A Brief Overview of Uncertainty Quantification and Error Estimation in Numerical Simulation

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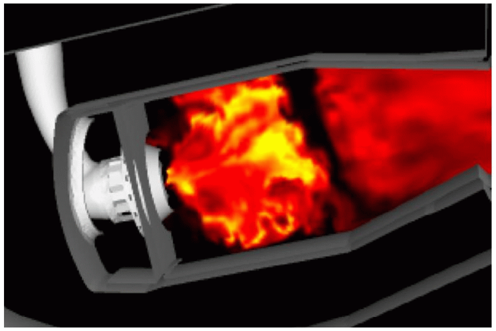
FAQs in Numerical Simulation

Example: Stanford ASC combustor calculation



- (Uncertainty) How accurately does a mathematical model describe the true physics and what is the impact of model uncertainty (structural or parametric) on outputs from the model?
- (Error Estimation) Given a mathematical model, how accurately is a specified output approximated by a given numerical method?
- (Reliability) Given a mathematical model and numerical method, can the error in numerical solutions and specified outputs be reliably estimated and controlled by adapting resources?

Uncertainty Quantification in Numerical Simulation

- Sources of uncertainty in numerical simulation.
- A simple Burger's equation example with 3 parametric sources of uncertainty.
- Mars atmospheric reentry with 130 input parametric sources of uncertainty.
- What can happen when sources of model uncertainty are not adequately understood.
- Some standard approaches to uncertainty quantification
- Uncertainty lectures
  - (Dr. Oberkampf) Uncertainty quantification using evidence theory.
  - (Prof. Ghanem) Error Budgets as a path from uncertainty to model validation.

Sources of Uncertainty in Simulation

Unfortunately, most numerical simulations of physical systems are rife with sources of uncertainty. Some examples include

- Geometrical uncertainty (Is the geometry exactly known?)
- Initial and boundary data uncertainty (Are initial/boundary conditions precisely known?)
- Structural uncertainty (Do the equations model the physics?)
  - Turbulence models
  - Combustion models
  - Number of moments in moment closure approximations
- Parametric uncertainty (How accurate are model parameters?)
  - Imperical equations of state and constitutive models
  - Reaction rates and relaxation times
  - Transport properties and catalycity

Uncertainty Quantification Approaches

Apply statistical techniques directly to simulations

- Monte Carlo simulation and variants
- Stratefied sampling
- Latin hypercube sampling
- Response surface method

Recast a mathematical model of a physical process as a stochastic PDE and solve using deterministic methods

- Perturbation expansion methods for random fields
- Stochastic operator expansions
- Polynomial Chaos methods (see Prof. Ghanem)

Simple Example: Burger's Equation

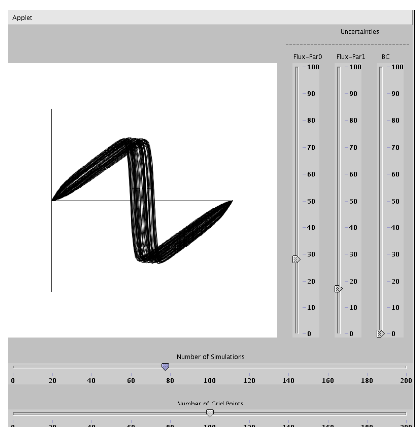
Example: Modified Burger's Equation

$$\begin{aligned} u_t + f(u)_x &= \nu\, u_{xx}, \quad (x,t) \in [0,1] \times \mathbf{R}_+ \\ u(x,0) &= sin(2\pi x) \end{aligned}$$

with 2-parameter flux

$$f(u) = c_0\, u + (1 + c_1)\, u^2/2 \ .$$

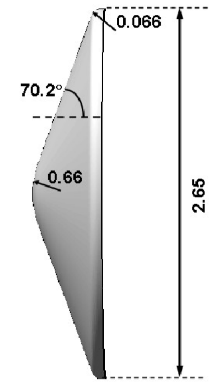
Applet: http://science.nas.nasa.gov/∼barth/stanford_workshop/PDE.hml



Example: Mars Atmospheric Entry

Example: Aerothermal CFD analysis of Mars atmospheric en

Uncertainty Analysis of Laminar Aeroheating Prediction for Mars Entries, Deepak Bose and Michael Wright (NASA Ames RC), AIAA Paper 2005-4682, 2005.



- Uncertainty analysis for peak forebody heating predicted using the DPLR CFD code
- 130 input parameters
- Monte Carlo sensitivity analysis used to "shortlist" important parameters
- Full Monte Carlo uncertainty analysis on shortlisted parameters
- Presentation courtesy of Michael Wright, Code TSA, NASA Ames.

Range Based Sensitivity Analysis

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Selected Input Parameters

Input category	Model	Parameter varied	No. of input parameters	Variability for sensitivity analysis
Dissociation reaction rates	$k = A_M T^{\eta} \exp(-D/T_a)$	A_M	40	1 order of magnitude
Exchange reaction rates	$k = A T^{\eta} \exp(-D/T_a)$	A	7	1 order of magnitude
Vibration-dissociation Coupling	$T_a = T^{\eta} T_V^{1-\eta}$	η	5	±0.15
V-T Relaxation time	Millikan and White	slope	40	±10%
Binary collision integral	$\Omega^{1,1}, \Omega^{2,2} = Af(T)$	A	36	±30%
Wall Catalysis		γ_{cat}, p_2	2	Entire range
		Total =	130	

Uncertainty Estimates

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Binary Collision Integrals :

Interaction	Uncertainty
CO_2–CO_2	20%
CO_2–CO	20%
CO_2–O	30%
CO–O	30%
CO–CO	20%
O–O	5%

Gaussian distribution

The uncertainty estimates are augmented by an additional 10% to account for non- ideal effects

Wall Catalycity :

Parameter	Uncertainty
γ_{cat} (Highly catalytic)	10^{-1}- 10^{0}
γ_{cat} (Moderately catalytic)	10^{-3}- 10^{-1}
γ_{cat} (Weakly catalytic)	10^{-4}- 10^{-3}
p_2	10^{-4}- 10^{0}

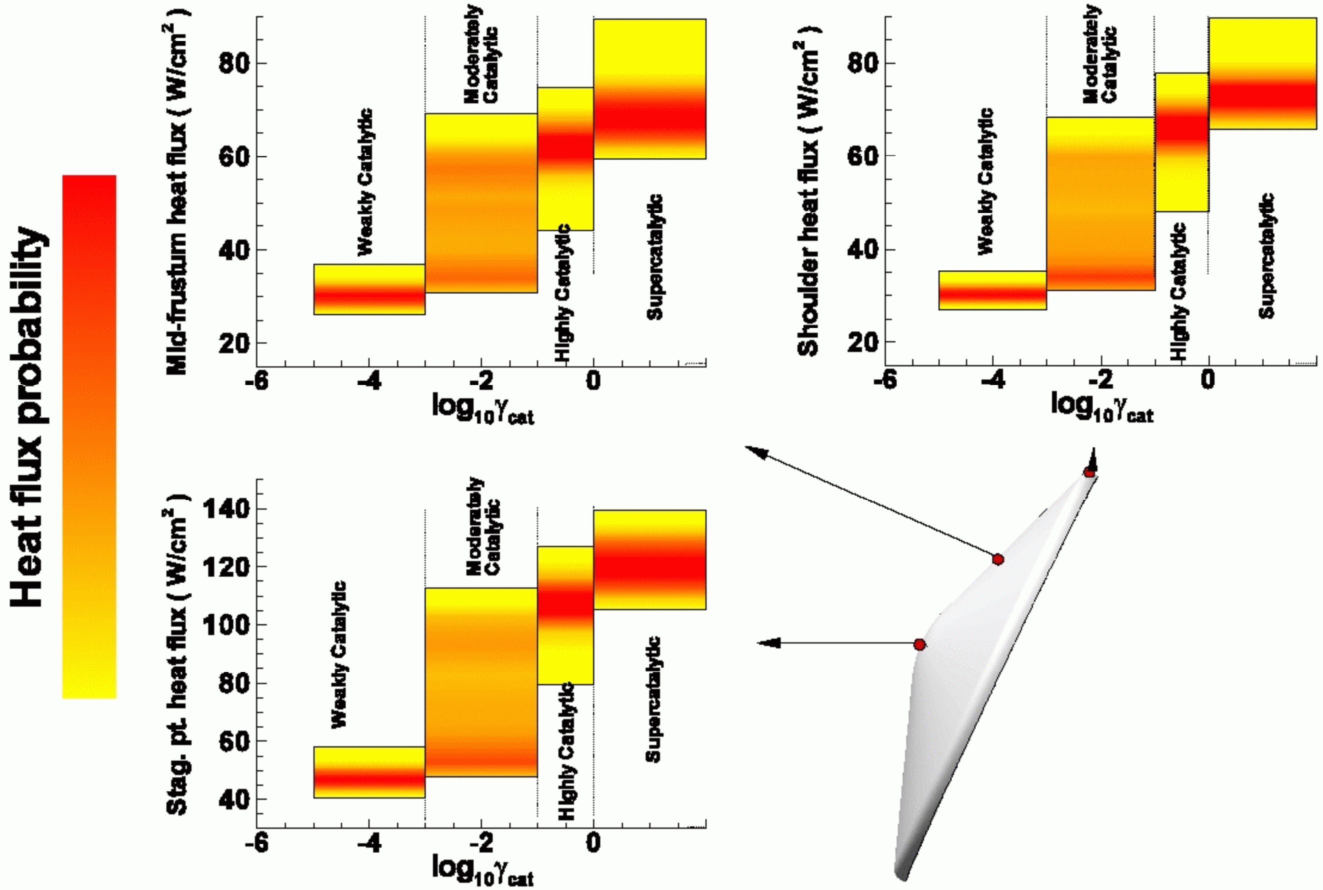
Uniform distribution

Chemical Reactions :

Reaction	Uncertainty
O_2+ O ⇔ 2O+ O	½ order
O_2+ CO ⇔ 2O+ CO	½ order

Gaussian distribution

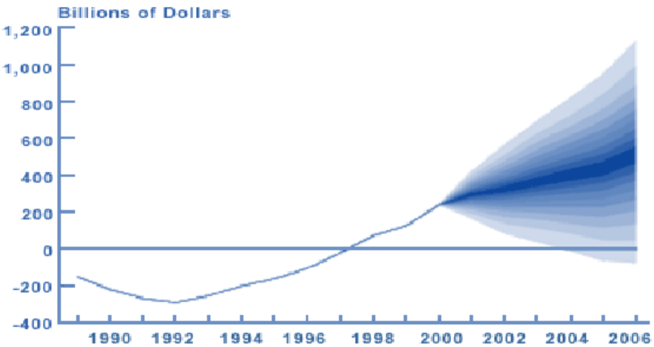
In a nutshell...



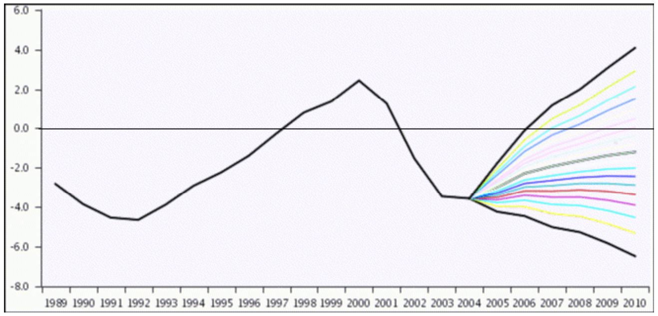
Uncertainty Quantification Gone Awry

Congressional Budget Office (CBO) budget projections

CBO Budget Uncertainty Fan in 2000:



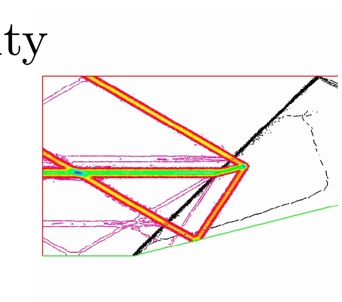
CBO Budget Uncertainty Fan in 2004:



Error Estimation Lectures

- (Prof. Peraire) 2-sided error bounds and accuracy certificates
  - Certifiably accurate computations
  - Error control via adaptivity

- (Prof. Houston) FEM error estimation for functionals via duality
  - Error representation for functionals $J(u)$ via duality
  - Weighted and unweighted error estimates
  - Error control via adaptivity



- (Barth) Error estimation for finite volume methods
  - Godunov finite volume methods rewritten as a Petrov-Galerkin FE method.
  - Applying standard error estimation techniques in the finite volume setting

Error Estimates for Functionals

Space-time hyperbolic PDE ($p^- = 1$ at inflow and $p^+ = 0$ at outflow):

$$\begin{aligned} \mathcal{L}\, u - f &= 0, \quad \text{(interior)} \\ p^-\,(u - g) &= 0, \quad \text{(initial/boundary data)} \end{aligned}$$

Weighted error estimates for functionals:

$$|J(u) - J(u_h)| \leq \sum_K |(r_h, \phi - \pi_h \phi)_K| + \sum_{\partial K} \langle j_h, \phi - \pi_h \phi \rangle_{\partial K}|$$

where

$$r_h \equiv \mathcal{L}\, u_h - f \quad \text{(Element Residual)}$$

$$j_h \equiv \begin{cases} p^-\,[u_h]_-^+ & \text{(Interior Jump Residual)} \\ p^-\,(g - u_h) & \text{(Boundary Jump Residual)} \end{cases}$$

Unweighted error estimates for functionals:

$$|J(u) - J(u_h)| \leq C_{\text{int}} C_{\text{stab}} \| h^s r_h \|, s > 0$$

Error Estimates via Duality

ϕ is solution of the infinite-dimensional *dual problem*. Suppose $\mathcal{V}$ is the space of H^s functions and $\mathcal{V}_h \subset \mathcal{V}$ a suitable finite-dimensional approximation space.

Abstract FEM method with weakly imposed BCs:

(Finite-Dimensional Primal Problem) Find $u_h \in \mathcal{V}^h$ such that

$$B(u_h, v) = (f, v) \ , \quad \forall v \in \mathcal{V}_h$$

(Infinite-Dimensional Dual Problem) Find $\phi \in \mathcal{V}$ such that

$$B(v, \phi) = (\psi, v) = J(v) \ , \quad \forall v \in \mathcal{V}$$

Assessing Computability

The dual solution and functional error estimates contain a wealth of information concerning *computability* of outputs.

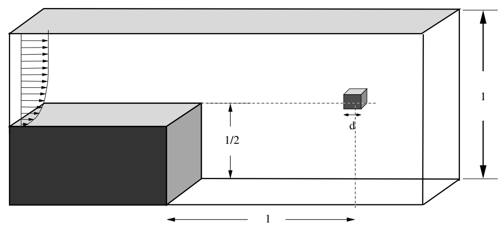
$$|J(u) - J(u_h)| \leq \sum_K |(r_h, \phi - \pi_h \phi)_K| + \sum_{\partial K} \langle j_h, \phi - \pi_h \phi \rangle_{\partial K}|$$

Clearly, the computability of outputs deteriorates as gradients of the dual solution grow in space and/or time.

An extreme example is fluid turbulence where the prospect of controlling pointwise errors deteriorates rapidly with increasing Reynolds number.

Computability of Outputs

Example: Backward facing step (Re=2000)



Suppose $J(u)$ is the streamwise velocity component averaged in cube in space and over a unit time interval, i.e.

$$J(u) = \int_9^{10} \int_{d \times d \times d} u_1 dx^3 dt$$

Computability Outputs

Hoffman and Johnson (2002) have computed solutions of the backward facing step problem using a FEM method with linear elements for incompressible flow.

In velocity and pressure variables, (V, p), the following error estimate for functionals is readily obtained in terms of the dual solution (ψ, ϕ)

$$
\begin{aligned}
|J(V,p) - J(V_h, p_h)| \quad &\leq \quad C\|\dot{\psi}\|\Delta t\, r_0(V,p)\| \\
&+ \quad C\|D^2\phi\|\|h^2\, r_0(V,p)\| \\
&+ \quad C\|\dot{\phi}\|\|\Delta t\, r_1(V,p)\| \\
&+ \quad C\|D\phi\|\|h\, r_1(V,p)\|
\end{aligned}
$$

where r_i are element residuals.

Computability Outputs

The following stability factors have been computed by Hoffman and Johnson (2002) for the backward facing step problem:

d	$\|\|\dot{\psi}\|\|$	$\|\|\nabla\psi\|\|$	$\|\|\nabla\phi\|\|$	$\|\|\dot{\phi}\|\|$
1/8	124.0	836.0	138.4	278.4
1/4	39.0	533.4	48.9	46.0
1/2	10.5	220.3	16.1	25.2

These results clearly show the deterioration in computability as the box width is decreased.

Concluding Remarks

- Due to the vast increases in computing power, it's an exciting time in scientific computation.
- The time is right to advance the state-of-the-art in scientific computing to a new level.
- The ability to quantify uncertainty and numerical errors in large scale computations is *the* missing piece of the puzzle.