

Space-Time DG

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Example Dual Problems

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Periodic Cylinder Flow

Concluding Remarks

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

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Time Dependent Flow Problems

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Concluding Remarks 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?







Helicopter Aerodynamics³ Launch Vehicle Analysis² Abort Systems Analysis¹ ¹POC: S. Rogers, ²POC: G. Klopfer, ³POC: N. Chaderjian (NASA) $\Rightarrow e = e = e = e = e$



Overview

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Concluding Remarks

- 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 uncertaintly 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

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



- 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?

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Nonlinear Conservation Law Systems

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Concluding Remarks Conservation law system in $\mathbf{R}^{d \times 1}$

$$\mathbf{u}_{t}$$
 + div $\mathbf{f} = \mathbf{0}$, $\mathbf{u}, \mathbf{f}_{i} \in \mathbf{R}^{m}$ $i = 1, \dots, d$

Convex entropy extension

 $U_{t} + \operatorname{div} F \leq 0, \quad U, F_i \in \mathbf{R}$

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Space-Time Discontinuous Galerkin Formulation

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Concluding Remarks 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 $\mathbf{w}_h \in \mathcal{V}^h$

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

$$B^{n}(\mathbf{v}, \mathbf{w})_{\mathrm{DG}} = \int_{I^{n}_{K \in \mathcal{T}}} \int_{K} -(\mathbf{u}(\mathbf{v}) \cdot \mathbf{w}_{,t} + \mathbf{f}^{i}(\mathbf{v}) \cdot \mathbf{w}_{,x_{i}}) \, dx \, dt$$

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

+
$$\int_{\Omega} \left(\mathbf{w}(t_{-}^{n+1}) \cdot \mathbf{u}(\mathbf{v}(t_{-}^{n+1})) - \mathbf{w}(t_{+}^{n}) \cdot \mathbf{u}(\mathbf{v}(t_{-}^{n})) \right) \, dx$$

- Proposed by Reed and Hill (1973), LeSaint and Raviart (1974) and further developed for conservation laws by Cockburn and Shu (1990)
- u the conservation variables, v the symmetrization variables
- h a numerical flux function, $h(v_-,v_+;n)=-h(v_+,v_-;-n),$ $h(v,v;n)=f(v)\cdot n$

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The Discontinuous in Time Approximation Space

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Concluding Remarks

- 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.



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Concluding Remarks

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

$$\int_{\Omega} U(\mathbf{u}^*(t^0_-)) \, dx \leq \int_{\Omega} U(\mathbf{u}(\mathbf{v}_h(x, t^N_-))) \, dx \leq \int_{\Omega} U(\mathbf{u}(\mathbf{v}_h(x, t^0_-))) \, dx$$
$$\mathbf{u}^*(t^0_-) = \frac{1}{\max(\Omega)} \int_{\Omega} \mathbf{u}(\mathbf{v}_h(x, t^0_-)) \, dx$$

whenever the numerical flux satisfies the system extension of Osher's famous "E-flux" condition

$$\left| \begin{bmatrix} \mathbf{v} \end{bmatrix}_{x_{-}}^{x^{+}} \cdot \left(\mathbf{h}(\mathbf{v}_{-},\mathbf{v}_{+};\mathbf{n}) - \mathbf{f}(\mathbf{v}(\theta)) \cdot \mathbf{n} \right) \leq 0 \ , \ \forall \theta \in [0,1] \ , \mathbf{v}(\theta) = \mathbf{v}_{-} + \theta[\mathbf{v}]_{-}^{+} \right|$$

 Several flux functions satisfy this technical condition when recast in entropy variables, e.g. Lax-Friedrichs, HLLE, Roe with modifications, etc.



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Concluding Remarks Suppose **u**, **v** remains bounded in the sense

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

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

L₂ 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

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

Norm control [Babuska and Miller, 1984]

 $\|\mathbf{u} - \mathbf{u}_h\| < \text{tolerance}$

• Functional output control [Erickson et. al. (1995), Becker and Rannacher, 1997]

 $|J(\mathbf{u}) - J(\mathbf{u}_h)| < \text{tolerance} \ , \ \ J(\mathbf{u}) : \mathbf{R}^m \mapsto \mathbf{R}$

Example functional outputs:

- Time-averaged lift force, drag force, pitching moments
- Average flux rates through specified surfaces
- Weighted-average functionals of the form

$$J_{\Psi}(\mathbf{u}) = \int_{T_0}^{T_1} \int_{\Omega} \Psi(x, t) \cdot N(\mathbf{u}) dx dt$$

for some user-specified weighting $\Psi(x, t)$ and nonlinear function N(u)



Error Representation: Linear Case

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Concluding Remarks Assume $\mathcal{B}(\cdot, \cdot)$ bilinear and $J(\cdot)$ linear.

<u>Primal Numerical Problem</u>: Find $\mathbf{u}_h \in \mathcal{V}_h^{\mathrm{B}}$ such that

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

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

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

$$J(\mathbf{u}) - J(\mathbf{u}_h) = J(\mathbf{u} - \mathbf{u}_h)$$
 (linearity of J)

$$= B(\mathbf{u} - \mathbf{u}_h, \Phi)$$
 (dual problem)

$$= B(\mathbf{u} - \mathbf{u}_h, \Phi - \pi_h \Phi)$$
 (Galerkin orthogonality)

$$= B(\mathbf{u}, \Phi - \pi_h \Phi) - B(\mathbf{u}_h, \Phi - \pi_h \Phi)$$
 (linearity of B)

$$= F(\Phi - \pi_h \Phi) - B(\mathbf{u}_h, \Phi - \pi_h \Phi)$$
 (primal problem)

Final error representation formula:

 $J(\mathbf{u}) - J(\mathbf{u}_h) = F(\Phi - \pi_h \Phi) - B(\mathbf{u}_h, \Phi - \pi_h \Phi)$

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Estimating $\Phi - \pi_h \Phi$:

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Concluding Remarks 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 S uli, 2003]

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Extrapolation from coarse grids



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Concluding Remarks Mean-value linearized forms:

$$\begin{split} \mathcal{B}(\mathbf{u},\mathbf{v}) &= \mathcal{B}(\mathbf{u}_h,\mathbf{v}) + \overline{\mathcal{B}}(\mathbf{u}-\mathbf{u}_h,\mathbf{v}) \quad \forall \ \mathbf{v} \in \mathcal{V}^{\mathrm{B}} \\ J(\mathbf{u}) &= J(\mathbf{u}_h) + \overline{J}(\mathbf{u}-\mathbf{u}_h), \end{split}$$

Example: $\mathcal{B}(u, v) = (L(u), v)$ with L(u) differentiable

$$L(u_B) - L(u_A) = \int_{u_A}^{u_B} \frac{dL}{du} = \int_{u_A}^{u_B} \frac{dL}{du} du$$
$$= \int_0^1 \frac{dL}{du} (\tilde{u}(\theta)) d\theta \cdot (u_B - u_A) = \overline{L}_{,u} \cdot (u_B - u_A)$$

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

$$\begin{aligned} \mathcal{B}(\mathbf{u},\mathbf{w}) &= \mathcal{B}(\mathbf{u}_h,\mathbf{w}) + (\overline{L}_{,\mathbf{u}} \cdot (\mathbf{u} - \mathbf{u}_h),\mathbf{w}) \\ &= \mathcal{B}(\mathbf{u}_h,\mathbf{w}) + \overline{\mathcal{B}}(\mathbf{u} - \mathbf{u}_h,\mathbf{w}) \quad \forall \mathbf{v} \in \mathcal{V}^{\mathrm{B}} \end{aligned}$$



Error Representation: Nonlinear Case

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

Primal numerical problem: Find $\mathbf{u}_h \in \mathcal{V}_h^{\mathrm{B}}$ such that

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

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

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

$$J(\mathbf{u}) - J(\mathbf{u}_{h}) = \overline{J}(\mathbf{u} - \mathbf{u}_{h})$$
(mean value J)

$$= \overline{\mathcal{B}}(\mathbf{u} - \mathbf{u}_{h}, \Phi)$$
(dual problem)

$$= \overline{\mathcal{B}}(\mathbf{u} - \mathbf{u}_{h}, \Phi - \pi_{h}\Phi)$$
(Galerkin orthogonality)

$$= \mathcal{B}(\mathbf{u}, \Phi - \pi_{h}\Phi) - \mathcal{B}(\mathbf{u}_{h}, \Phi - \pi_{h}\Phi)$$
(mean value \mathcal{B})

$$= F(\Phi - \pi_{h}\Phi) - \mathcal{B}(\mathbf{u}_{h}, \Phi - \pi_{h}\Phi),$$
(primal problem)

Final error representation formula:

$$J(\mathbf{u}) - J(\mathbf{u}_h) = F(\Phi - \pi_h \Phi) - \mathcal{B}(\mathbf{u}_h, \Phi - \pi_h \Phi)$$

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Refinement Indicators

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Concluding Remarks Space-time error representation formula

$$B_{\mathrm{DG}}(\mathbf{v}_h, w) - F_{\mathrm{DG}}(\Phi - \pi_h \Phi) = \sum_{n=0}^{N-1} \sum_{Q^n} B_{\mathrm{DG},Q^n}(\mathbf{v}_h, \Phi - \pi_h \Phi) - F_{\mathrm{DG},Q^n}(\Phi - \pi_h \Phi)$$

Stopping Criteria:

$$|J(\mathbf{u}) - J(\mathbf{u}_h)| = \left| \sum_{n=0}^{N-1} \sum_{Q^n} B_{\mathrm{DG},Q^n}(\mathbf{v}_h, \Phi - \pi_h \Phi) - F_{\mathrm{DG},Q^n}(\Phi - \pi_h \Phi) \right|$$

Refinement/Coarsening Indicator:

$$|J(\mathbf{u}) - J(\mathbf{u}_h)| \leq \sum_{n=0}^{N-1} \sum_{Q^n} \underbrace{|B_{\mathrm{DG},Q^n}(\mathbf{v}_h, \Phi - \pi_h \Phi) - F_{\mathrm{DG},Q^n}(\Phi - \pi_h \Phi)|}_{\mathrm{refinement indicator},\eta_{Q^n}}$$

Fixed fraction mesh adaptation:

 Refine a fixed fraction of element indicators, η_{Qⁿ}, that are too large and coarsen a fixed fraction of element indications that are too small.

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Example: A Scalar Time-Dependent PDE

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



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

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P2 space-time elements P3 space-time elements

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Example: A Scalar Time-Dependent PDE

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Concluding Remarks 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

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

$$J(\mathbf{u}) - J(\mathbf{u}_h) = \sum_{n=N-1}^{0} \sum_{K} F_{\mathrm{DG},Q^n}(\Phi - \pi_h \Phi) - B_{\mathrm{DG},Q^n}(\mathbf{v}_h, \Phi - \pi_h \Phi)$$
$$|J(\mathbf{u}) - J(\mathbf{u}_h)| \le \sum_{n=N-1}^{0} \sum_{K} |F_{\mathrm{DG},Q^n}(\Phi - \pi_h \Phi) - B_{\mathrm{DG},Q^n}(\mathbf{v}_h, \Phi - \pi_h \Phi)$$



Dual defect, $\Phi - \pi \Phi$

Error estimate buildup

r
 bump function



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Example: Euler flow past multi-element airfoil geometry. $M = .1, 5^{\circ}$ AOA.

				equivalent uniform
lift coefficient	lift coefficient	refinement		refinement
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$5.156 \pm .147$	$5.156 \pm .346$	0	5000	5000
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$5.287 \pm .006$	$5.287 \pm .024$	2	18000	80000
$5.291\pm.002$	$5.291\pm.007$	3	27000	320000



Error reduction during mesh adaptivity



Adapted mesh (18000 elements)

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Primal-Dual Problems in Fluid Mechanics

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Subsonic Euler flow, $M = .10, 5^{\circ}$ AOA, Lift force functional.







Primal Mach number

Dual x-momentum

Adapted Mesh

Adapted Mesh

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Transonic Euler flow, M = .85, 2° AOA, Lift force functional.



Primal density

Dual density



Software Implementation and extension to the Navier-Stokes Eqns

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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.

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• High-order accuracy demonstrated in both space and space-time



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Concluding Remarks 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.

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



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
- Calculated the estimated functional error and compare with a reference calculation using cubic elements

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Mean Drag for Cylinder Flow

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$$J_{\rm drag}(u) = \int_0^T \int_{\Gamma_{\rm wall}} ({
m Force} \cdot \hat{t}_{
m drag}) \, \Psi(t) \, dx \, dt$$

Example: Cylinder flow at Re=300

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





Dual defect, $\phi^{(x-mom)} - \pi_h \phi^{(x-mom)}$.



Mean Drag Dual Problems at Re=300 and Re=1000

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Dual problem at Re=300

Dual problem at Re=1000

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Mean Drag for Cylinder Flow at Re=1000

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Error representation buildup during the backward in time dual integration





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Adapted mesh from element indicators averaged over a period P



Coarse mesh (12K elements)



2 level refined mesh (20K elements)



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Concluding Remarks Cylinder flow at Re=3900 and 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".





Re=10000

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Re=3900

Growth of Dual Problems

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Growth of drag functional dual solution Φ with increasing Reynolds number

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A Closing Note on the Use of Dual Problems in Uncertainty Quantification

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Concluding Remarks 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.



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Concluding Remarks Given a nonlinear PDE system with solution $\mathbf{u} \in \mathbf{R}^m$ depending on *n*-dimensional random vector, $\omega \in \mathcal{P} \subset \mathbf{R}^n$

 $L\mathbf{u}(x;\omega) = \mathbf{f}$

and output functional

$$J(\mathbf{u};\omega):\mathbf{R}^m\times\mathbf{R}^n\to\mathbf{R}$$

calculate statistics of the functional such as expectation

$$E[J] = \int_{\mathcal{P}} J(\mathbf{u}; \omega) \, \rho df(\omega) \, d\omega = \int_0^1 J(\mathbf{u}; \omega(\mu)) \, d\mu$$

and variance

$$V[J] = E[J^2] - E[J]^2$$

using Monte Carlo (MC) or Quasi Monte Carlo (QMC) sampling.



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Higher Order Parameter Sampling (HOPS), Estep and Neckels (2006)

- Onvert the statistics integration problem to uniform MC sampling on a unit hypercube.
- 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 ϕ_i

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

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

$$\mathbf{g}_i^{\mathsf{T}} = \frac{\partial J}{\partial \omega}(\mathbf{x}, \omega_i) - \phi^{\mathsf{T}} \frac{\partial L}{\partial \omega}(\mathbf{x}, \omega_i)$$

④ Apply MC or QMC integration in each C_i using the linearized sampling formula for *fixed* values of J(**u**_i, ω_i) and **g**_i^T

$$J(\mathbf{u},\omega)\approx J(\mathbf{u}_i,\omega_i)+\mathbf{g}_i^T(\omega-\omega_i)$$

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Adaptive HOPS Surface

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Concluding Remarks Estep and Neckels then consider adaptive refinement to improve approximation properties of the HOPS surface.

Original HOPS surface



Adaptively refined HOPS surface



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Concluding Remarks

- 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

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- error control for general transient problems,
- dual problems in the presence of flow bifurcations.



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Error reduction during mesh adaptivity



Adapted mesh (18000 elements)

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Example: Ringleb Flow

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Schematic of Ringleb flow

Iso-Density contours



Discontinuous Galerkin

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NASA

Example: A Scalar Time-Dependent PDE

Space-Time DG

Tim Barth

Introduction

Cylinder Flow

Nonlinear Conservation Laws

Space-time DG

Error Representation

Scalar transport

Example Dual Problems

Navier-Stokes Formulatio

Periodic Cylinder Flow

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



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