0}^{N-1} \sum_{Q^n} B_{DG, Q^n}(v_h, \Phi - \pi_h \Phi) - F_{DG, Q^n}(\Phi - \pi_h \Phi) \right| \]

Refinement/Coarsening Indicator:

\[ |J(u) - J(u_h)| \leq \sum_{n=0}^{N-1} \sum_{Q^n} \left| B_{DG, Q^n}(v_h, \Phi - \pi_h \Phi) - F_{DG, Q^n}(\Phi - \pi_h \Phi) \right| \]

Fixed fraction mesh adaptation:

- Refine a fixed fraction of element indicators, \( \eta_{Q^n} \), that are too large and coarsen a fixed fraction of element indications that are too small.
Example: A Scalar Time-Dependent PDE

Circular transport, $\lambda = (y, -x)$, of bump data

\[
\begin{align*}
    u_t + \lambda \cdot \nabla u &= 0, \\
    u(x, 0) &= \Psi(1/10; x - x_0), \\
    x &\in [-1, 1]^2 \\
    x_0 &= (7/10, 0, 0)
\end{align*}
\]

Convergence, $\| u - u_h \|_{L^2(\Omega \times [0, T])}$
Example: A Scalar Time-Dependent PDE

A functional is chosen that averages the solution data in the space-time ball of radius 1/10 located at $x_c = (1/2, 1/2, 1.05)$ in space-time:

$$J(u) = \int_0^{1.15} \int_\Omega \Psi(1/10; x - x_c) \ u \ dx \ dt$$

$$J(u) - J(u_h) = \sum_{n=N-1}^{0} \sum_K F_{DG,n}(\Phi - \pi_h \Phi) - B_{DG,n}(v_h, \Phi - \pi_h \Phi)$$

$$|J(u) - J(u_h)| \leq \sum_{n=N-1}^{0} \sum_K |F_{DG,n}(\Phi - \pi_h \Phi) - B_{DG,n}(v_h, \Phi - \pi_h \Phi)|$$
Example: Euler flow past multi-element airfoil geometry. $M = .1$, 5° AOA.

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Error reduction during mesh adaptivity
Adapted mesh (18000 elements)
Primal-Dual Problems in Fluid Mechanics

**Subsonic Euler flow**, \( M = 0.10 \), 5° AOA, Lift force functional.

![Primal Mach number](image1)
![Dual x-momentum](image2)
![Adapted Mesh](image3)

**Transonic Euler flow**, \( M = 0.85 \), 2° AOA, Lift force functional.

![Primal density](image4)
![Dual density](image5)
![Adapted Mesh](image6)
Software Implementation and extension to the Navier-Stokes Eqns

Space-Time FEM:

- DG extension to the compressible Navier-Stokes equations using the symmetric interior penalty method of Douglas and Dupont, 1976) as described in Hartmann and Houston (2006)
- Implements the discontinuous Galerkin discretization in entropy variables.
- Unconditionally stable for all time step sizes
- Solves both the primal numerical problem and the jacobian linearized dual problem arising in space-time error estimation.
- High-order accuracy demonstrated in both space and space-time.
Dual Problems for Time Dependent Problems

Computing dual (backwards in time) problems looks expensive in terms of both storage and computation

- Storage of the primal time slices for use in the locally linearized dual problem.
- Approximation of the infinite-dimensional dual problem for the backwards in time dual problem.

Tremendous simplification arising for periodic flow problems with period $P$ when phase-independent functionals are utilized, e.g. mean drag

- Functional independent of the startup transient
- Only a small number of periods of the primal problem need be stored or recreated.
Task: Represent and estimate the error in the mean drag force coefficient

- Solve the primal problem using linear space-time elements
- Construct a smooth phase invariant functional measuring the mean drag force coefficient
- Solve the dual (backwards in time) problem using quadratic space-time elements
- Calculate the estimated functional error and compare with a reference calculation using cubic elements
Mean Drag for Cylinder Flow

\[ J_{\text{drag}}(u) = \int_0^T \int_{\Gamma_{\text{wall}}} (\text{Force} \cdot \hat{t}_{\text{drag}}) \psi(t) \, dx \, dt \]

Example: Cylinder flow at Re=300

Dual problem, \( \phi(x - \text{mom}) \)

Dual defect, \( \phi(x - \text{mom}) - \pi_h \phi(x - \text{mom}) \).
Mean Drag Dual Problems at Re=300 and Re=1000

Dual problem at Re=300

Dual problem at Re=1000
Error representation buildup during the backward in time dual integration
Adapted mesh from element indicators averaged over a period $P$

Coarse mesh (12K elements) 2 level refined mesh (20K elements)
Cylinder flow at $\text{Re}=3900$ and $\text{Re}=10000$ using quartic ($p = 4$) space-time elements.

- Choosing measurement problems that are not genuinely stationary produces rapidly growing dual problems and dependency on the initial data.

Dual solution corresponds to the average drag force over 3 approximate “periods”.

$\text{Re}=3900$          $\text{Re}=10000$
Growth of drag functional dual solution $\Phi$ with increasing Reynolds number
A Closing Note on the Use of Dual Problems in Uncertainty Quantification

Developing a capability to numerically compute primal/dual problems for compressible Navier-Stokes is a major undertaking.

Can this capability be reused in uncertainty quantification?

Estep and Neckels (2006) observed that dual problems can be used to build a piecewise linear response surface for use in Monte Carlo (MC) and Quasi Monte Carlo (QMC) sampling of uncertain outputs when the output of interest is a functional.
Evaluation of Uncertain Output Functionals

Given a nonlinear PDE system with solution \( u \in \mathbb{R}^m \) depending on \( n \)-dimensional random vector, \( \omega \in \mathcal{P} \subset \mathbb{R}^n \)

\[
Lu(x; \omega) = f
\]

and output functional

\[
J(u; \omega) : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}
\]

calculate statistics of the functional such as expectation

\[
E[J] = \int_{\mathcal{P}} J(u; \omega) \text{pdf}(\omega) \, d\omega = \int_0^1 J(u; \omega(\mu)) \, d\mu
\]

and variance

\[
\]

using Monte Carlo (MC) or Quasi Monte Carlo (QMC) sampling.
Higher Order Parameter Sampling (HOPS), Estep and Neckels (2006)

1. Convert the statistics integration problem to uniform MC sampling on a unit hypercube.

2. Partition the unit hypercube into smaller hypercube subdomains with size determined from accuracy of the linearized sampling formula.

3. In each hypercube subdomain $C_i$ center, calculate the primal solution $u_i$ and adjoint solution $\phi_i$

$$\left( \frac{\partial L}{\partial u}(x, \omega_i) \right)^T \phi_i = \left( \frac{\partial J}{\partial u}(x, \omega_i) \right)^T \rightarrow \mathcal{B}(w, \phi_i; \omega_i) = \mathcal{J}(w; \omega_i)$$

and the reduced sensitivity gradients (cf. A. Jameson, 1988)

$$g_i^T = \frac{\partial J}{\partial \omega}(x, \omega_i) - \phi^T \frac{\partial L}{\partial \omega}(x, \omega_i)$$

4. Apply MC or QMC integration in each $C_i$ using the linearized sampling formula for fixed values of $J(u_i, \omega_i)$ and $g_i^T$

$$J(u, \omega) \approx J(u_i, \omega_i) + g_i^T (\omega - \omega_i)$$
Estep and Neckels then consider adaptive refinement to improve approximation properties of the HOPS surface.

Original HOPS surface

Adaptively refined HOPS surface
Estimating and controlling numerical error in time-dependent calculations is fraught with difficulties

- growth in backward-in-time dual problems,
- loss of sharpness in error bounds.

The calculation of dual problems is computationally demanding

- storage of primal time slices,
- higher order solves of dual problem

Error representation/estimation results presented today barely scratch the surface

- error control for general transient problems,
- dual problems in the presence of flow bifurcations.
Example: Euler flow past multi-element airfoil geometry. $M = .1, 5^\circ$ AOA.

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Error reduction during mesh adaptivity

Adapted mesh (18000 elements)
Example: Ringleb Flow

Schematic of Ringleb flow

Iso-Density contours

Discontinuous Galerkin
Circular transport, \( \lambda = (y, -x) \), of bump data

\[
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    x &\in [-1, 1]^2
\end{align*}
\]

\( x_0 = (7/10, 0, 0) \)

Primal numerical problem

Convergence, \( \| u - u_h \|_{L_2(\Omega \times [0, T])} \)