Gradient-based Approaches for Sensitivity Analysis and Uncertainty Quantification within Hypersonic Flows

Ph.D. Defense

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Background

- Utility of simulation has dramatically expanded over the past 30 years.
  - Driven by increased computational resources and improved algorithms
  - Simple design tools $\rightarrow$ Accurate Predictive Simulation
- Computational Science increasingly viewed as third branch of Science
  - Theory
  - Experiment
  - **Simulation**
- Increased capability has made simulation critical for situations where experiment is difficult/impossible to obtain
  - Hypersonic Flow
  - Nuclear Reactor Design
- Simulations must be able to supply confidence measure/uncertainty to enable design and decision making.

Uncertainty Quantification (UQ)

- Problem: Determine uncertainty of simulation results based on uncertainties within the simulation.
- Multiple sources of uncertainty:
  - Random Elements in simulation
  - **Physical Parameters**
  - Manufacturing Tolerances
  - Modeling inadequacies
  - **Boundary Conditions**
  - Initial Conditions
- Goal: Calculate Statistics/Interval of simulation outputs
- Traditionally requires running large number of simulations (~ 1000)
  - Prohibitively expensive for complex simulations
- Must reduce cost to enable use of UQ in design/certification process

Sensitivity Analysis (SA)

- Problem: Determine the effect of parameters on simulation outputs.
- Closely related discipline to Uncertainty Quantification (UQ)
- Provides means of improving results by:
  - Identifying the most critical parameters
  - Determining contribution to output uncertainty
  - Providing focus for further experiments
- Global Analysis: Calculate Correlation between input and output
- Localized Analysis: Partial derivative of output w.r.t. inputs
  - Applicable beyond sensitivity analysis
  - Can be viewed as gradient of output w.r.t inputs

Motivation

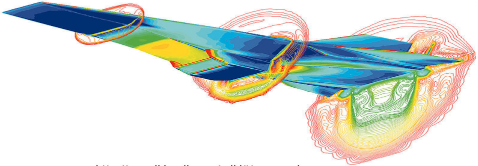
Observations:

- For practical CFD 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 and sensitivity analysis.

Hypersonic Flow

- Hypersonic Flow roughly defined as $M > 5$
- Characterized by:
  - Strong Shocks
  - Internal Energy Modes (Rotational, Vibrational, Electronic)
  - Chemical Reactions
- Non-equilibrium chemistry requires each species to be modeled
- Thermal non-equilibrium requires individual energy modes to be solved independently
- Models can require hundreds of parameters to define (Arrhenius Reaction Coefficients, Curve fits, etc.)



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

Physical Model

- Five Species, Two Temperature Real Gas Model for Air
  - Accounts for Molecular dissociation: N_2, O_2, N, O, NO
  - Energy described by translation-rotational temperature and vibrational-electronic temperature
- Compressible Navier Stokes Equations:

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

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

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

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

Physical Model

- Constitutive Law's:

$$\rho_s \tilde{V}_s = -\rho D_s \nabla c_s \qquad \text{Fick's Law}$$

$$\underline{\tau} = \mu(\nabla\vec{u} + \vec{u}\nabla) - \frac{2}{3}\mu\nabla\cdot\vec{u}\underline{I} \qquad \text{Newtonian Fluid}$$

$$\vec{q} = -k\nabla T \qquad \text{Fourier's Law}$$

$$\vec{q_v} = -k_v\nabla T_v$$

- Equations of State:

$$\frac{C_v^s(T)M_s}{\bar{R}} = A^i_{o,s} + A^i_{1,s}T + A^i_{2,s}T^2 + A^i_{3,s}T^3 + A^i_{4,s}T^4 \qquad \text{(Caloric)}$$

$$P(\rho, T) = \rho\sum_s c_s\frac{\bar{R}}{M_s}T \qquad \text{(Thermal)}$$

Transport Model

- Defines: $\mu = \mu(T, \rho_s)$, $k = k(T, \rho_s)$, $k_v = k_v(T, \rho_s)$, $D_s = D_s(T, \rho_s)$
- Calculated using Collision integrals (cross-sections) for each interaction $\Omega_{s,r}^{k,k}$
- Specified at 2000 K and 4000 K and interpolated using:

$$log_{10}(\Omega_{s,r}^{k,k}) = log_{10}(\Omega_{s,r}^{k,k})_{2000} + \left[log_{10}(\Omega_{s,r}^{k,k})_{4000} - log_{10}(\Omega_{s,r}^{k,k})_{2000}\right] \frac{ln(T) - ln(2000)}{ln(4000) - ln(2000)}$$

- 15 interactions possible giving 60 total model parameters
- Effect of curve shifts accounted for using parameter $A_{s,r}^{k}$:

$$\Omega_{s,r}^{k,k}(T) = A_{s,r}^{k} \hat{\Omega}_{s,r}^{k,k}(T)$$

Chemical Kinetics Model

- Net creation/destruction of each species ω_s:

$$\omega_s = M_s \sum_r (\beta_{s,r} - \alpha_{s,r})(R_{f,r} - R_{b,r})$$

- Reaction Rates specified using Law of Mass Action:

$$R_{f,r} = 1000 \left[k_{f,r} \prod_s (0.001\rho_s / M_s)^{\alpha_{s,r}} \right]$$

- Rate Coefficients $k_{f,r}$ and $k_{b,r}$ given by Arrhenius relation (Dunn-Kang Model)

$$k_{f,r} = C_{f,r} T_a^{\eta_{f,r}} e^{-\frac{E_{f,r}}{k_B T_a}} \qquad k_{b,r} = C_{b,r} T_a^{\eta_{b,r}} e^{-\frac{E_{b,r}}{k_B T_a}}$$

- 17 reactions total, 34 parameters: $log_{10}(k_r/k_o) = \xi_r$

CFD Solver

- Equations solved numerically in two dimensions using in-house developed finite-volume solver
- Capable of solving on unstructured triangles/quadrilaterals
- Solution marched to steady state using implicit pseudo-time stepping

$$\mathbf{J}(\mathbf{U}^n, \mathbf{U}^{n-1}) = \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t} + \mathbf{R}(\mathbf{U}^n)$$

- Newton's Method used to solve nonlinear equation at each time-step:

$$\delta \mathbf{U}^k = -\left[P\right]^{-1} \mathbf{J}(\mathbf{U}^k, \mathbf{U}^{n-1})$$
$$\mathbf{U}^{k+1} = \mathbf{U}^k + \lambda \delta \mathbf{U}^k$$

- Jacobi or line-preconditioned GMRES used to invert Jacobian

Spatial Discretization

- Gradient reconstruction of primitives
- Green-Gauss contour integration used to calculate gradients
- Smooth Van Albada Limiter with Pressure Switch used:

$$\Psi_k = max(0, 1 - K\nu_k)\frac{1}{\Delta^-}\frac{(\Delta^{+^2} + \varepsilon^2)\Delta^- + 2\Delta^{-^2}\Delta^+}{\Delta^{+^2} + 2\Delta^- + \Delta^-\Delta^+ + \varepsilon^2}$$

$$\nu_i = \frac{\sum_k |P_R - P_L|}{\sum_k P_R + P_L}$$

- Face based Gradients calculated using averaging and correction term:

$$\nabla \mathbf{V}_k = \tilde{\nabla}\mathbf{V} + \frac{\mathbf{V}_R - \mathbf{V}_L - \tilde{\nabla}\mathbf{V} \cdot \Delta\vec{T}}{|\Delta\vec{T}|}\frac{\Delta\vec{T}}{|\Delta\vec{T}|}$$

- Inviscid Flux Calculated Using AUSM+UP flux function with Frozen Speed of Sound

Real Gas Results

- 5 km/s cylinder test case
- Fixed Wall temperature
- Super-catalytic Wall
- Results compared with LAURA (Same Mesh)
- Park Chemical Kinetics Model

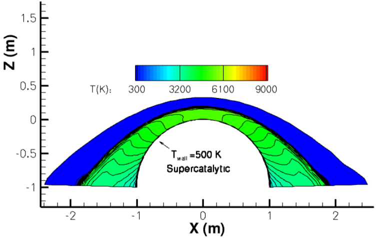
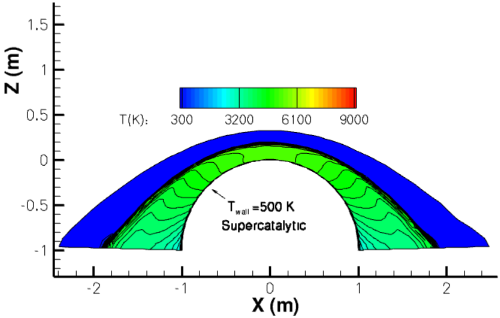
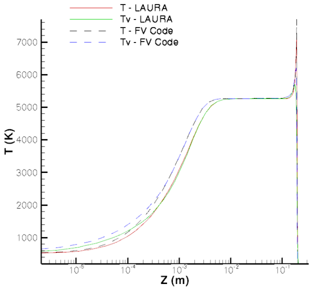
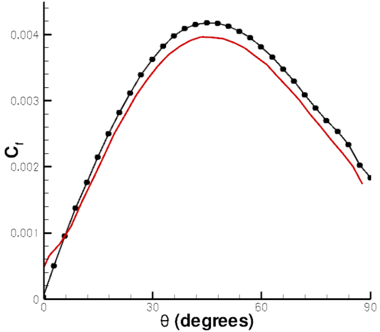


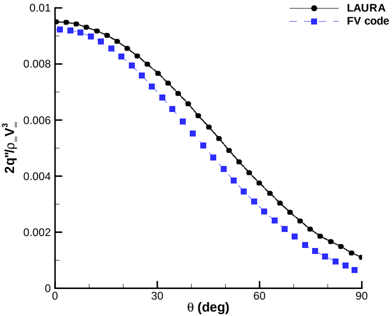
Table: Benchmark Flow Conditions

$$
\begin{aligned}
V_\infty &= 5\ km/s \\
\rho_\infty &= 0.001\ kg/m^3 \\
T_\infty &= 200\ K \\
T_{wall} &= 500\ K \\
M_\infty &= 17.605 \\
Re_\infty &= 753{,}860 \\
Pr_\infty &= 0.72
\end{aligned}
$$


Z (m)
1.5
1
0.5
0
-0.5
-1
T(K): 300 3200 6100 9000
T_{wall} =500 K
Supercatalytic
-2 -1 0 1 2
X (m)


T - LAURA
Tv - LAURA
T - FV Code
Tv - FV Code
T (K)
7000
6000
5000
4000
3000
2000
1000
Z (m)


0.004
0.003
0.002
0.001
0
C_f
0
30
60
90
θ (degrees)


LAURA
FV code
0.01
0.008
0.006
0.004
0.002
0
$2q''/\rho_\infty V^3_\infty$
0
30
60
90
θ (deg)

Sensitivity Derivation

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

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

- Objective and Constraint may be differentiated using the Chain rule

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

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

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

Sensitivity Derivation

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

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

- Transpose Equation (Adjoint Sensitivity Equation)

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

- Flow Adjoint (Independent of D):

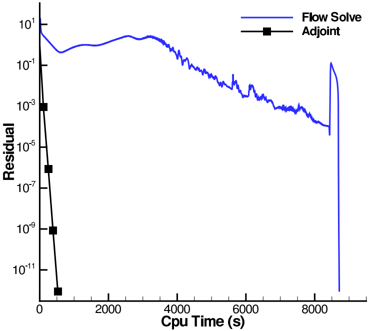
$$\mathbf{\Lambda} = -\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-\mathbf{T}} \frac{\partial \mathbf{L}}{\partial \mathbf{U}}^{\mathbf{T}}$$

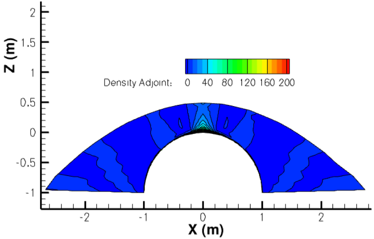
- Solved Using Defect Correction combined with line-preconditioned GMRES:

$$[P]^T \delta \mathbf{\Lambda}^k = -\frac{\partial L}{\partial \mathbf{U}}^T - \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T \mathbf{\Lambda} = -R_{\mathbf{\Lambda}}(\mathbf{\Lambda}^k)$$
$$\mathbf{\Lambda}^{k+1} = \mathbf{\Lambda}^k + \lambda \delta \mathbf{\Lambda}^k$$

Flow Adjoint

- Single Adjoint gives derivative of one output w.r.t. all inputs
- Because linear, Adjoint about 40 times faster than flow solve
- Implemented with Automatic-differentiation (Tapenade)
- Approximately 100 vectors per GMRES restart, 527 total Mat-vec.





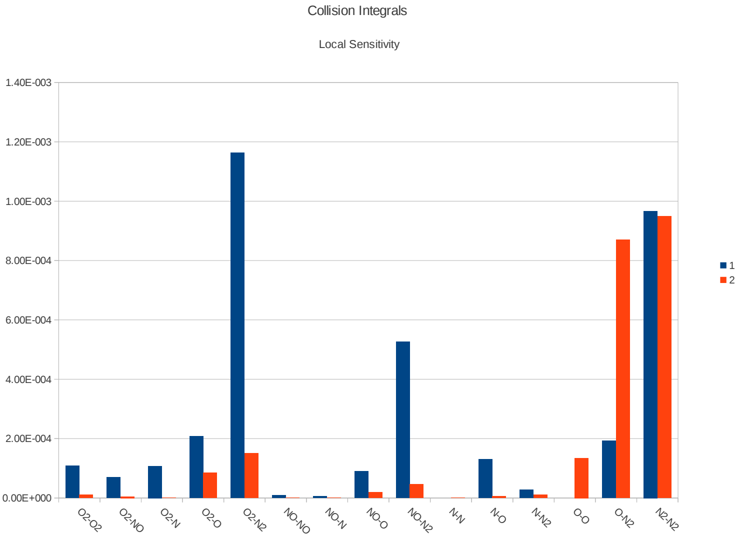
Local Sensitivity Analysis

- Using derivative values, the local effect of each parameter can be determined directly
- Integrated Surface heating used as objective:

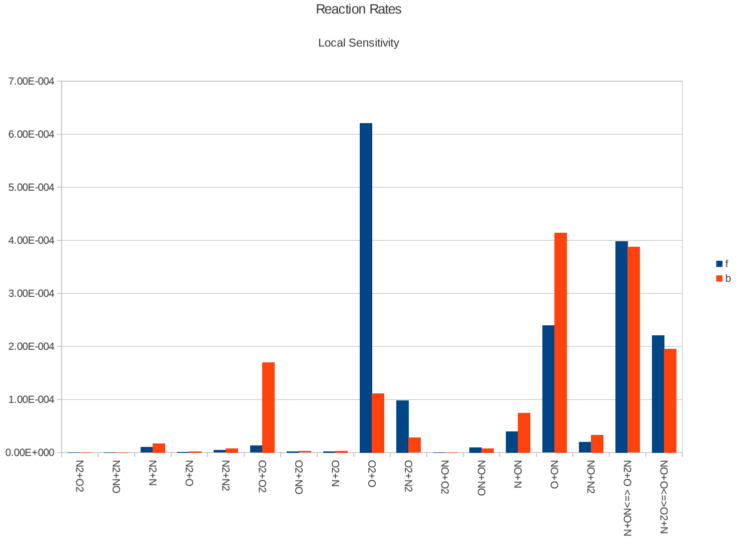
$$L = -\frac{\int_{\partial\Omega} k\nabla T \cdot \vec{n} + k_v \nabla T_v \cdot \vec{n} dA}{\frac{1}{2}\rho_\infty V_\infty^3}$$

- Effect of Collision integrals, reaction rate coefficients and freestream values analyzed (66 total)
- Requires a single flow and adjoint solution

Local Sensitivity Analysis



Local Sensitivity Analysis



Global Sensitivity Analysis

- Local analysis gives effect to infinitesimal change in parameters
- Does not account for interference effects or large perturbations
- Global sensitivity analysis gives average effect over design space
- Calculated via Monte Carlo sampling (6,331 for this case)

$$r_i = \frac{cov(D_i, y)}{\sigma_{D_i}\sigma_y}$$

- Design space given by the uncertainty space of 66 parameters: (Assumed normal distribution)

Number	Variable	Mean	Standard Deviations
1	$\rho_\infty \ (kg/m^3)$	1×10^{-3}	5%
2	$V_\infty (m/s)$	5000	15.42
3-17	A^1_{s-r}	1	5%
18-32	A^2_{s-r}	1	5%
33-49	ξ_f	0	0.25
50-66	ξ_b	0	0.25

Local vs. Global

- Importance ranking and contribution to variance compared
- Variance contribution given by square of correlation coefficient
- Local and Global show significant disagreement

Rank	Variable	Local	Global	Local
1	ρ_∞	1	0.60055	0.43230
2	$O_2 + O \leftrightarrows 2O + O$ (f)	2	1.0610×10^{-1}	1.7490×10^{-1}
3	$NO + O \leftrightarrows N + 2O$ (b)	3	5.1914×10^{-2}	7.7560×10^{-2}
4	O2-N2 (k=1)	7	4.2121×10^{-2}	2.4524×10^{-2}
5	N2-N2 (k=1)	10	3.1617×10^{-2}	1.6956×10^{-2}
6	$O_2 + O_2 \leftrightarrows 2O + O_2$ (b)	13	2.1621×10^{-2}	1.3120×10^{-2}
7	$N_2 + O \leftrightarrows NO + N$ (f)	4	2.0647×10^{-2}	7.2017×10^{-2}
8	N2-N2 (k=2)	11	1.9019×10^{-2}	1.6354×10^{-2}
9	O-N2 (k=2)	12	1.3874×10^{-2}	1.3714×10^{-2}
10	$N_2 + O \leftrightarrows NO + N$ (b)	5	1.2155×10^{-2}	6.8076×10^{-2}

Gradient-based Global Sensitivity Analysis

- Sampling-based GSA too expensive for complex simulation
- Build function approximating output based on small number of results (regression):

$$y(D) = \sum_s \beta_s \Psi_s(D)$$

- Requires simulation data for each term in regression:

$$S = \frac{(d+p)!}{d!p!}$$

- Gradients included to reduce required number of simulations (provides $d+1$ pieces of information)

$$N \geq \lceil \frac{(d+p)!}{d!p!(d+1)} \rceil$$

Gradient-based Global Sensitivity Analysis

- Limiting to $p = 2$ gives linear growth with dimension ($d + 2$ typical)
- Derivative matching included in collocation matrix

$$\begin{bmatrix} \Psi_1(D_1) & \Psi_2(D_1) & \cdots & \Psi_s(D_1) \\ \frac{\partial \Psi_1(D_1)}{\partial D_1} & \frac{\partial \Psi_2(D_1)}{\partial D_1} & \cdots & \frac{\partial \Psi_s(D_1)}{\partial D_1} \\ \vdots & \ddots & \ddots & \vdots \\ \frac{\partial \Psi_1(D_1)}{\partial D_d} & \frac{\partial \Psi_2(D_1)}{\partial D_d} & \cdots & \frac{\partial \Psi_s(D_1)}{\partial D_d} \\ \vdots & \ddots & \ddots & \vdots \\ \Psi_1(D_N) & \Psi_2(D_N) & \cdots & \Psi_s(D_N) \\ \frac{\partial \Psi_1(D_N)}{\partial D_1} & \frac{\partial \Psi_2(D_N)}{\partial D_1} & \cdots & \frac{\partial \Psi_s(D_N)}{\partial D_1} \\ \vdots & \ddots & \ddots & \vdots \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_s \end{bmatrix} = \begin{bmatrix} y(D_1) \\ \frac{\partial y(D_1)}{\partial D_1} \\ \vdots \\ \frac{\partial y(D_1)}{\partial D_d} \\ \vdots \\ y(D_N) \\ \frac{\partial y(D_N)}{\partial D_1} \\ \vdots \end{bmatrix}$$

- Coefficients determined using least squares

Gradient-based Global Sensitivity Analysis

- Global Sensitivity using 68 function/gradients
- Hermite Polynomial basis with maximum order 2
- Correlation calculated by sampling from regression
- Better agreement in terms of ranking and contribution
- Used for dimension reduction for uncertainty quantification

Rank	Variable	Global	Regression	Global
1	ρ_∞	1	0.56879	0.60055
2	$O_2 + O \leftrightarrows 2O + O$ (f)	2	1.0002×10^{-1}	1.0610×10^{-1}
3	$O_2 + O_2 \leftrightarrows 2O + O_2$ (b)	6	5.7669×10^{-2}	2.1621×10^{-2}
4	$NO + O \leftrightarrows N + O + O$ (b)	3	4.0057×10^{-1}	5.1914×10^{-2}
5	N2-N2 (k=1)	5	3.7461×10^{-2}	3.1617×10^{-2}
6	O2-N2 (k=1)	4	3.3299×10^{-2}	4.2121×10^{-2}
7	N2-N2 (k=2)	8	2.1163×10^{-2}	1.9019×10^{-2}
8	O-N2 (k=2)	9	1.7395×10^{-2}	1.3874×10^{-2}
9	V_∞	14	1.3497×10^{-2}	4.8401×10^{-3}
10	$O_2 + O \leftrightarrows 2O + O$ (b)	13	1.1734×10^{-2}	7.4280×10^{-3}

Uncertainty Quantification

- 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
  - Linear Extrapolation
  - Least-squares 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
- Surrogates tested by comparing with Monte Carlo results
- Uncertainty of integrated surface heating for $5 km/s$ cylinder predicted based on 66 inputs

Kriging Model

- Assumes data obey Gaussian Process

$$y = N(m(x), K(x, x'; \theta))$$

- Training based on simulation results $Y(\vec{X})$
- Output predictions given by sampling from conditional distribution:

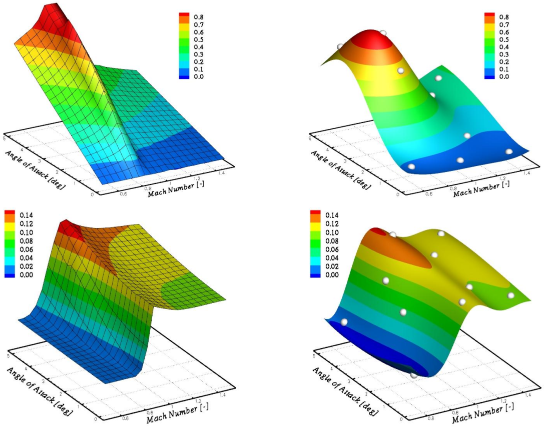
$$y^* | \vec{X}, Y, m(x) = m(x) + k_*^T K^{-1}(Y - m(x))$$

- Gradients included by extending covariance matrix:

$$\underline{K} = \begin{bmatrix} cov(Y, Y) & cov(Y, \nabla Y) \\ cov(\nabla Y, Y) & cov(\nabla Y, \nabla Y) \end{bmatrix}$$

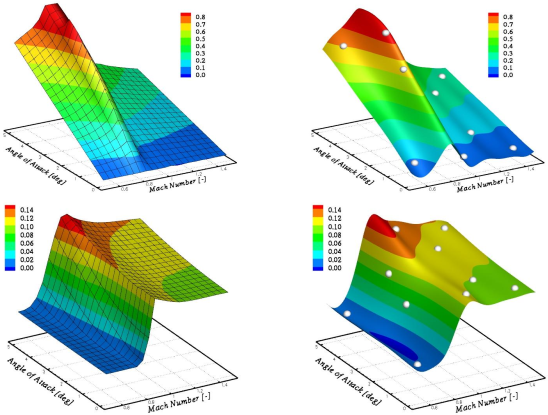
- Dimension reduction based on SA employed to limit required number of training points
- Mean function, $m(x)$, given as $p = 2$ regression or constant

Kriging Model



Flight Envelope Calculations* - Function Only

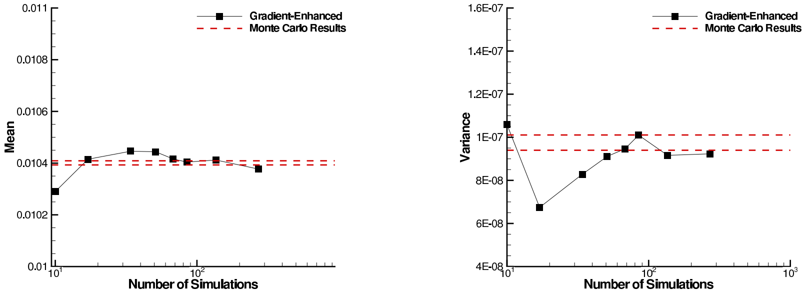
*(courtesy of Wataru Yamazaki)



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

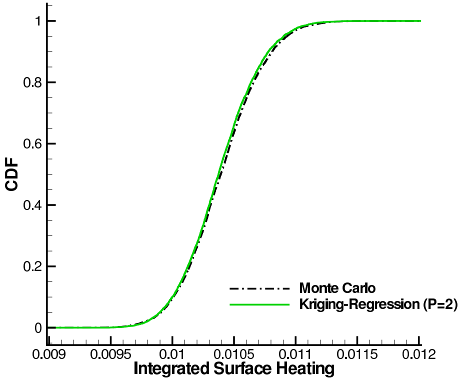
Kriging Model

- Dimension reduced to 15 based on Monte Carlo GSA
- Surrogate Performance measured based on Statistic prediction
- Constant mean function used



Kriging Model

- Dimension reduced to 17 based on regression GSA
- Regression used as Kriging Mean function
- 68 function/gradient evaluations



Method Comparison

- Methods compared based on cost and statistic predictions
- Kriging Methods give most accurate results
- Significant Cost reduction possible (6331 f vs. 68 f/g)

Method	Mean	Variance	95% CI	F/G Cost
Moment Method	1.0370E-002	1.3790E-007	±7.1616%	1
Linear Extrapolation	1.0369E-002	1.3412E-007	±7.0638%	1
P=1 Regression	1.0497E-002	8.8273E-008	±5.6610%	10
P=2 Regression	1.0370E-002	8.6692E-008	±5.6786%	68
Kriging-Trunc.-17D	1.0446E-002	1.0227E-007	±6.1228%	68
Kriging-Reg.-17D	1.0384E-002	9.2394E-008	±5.8543%	68
Monte Carlo-L	**1.0393E-002**	**9.3979E-008**	**±5.8994%**	**6331**
Monte Carlo-U	**1.0409E-002**	**1.0106E-007**	**±6.1083%**	

Gradient-based Epistemic Uncertainty Quantification

- Represents lack of knowledge about parameter, only interval can be specified
- Goal: Determine Output Interval based on input intervals
- Dominant form of uncertainty for hypersonic flow, need methods for high dimension
- Typically quantified by sampling (LHS) over variable combinations ($\sim 3^d$)
- Gradient-enhanced surrogates can be employed for sampling approaches
- Can also be cast as constrained optimization problem

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

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

- Gradient-based Optimization can be used to reduce cost

Gradient-based Epistemic Uncertainty Quantification

- Linear method for interval calculation possible with single function/gradient

$$y_o = f(x_o)$$
$$\Delta_y = \sum_{i=1}^{d} \left| \frac{\partial f}{\partial x_i}\bigg|_{x_o} \Delta_{x_j} \right|$$
$$[y_{max}, y_{min}] = [y_o + \Delta_y, y_o - \Delta_y]$$

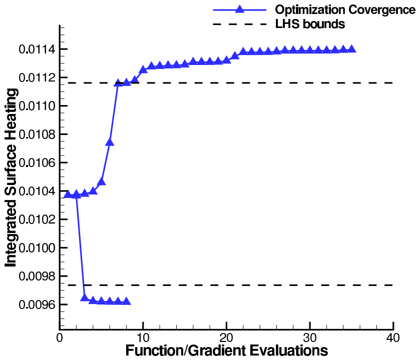
- Quasi-Newton Method for optimization (namely L-BFGS)
  - Requires function/gradient for each iteration
  - Can give optimal scaling as dimension expands
  - Hessian matrix approximated using previous gradient values
  - Local in Nature
- Epistemic UQ requires global min/max; however, local optimization appears sufficient for hypersonic problem

Epistemic UQ results - 8 dimensions

- Collision integrals treated as epistemic (20% interval width)
- Methods tested using 8 uncertain parameters
- Validated using LHS with 3 points per dimension (6,561 samples)
- Linear (1 f/g) and optimization ($\sim$ 40 f/g) produce more accurate interval

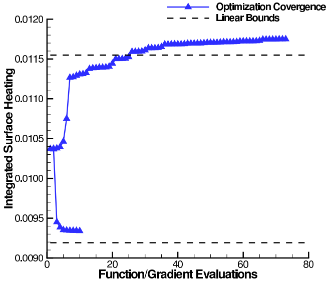
	Linear Method	LHS interval	Optimization
Center	1.0370E-002	1.0449E-002	1.0506E-002
Interval Half Width	8.6634E-004	7.1266E-004	8.8912E-004
Upper	1.1237E-002	1.1161E-002	1.1395E-002
Lower	9.5040E-003	9.7361E-003	9.6168E-003
Percentage	8.35%	6.82%	8.46%

Epistemic UQ results - 8 dimensions



- Optimization more correct result as it satisfies problem statement
- More extensive sampling gives bounds approaching optimization

- Optimization/Linear analysis can be applied to large dimension
- Number of parameters expanded to all collision integrals (30 total)
- Methods produce similar interval estimates



	Linear Method	Optimization
Center	1.0370E-002	1.0543E-002
Half Width	1.1787E-003	1.2031E-003
Upper	1.1549E-002	1.1746E-002
Lower	9.1916E-003	9.3400E-003
Percentage	11.37%	11.41%

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

Nested Sampling

Define:

- α are aleatory variables
- β are epistemic variables
- $L(\alpha, \beta)$ is simulation output

Nested Sampling:

- Extract β realization for $i = 1, N_r$
  - Sample over α for $j = 1, N_s$
    - Run simulation
    - Compute $L(\alpha, \beta)$
  - Characterize output distribution associated with varying α
- Examine statistics over all realizations (determine worst-case)

Cost-Reduction Strategies

- Nested sampling can be performed inexpensively based on surrogate
- Optimization/Surrogate should scale to higher dimension for large number of epistemic variables
- Two choices for ordering
  - Use optimization to determine min/max of statistic
  - **Use sampling to determine statistic of min/max**
- **Statistics-of-Intervals**
  - Solve multiple optimization problems for different α samples:

$$L_{min}(\alpha) = \min_{\beta} L(\alpha, \beta)$$

$$L_{max}(\alpha) = \max_{\beta} L(\alpha, \beta)$$

  - Construct surrogate (Kriging model) for $L_{min}(\alpha)$ and $L_{max}(\alpha)$
  - Calculate statistics based on sampling over α from surrogate model

Fay-Riddell Heating Results

Fay-Riddell Stagnation Heating Correlation:

$$q'' = 0.76(Pr_w)^{-0.6}(\rho_w \mu_w)^{0.1}(\rho_e \mu_e)^{0.4}\sqrt{\left(\frac{dU_e}{dx}\right)}(h_{o,e} - h_w)\left[1 + (Le^{0.52} - 1)\left(\frac{h_D}{h_{o,e}}\right)\right]$$

$$\left(\frac{dU_e}{dx}\right) = \frac{1}{R_N}\sqrt{2\frac{p_e - p_\infty}{\rho_e}}$$

$$h_D = \sum_i C_{i,e}\Delta h^o_{f,i}$$

- Properties at boundary layer edge determined by normal shock relations
- Composition determined with statistical thermodynamics
- Transport Quantities calculated from collision integrals
- 5 km/s flow over cylinder considered

Fay-Riddell Heating Results

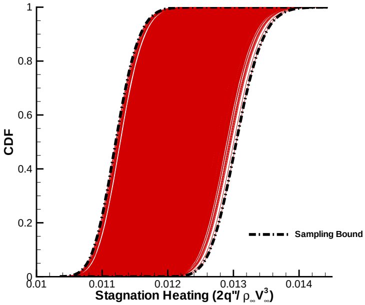
Uncertain Parameters:

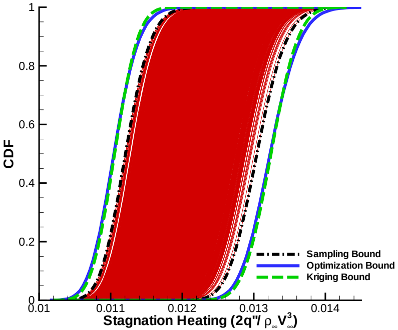
Variable	Type	Uncertainty
ρ_∞ (kg/m^3)	Aleatory	$\pm 10\%$ $(\sigma = 5\%)$
$V_\infty (m/s)$	Aleatory	± 30.84 $(\sigma = 15.42)$
$\Omega^{1,1}_{N2-N2}, \Omega^{2,2}_{N2-N2}$	Epistemic	$\pm 20\%$
$\Omega^{1,1}_{N2-N}, \Omega^{2,2}_{N2-N}$	Epistemic	$\pm 20\%$
$\Omega^{1,1}_{N2-O}, \Omega^{2,2}_{N2-O}$	Epistemic	$\pm 20\%$
$\Omega^{1,1}_{N2-O2}, \Omega^{2,2}_{N2-O2}$	Epistemic	$\pm 20\%$

- 10 total uncertain parameters (2 aleatory, 8 epistemic)
- Nested Sampling used for Validation
- 3 samples per dimension for epistemic variables (6,561 total)
- 5000 samples used for aleatory variables

Fay-Riddell Heating Results

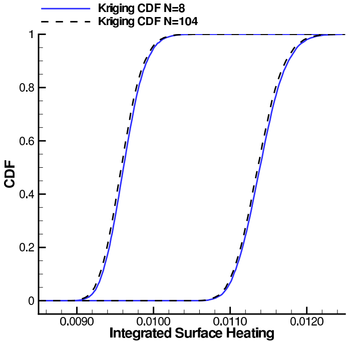
- Each β realization has associated CDF curve (30 million samples)
- Bounding CDF curves determined by optimization over β for fixed α
- Kriging model built from 4 pairs of optimization results
- 30 million function evaluations reduced to 157 function/gradient





Real Gas CFD Mixed Results

- CDF for bounds can be created from Kriging Model
- CDF created with Kriging model based on 8 ($\sim$ 500 f/g) and 104 (6176 f/g) pairs of optimizations
- CDF curves virtually identical, implying convergence of Kriging predictions



Real Gas CFD Mixed Results

- Multiple Optimizations used to approximate combined results
- Kriging model constructed for min and max values
- Monte Carlo performed on Kriging surrogate
- $99th$ percentile of Min/Max predicted

Training Data Size	F/G Evaluations	99^{th} percentile of Min	99^{th} percentile of Max
8	~ 500	1.017556×10^{-2}	1.206949×10^{-2}
15	~ 900	1.016681×10^{-2}	1.207132×10^{-2}
23	~ 1400	1.018928×10^{-2}	1.207939×10^{-2}
52	~ 3000	1.020232×10^{-2}	1.210513×10^{-2}
104	6176	1.020243×10^{-2}	1.210416×10^{-2}

- Statistic converges with handful of optimization results
- SOI method allows mixed UQ when nested strategy prohibitively expensive

Conclusions and Contributions

- Developed a two-dimensional hypersonic flow solver with adjoint capability
  - Five species, two temperature non-equilibrium real gas model
  - Adjoint implemented with automatic differentiation (Tapenade)
- Utilized gradient information for sensitivity analysis to identify most important model parameters and contributions to uncertainty
  - Derivative allows rapid localized sensitivity analysis
  - Global sensitivity analysis accelerated with sampling from gradient-enhanced regression
- Demonstrated gradient-based uncertainty quantification for hypersonic simulation

Conclusions and Contributions

- 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.

Future Work

- Methods should be applied to a wider variety of simulations and test cases
- Extend proposed methods to higher dimension and multiple outputs
- Explore Hessian for hypersonic flow due to extremely low cost of linear solution
  - Incorporate Hessian into surrogate construction
  - Apply more sophisticated optimization algorithms
- Kriging-based efficient global optimization for epistemic uncertainty
- Explore strategies to account for other types of uncertainty, such as model discrepancy and numerical errors.
- Utilize uncertainty information within optimization and solution adaptation

Questions?

Supplemental Material

Kriging Models

- Built upon assumption of gaussian process:

$$y(x) = N(m(x), K(x, x'; \theta)) \tag{1}$$

- $m(x)$ is the mean function
  - Can be explicitly defined and combined with zero mean GP
  - Form can be assumed and included into construction (Universal Kriging)
- $K(x, x'; \theta)$ is the covariance between data points
  - For Kriging, function of distance between points
  - Optimal parameters θ determined by based on simulation observations and likelihood equation
- Kriging output is a GP and predictions have associated distributions

Gradient Enhancement

- Covariance Matrix extended to block matrix

$$\underline{K} = \begin{bmatrix} cov(Y,Y) & cov(Y,\nabla Y) \\ cov(\nabla Y, Y) & cov(\nabla Y, \nabla Y) \end{bmatrix}$$

- Function/Function

$$cov(y,y') = k(\vec{x},\vec{x}').$$

- Derivative/Function

$$cov(\frac{\partial y}{\partial x_k}, y') = \frac{\partial}{\partial x_k} k(\vec{x},\vec{x}').$$

- Derivative/Derivative

$$cov(\frac{\partial y}{\partial x_k}, \frac{\partial y'}{\partial x_l'}) = \frac{\partial^2}{\partial x_k \partial x_l'} k(\vec{x},\vec{x}').$$

- Covariance Function must now be twice differentiable

Covariance Functions

- Covariance Function product of 1D functions

$$k(\vec{x},\vec{x}';\theta) = \sigma^2 \prod_{i=1}^{d} k_i(x_i - x_i';\theta_i)$$

- One dimensional Functions
  - Squared Exponential:

$$k_i(x_i - x_i') = e^{-\left(\frac{x_i - x_i'}{\theta_i}\right)^2}$$

  - Matern Function $\nu = \frac{3}{2}$:

$$k_i(x_i - x_i') = \left(1 + \sqrt{3}\left|\frac{x_i - x_i'}{\theta_i}\right|\right) e^{-\sqrt{3}\left|\frac{x_i - x_i'}{\theta_i}\right|}$$

  - Matern Function $\nu = \frac{5}{2}$:

$$k_i(x_i - x_i') = \left(1 + \sqrt{5}\left|\frac{x_i - x_i'}{\theta_i}\right| + \frac{5}{3}\left|\frac{x_i - x_i'}{\theta_i}\right|^2\right) e^{-\sqrt{5}\left|\frac{x_i - x_i'}{\theta_i}\right|}$$

Covariance Functions

- Cubic Spline 1:

$$k_i(x_i - x_i') = \begin{cases} 1 - 15\left|\frac{x_i - x_i'}{\theta_i}\right|^2 + 30\left|\frac{x_i - x_i'}{\theta_i}\right|^3 & \text{for } 0 \le \left|\frac{x_i - x_i'}{\theta_i}\right| \le 0.2 \\ 1.25\left(1 - \left|\frac{x_i - x_i'}{\theta_i}\right|\right)^3 & \text{for } 0.2 \le \left|\frac{x_i - x_i'}{\theta_i}\right| \le 1 \\ 0 & \text{for } \left|\frac{x_i - x_i'}{\theta_i}\right| \ge 1 \end{cases}$$

- Cubic Spline 2:

$$k_i(x_i - x_i') = \begin{cases} 1 - 6\left|\frac{x_i - x_i'}{\theta_i}\right|^2 + 6\left|\frac{x_i - x_i'}{\theta_i}\right|^3 & \text{for } 0 \le \left|\frac{x_i - x_i'}{\theta_i}\right| \le 0.5 \\ 2\left(1 - \left|\frac{x_i - x_i'}{\theta_i}\right|\right)^3 & \text{for } 0.5 \le \left|\frac{x_i - x_i'}{\theta_i}\right| \le 1 \\ 0 & \text{for } \left|\frac{x_i - x_i'}{\theta_i}\right| \ge 1 \end{cases}$$

- Gives sparse covariance matrix/better condition number for Large sample size

GEUK Details

- Covariance Parameters determined via Maximum Likelihood:

$$\log(p(y|X;\theta)) = -\frac{1}{2}[Y^T \delta Y^T]\underline{K}^{-1}\begin{bmatrix} Y \\ \delta Y \end{bmatrix} + \frac{1}{2}[Y^T \delta Y^T]\underline{C}\begin{bmatrix} Y \\ \delta Y \end{bmatrix} - \frac{1}{2}log|P| - \frac{1}{2}log|M| - \frac{1}{2}log|\underline{A}| - \frac{nd+n-s}{2}log 2\pi$$

- Optimization carried out using Pattern search or simplex
- Most Expensive and Problematic part of Surrogate Construction
  - Optimization problem scales with dimension
  - Covariance Matrix inversion $O(n^3 d^3)$ if dense
  - Improvements possible with sparse covariance and better optimization algorithm

Regression Basis

- Hermite Polynomials used as Basis
- Basis set is truncated based on sensitivity analysis (High order used for most sensitive parameters)
- Derivatives included in Basis to reduce number of required samples
- Parameters assumed to follow GP:

$$\hat{\beta} = \left([H^T G^T] \underline{K}^{-1} \begin{bmatrix} H \\ G \end{bmatrix} \right)^{-1} [H^T G^T] \underline{K}^{-1} \begin{bmatrix} Y \\ \delta Y \end{bmatrix}$$

- Function predictions:

$$y_* | \vec{X}, Y, \delta Y = [k_*^T w_*^T] \underline{K}^{-1} \begin{bmatrix} Y \\ \delta Y \end{bmatrix} + \left(h(\vec{x}_*) - [k_*^T w_*^T] \underline{K}^{-1} \begin{bmatrix} H \\ G \end{bmatrix} \right) \hat{\beta}$$

- Variance Prediction

$$V[y_*] = cov(\vec{x}_*, \vec{x}_*) - k_*^T K^{-1} k_* + R(\vec{x}_*) A^{-1} R(\vec{x}_*)^T. \qquad (2)$$

Linear Methods

- Fast statistic approximations possible with single function/gradient:

$$\mu = y(\bar{x})$$

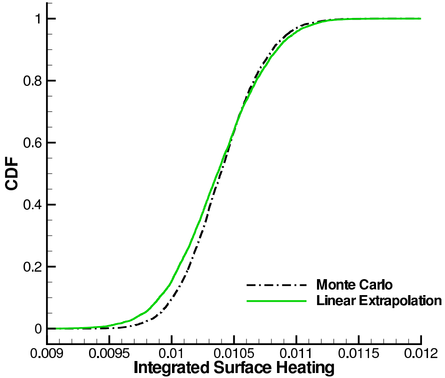
$$\sigma^2 = \sum_{i=1}^{d} \frac{\partial y}{\partial x_i}^2 \sigma_{x_i}^2$$

- Taylor series can be used when arbitrary statistic required:

$$y_{lin}(x) = y(\bar{x}) + \left.\frac{\partial y}{\partial x_i}\right|_{\bar{x}} (x_i - \bar{x}_i)$$

Statistic	Momnet Method	Linear Extrapolation	Monte Carlo Lower	Monte Carlo Upper
Mean	1.0370E-002	1.0369E-002	1.0393E-002	1.0409E-002
Variance	1.3790E-007	1.3412E-007	9.3979E-008	1.0106E-007
Std. Deviation	3.7134E-004	3.6622E-004	3.0656E-004	3.1789E-004
95% CI	±7.1616%	±7.0638%	±5.8994%	±6.1083%

Linear Methods



- Given extreme cost savings, accuracy likely sufficient for optimization
- Accurate uncertainty predictions require more sophisticated surrogates

Validity of Optimization

- Optimization bounds appear overly conservative
- As samples per dimension increases, sampling bounds approach optimization bounds
- Property demonstrated in 6 dimensions (2 aleatory, 4 epistemic)