Gradient-based Methods for Rapid Uncertainty Quantification in Hypersonic Flows

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July 26, 2012

Uncertainty Quantification for Engineering Simulations

- Engineering Simulation: Characterize the performance of a specified system using the relevant physics
  - Maps design parameters to output metrics using governing equations.
- Simulation primary design tool when experimental data expensive, impractical to obtain.
- For decision making, the uncertainty of the simulation must be quantified.
  - Allows confidence interval for results
  - Identifies limitations of the simulation
  - Enable design under uncertainty
- Traditional approaches for Uncertainty Quantification (UQ) rely on exhaustive sampling
  - Prohibitively expensive for complex problems.
- The cost of uncertainty quantification must be reduced to enable widespread use.

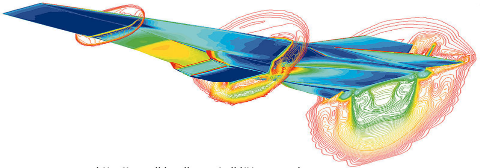
Characteristics of Engineering Simulations

- For many engineering simulations, interested in limited number of outputs
  - Number of inputs $\ggg$ Number of simulation outputs
- Simulation outputs typically vary smoothly as inputs vary
- Additional information provided by Gradients
  - Approximately same computational cost of simulations
  - Single adjoint gives derivative of single output w.r.t all inputs
- Adjoint capability increasingly available in commercial solvers for error estimation and optimization.

Gradient Information can be used to reduce the cost associated with uncertainty quantification.

Hypersonic CFD Overview

- Hypersonic Flow roughly defined as $M > 5$
- Important in aerospace applications, like propulsion and
  Atmospheric Re-entry
- Characterized by:
  - Strong Shocks
  - Internal Energy Modes (Rotational, Vibrational, Electronic)
  - Chemical Reactions
- Non-equilibrium thermodynamics requires each species/energy mode to be modeled individually
- Models can require hundreds to thousands of parameters to define (Arrhenius Reaction Coefficients, Curve fits, etc.)



http://en.wikipedia.org/wiki/Hypersonic

Physical Model

- Navier Stokes Equations for Non-equilibrium Flow:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \vec{U}) = -\nabla \cdot (\rho_s \vec{V}_s) + \omega_s$$

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho \vec{U} \otimes \vec{U}) = -\nabla P + \nabla \cdot \underline{\tau}$$

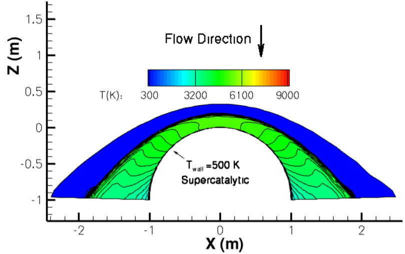
$$\frac{\partial \rho e_t}{\partial t} + \nabla \cdot (\rho h_t U) = \nabla \cdot (\underline{\tau} \vec{u}) - \nabla \cdot \vec{q} - \nabla \cdot \vec{q}_v - \nabla \cdot \left(\sum_s h_{t,s} \rho_s \tilde{V}_s \right)$$

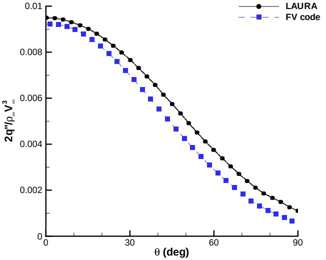
$$\frac{\partial \rho e_v}{\partial t} + \nabla \cdot (\rho e_v U) = Q_{T-V} + \sum_s e_{v,s} \omega_s - \nabla \cdot \left(\sum_s h_{v,s} \rho_s \tilde{V}_s \right) - \nabla \cdot \vec{q}_v$$

- Equations are deterministic; however, the model parameters introduce uncertainty into the output.

Hypersonic Example Case

- 5 km/s Flow (Mach 17.605) over a Blunt body at approximately 200,000 Ft
- 5 species, 2 temperature real gas model
    - Chemical Components: N_2, O_2, NO, N, O
    - Temperatures: Translational-rotational, Vibrational-electronic
- Simulation performed by in-house developed two dimensional, finite volume solver with adjoint capability
- Interested in surface heating of the body.





Uncertainty Quantification (UQ) for Hypersonics

- Multiple sources of uncertainty:
  - Physical Parameters
  - Manufacturing Tolerances
  - Modeling inadequacies
  - Boundary Conditions
  - Initial Conditions
  - Random Elements in simulation
- For deterministic simulations:
  - $L = F(\vec{D})$ where F represents the simulation
  - L only becomes uncertain when $\vec{D}$ is uncertain
- Traditional UQ methods extract multiple realizations of L based on samples of $\vec{D}$.
- By providing additional information about the mapping F, the gradient $\frac{dL}{dD}$ can be used to accelerate UQ.

Sensitivity Derivation

- Let the objective (L) and constraint ($R = 0$) have following functional dependence

$$L = L(D, \mathbf{U}(D)) \tag{1}$$
$$\mathbf{R} = \mathbf{R}(D, \mathbf{U}(D)) = 0 \tag{2}$$

- Objective and Constraint may be differentiated using the Chain rule

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathbf{U}}\frac{\partial \mathbf{U}}{\partial D} \tag{3}$$
$$\frac{d\mathbf{R}}{dD} = \frac{\partial \mathbf{R}}{\partial D} + \frac{\partial \mathbf{R}}{\partial \mathbf{U}}\frac{\partial \mathbf{U}}{\partial D} = 0 \tag{4}$$

- Solve Constraint Equation for $\frac{\partial \mathbf{U}}{\partial D}$ (Independent of L):

$$\frac{\partial \mathbf{U}}{\partial D} = \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1}\frac{\partial \mathbf{R}}{\partial D} \tag{5}$$

Sensitivity Derivation (cont.)

- Forward Sensitivity Equation Given by (Tangent Linear Model):

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} - \frac{\partial L}{\partial \mathbf{U}} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1} \frac{\partial \mathbf{R}}{\partial D} \tag{6}$$

- Transpose Equation (Adjoint Sensitivity Equation)

$$\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} - \frac{\partial \mathbf{R}}{\partial D}^{T} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-T} \frac{\partial L}{\partial \mathbf{U}}^{T} \tag{7}$$

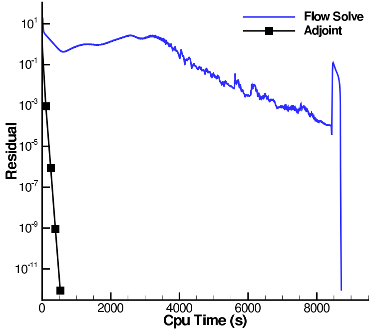
- Flow Adjoint (Independent of D):

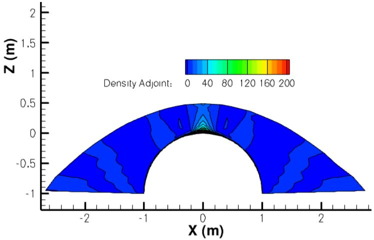
$$\mathbf{\Lambda} = -\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-\mathbf{T}} \frac{\partial \mathbf{L}}{\partial \mathbf{U}}^{\mathbf{T}} \tag{8}$$

- Derivatives calculated via Automatic Differentiation (Tapenade)
- Expense of calculating flow adjoint comparable to cost of primal
- All components of the gradient calculated with single adjoint.

Flow Adjoint

- Because linear, Adjoint can be mucher faster for highly nonlinear problems
- Adjoint Solve approximately 40 times faster than flow solve
- Represents the impact of a flow variable on the objective





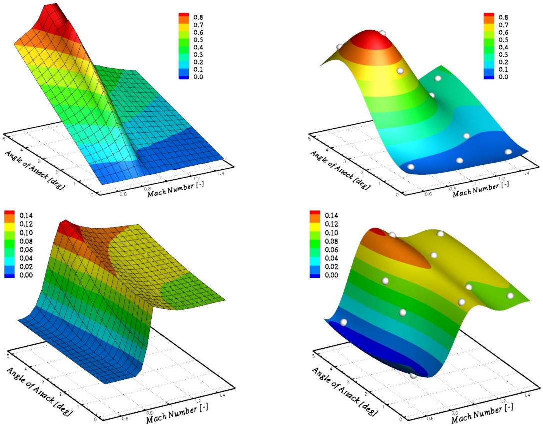
Forms of Uncertainty

- Different Forms of Uncertainty:
  1. **Aleatory**:
     - Due to inherent randomness
     - Specified with probability distribution
     - Quantified using Monte Carlo Sampling ($\sim 10^3 - 10^4$)
  2. **Epistemic**:
     - Due to lack of knowledge about exact value
     - Specified by interval
     - Quantified using Latin Hypercube sampling ($\sim 3^d$)
  3. **Mixed**:
     - Inputs have different forms
     - Quantified using Mixed Sampling ($\sim 3^{d+8}$)
     - Output distribution has interval
- Each form extremely expensive to quantify for complex simulations (Aleatory $\lll$ Epistemic $\lll$ Mixed)
- Different Gradient-based strategies used for each

Gradient-based Aleatory Uncertainty

- Goal: Determine simulation output distribution based on input distributions
- For limited number of outputs, replace simulation with inexpensive surrogate based on small number of results
  - $L = F(\vec{D}) \approx \tilde{F}(\vec{D})$ where $\tilde{F}$ is inexpensive to evaluate.
  - $\tilde{F}$ can be built based on a limited number of simulation results
  - Examples: Interpolation, Polynomial regression, Gaussian Process Regression (Kriging)
- Amount of data required to train accurate surrogate increases exponentially fast with dimension. Address by:
  - Utilizing SA to reduce dimension
  - Incorporating Gradient information into surrogate construction
- Distribution of output is found with Monte Carlo Sampling, replacing simulation evaluations with the surrogate.

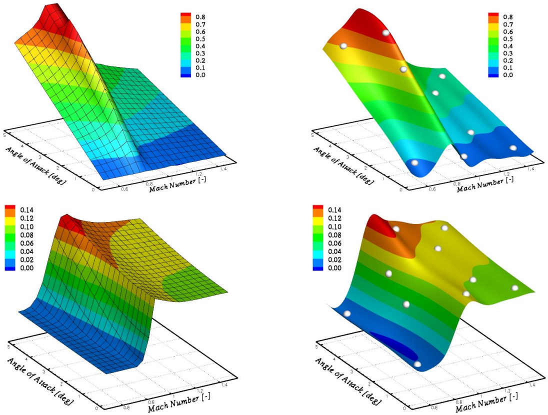
Kriging Model



Flight Envelope Calculations* - Function Only

*(courtesy of Wataru Yamazaki)

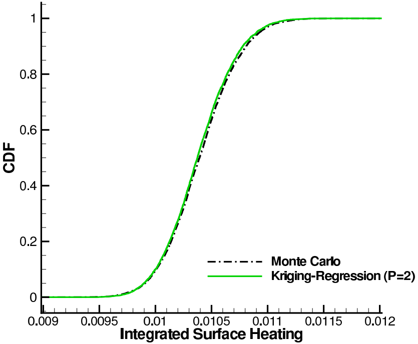
Kriging Model



Flight Envelope Calculations - Gradient Enhancement
*(courtesy of Wataru Yamazaki)

Gradient-based Aleatory UQ Results

- 5 km/s Flow test case with 66 uncertain Parameters
- Uncertainty in integrated surface heating evaluated
- Distribution from 5000 simulation results compared with Kriging Model with 68 function/gradient evaluations in 15 dimensions

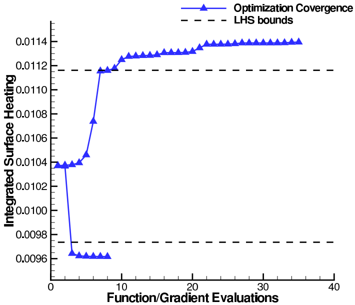


Gradient-based Epistemic Uncertainty Quantification

- Goal: Determine Output Interval based on input intervals
- Dominant form of uncertainty for hypersonic flow, need methods for high dimension
- Cast as bound constrained optimization problem: Given input intervals, determine min and max values.

$$y_{min} = \min_{x \in I} f(x)$$
$$y_{max} = \max_{x \in I} f(x)$$

- Gradient-based Optimization (L-BFGS) can be used to reduce cost

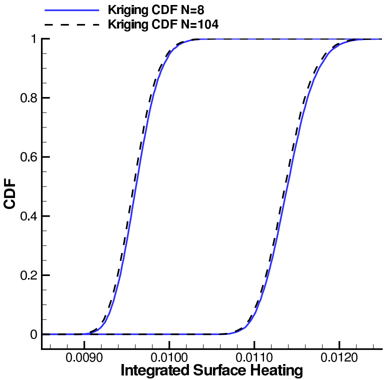


- Uncertainty in Transport Parameters ($\pm 20\%$)
- Optimization more correct result (Local Optimization sufficient)
- $6,561$ function evaluations reduced to ~ 40 function/gradient
- Exponential Scaling of sampling reduced to tractable optimization problem (applicable for high dimension)

Gradient-based Mixed Aleatory/Epistemic

- Variables have either aleatory or epistemic uncertainty
- **Goal**: Determine range containing output with specified probability (P-Box) and separate the contribution from each source
- Typical situation for simulation as complete knowledge rare
- Nested sampling traditionally used; however,
  - For hypersonic flows, number of epistemic variables much greater than number of aleatory variables
  - Expensive of nested sampling increases rapidly with number of epistemic variables
  - Prohibitively expensive for all but explicit functions
- Combine surrogate approaches with gradient-based optimization for rapid mixed UQ
  - Create surrogate for multiple optimization results to determine statistics of the interval

- CDF for bounds can be created from Kriging Model (with 8 to 104 sets of optimization results)
- $\sim$ 500 F/G vs over 30 million for nested sampling



Gradient-based method allowed UQ when traditional was intractable

Conclusions

- Each type of uncertainty addressed with gradient-enhanced method
  1. **Aleatory**:
     - Applied gradient-enhanced surrogate models for aleatory uncertainty
     - Dimension reduction based on global sensitivity analysis
     - Factor of 100 savings compared to Monte Carlo sampling
  2. **Epistemic**:
     - Gradient-based optimization used to determine output interval
     - Assuming local sufficient, optimization moves scaling from exponential to linear
  3. **Mixed**:
     - New combined surrogate-optimization approach developed
     - Optimizations performed for epistemic variables, surrogate created over aleatory
- For each scenario, significant cost savings compared with traditional approaches
- Gradient-based Epistemic/Mixed approaches enabled quantification when sampling is impossible.

Acknowledgments

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