Uncertainty Quantification in Viscous Hypersonic Flows using Gradient Information and Surrogate Modeling

Brian A. Lockwood, Markus P. Rumpfkeil, Wataru Yamazaki and Dimitri J. Mavriplis

Mechanical Engineering
University of Wyoming

January 4, 2010

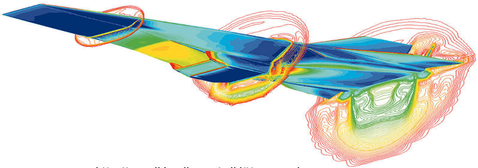
Outline

Outline

- Motivation and Introduction
- Overview of physical models and solver
- Sensitivity derivation and example results
- Perfect Gas Case Study
- Preliminary Real Gas
- Conclusions and Future Work

Hypersonics Overview

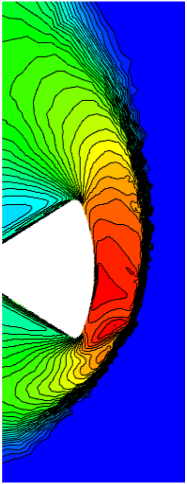
- Hypersonic Flow roughly defined as $M > 5$
- Characterized by:
  - Strong Shocks
  - Internal Energy Modes (Vibrational, Electronic)
  - Chemical Reactions
- Simulations are Nonlinear and Numerically Stiff
- Require Empirical Relations/Experimental Constants
- Models can require hundreds of parameters to define (Arrhenius Reaction Coefficients, Curve fits, etc.)



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

Introduction

- Sensitivity/Uncertainty Quantification currently based on sampling
  - Thousands of flow solutions required
  - Computationally expensive
- Localized Sensitivity Derivative calculated using flow adjoint
  - Same Computational Cost of Flow Solve
  - Single Adjoint gives Sensitivity of single output w.r.t all inputs
  - Useful for Optimization and Uncertainty



Flow Solver Details

- Compressible Navier Stokes Equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \vec{F}(\mathbf{U}) = \nabla \cdot \vec{F}_v(\mathbf{U}) + \mathbf{S}(\mathbf{U}) \qquad (1)$$

- Steady, Two dimensional, cell-centered finite volume solver using unstructured triangles and/or quadrilaterals
- Solver uses a fully implicit, pseudo-time stepping method
- Perfect gas and 5 Species, 2 Temperature Real gas model examined
    - Chemical Components: N_2, O_2, NO,N,O
    - Temperatures: Translational-rotational, Vibrational-electronic

Physical Model

- Perfect gas variables

$$\mathbf{U} = \left\{ \begin{array}{c} \rho \\ \rho\vec{u} \\ \rho e_t \end{array} \right\} \quad \vec{F} = \left\{ \begin{array}{c} \rho\vec{u} \\ \rho\vec{u} \otimes \vec{u} + P \\ \rho\vec{u} h_t \end{array} \right\} \quad \vec{F}_v = \left\{ \begin{array}{c} 0 \\ \underline{\tau} \\ \underline{\tau} \cdot \vec{u} - \vec{q} \end{array} \right\}$$

- Sutherland's Law used for viscosity
- 5 Model Parameters required to define model:
  - Ratio of Specific Heats γ
  - Reynolds Number
  - Prandtl Number
  - Two constants within Sutherland's Law

Physical Model

- Five species, Two Temperature Real Gas Model

$$\mathbf{U} = \left\{ \begin{array}{c} \rho_s \\ \rho\vec{u} \\ \rho e_t \\ \rho e_v \end{array} \right\} \quad \vec{F} = \left\{ \begin{array}{c} \rho_s\vec{u} \\ \rho\vec{u}\otimes\vec{u} + P \\ \rho\vec{u}h_t \\ \rho\vec{u}h_v \end{array} \right\} \quad \mathbf{S} = \left\{ \begin{array}{c} \omega_s \\ 0 \\ 0 \\ \sum_s \omega_s \hat{D}_{v,s} + Q_{T-V} \end{array} \right\}$$

$$\vec{F}_v = \left\{ \begin{array}{c} -\rho_s \tilde{V}_s \\ \underline{\mathcal{T}} \\ \underline{\mathcal{T}} \cdot \vec{u} - \vec{q} - \vec{q}_v - \sum_s h_{t,s}\rho_s \tilde{V}_s \\ -\sum_s h_{v,s}\rho_s \tilde{V}_s - \vec{q}_v \end{array} \right\}$$

- Dunn-Kang chemical kinetics model used
- Transport quantities calculated using curve fits from Blottner *et al*
- Approximately 250 constants required to define physical model

Solver Description

- Solution marched to steady state using implicit pseudo-time stepping
- Method of Lines:

$$\frac{d\mathbf{U}}{dt} + \mathbf{R}(\mathbf{U}) = 0 \qquad (2)$$

- Unsteady residual given by:

$$\mathbf{J}(\mathbf{U}^n, \mathbf{U}^{n-1}) = \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t} + \mathbf{R}(\mathbf{U}^n) \qquad (3)$$

- Nonlinear equation $\mathbf{J}(\mathbf{U}^n, \mathbf{U}^{n-1}) = 0$ solved approximately at each time step using Inexact Newton

$$[P]\,\delta\mathbf{U}^k = -\mathbf{J}(\mathbf{U}^k, \mathbf{U}^{n-1}) \qquad (4)$$

$$\mathbf{U}^{k+1} = \mathbf{U}^k + \lambda\delta\mathbf{U}^k \qquad (5)$$

Sensitivity Derivation

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

$$L = L(D, \mathbf{U}(D)) \quad (6)$$
$$\mathbf{R} = \mathbf{R}(D, \mathbf{U}(D)) = 0 \quad (7)$$

- Objective and Constraint may be differentiated using the Chain rule

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial D} \quad (8)$$
$$\frac{d\mathbf{R}}{dD} = \frac{\partial \mathbf{R}}{\partial D} + \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial D} = 0 \quad (9)$$

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

$$\frac{\partial \mathbf{U}}{\partial D} = \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1} \frac{\partial \mathbf{R}}{\partial D} \quad (10)$$

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

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} - \frac{\partial L}{\partial \mathbf{U}} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-1} \frac{\partial \mathbf{R}}{\partial D} \tag{11}$$

- Transpose Equation (Adjoint Sensitivity Equation)

$$\frac{dL}{dD}^{T} = \frac{\partial L}{\partial D}^{T} - \frac{\partial \mathbf{R}}{\partial D}^{T} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-T} \frac{\partial L}{\partial \mathbf{U}}^{T} \tag{12}$$

- Flow Adjoint (Independent of D):

$$\mathbf{\Lambda} = -\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{-\mathbf{T}} \frac{\partial \mathbf{L}}{\partial \mathbf{U}}^{\mathbf{T}} \tag{13}$$

- Solved Using Defect Correction:

$$[P]^{T} \delta \mathbf{\Lambda}^{k} = -\frac{\partial L}{\partial \mathbf{U}}^{T} - \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^{T} \mathbf{\Lambda} = -R_{\mathbf{\Lambda}}(\mathbf{\Lambda}^{k}) \tag{14}$$

$$\mathbf{\Lambda}^{k+1} = \mathbf{\Lambda}^{k} + \lambda \delta \mathbf{\Lambda}^{k} \tag{15}$$

Demonstration Flow Results

- 5 km/s cylinder test case
- Fixed Wall temperature
- Super-catalytic Wall
- Results compared with LAURA (NASA Code used for Re-entry Vehicles)

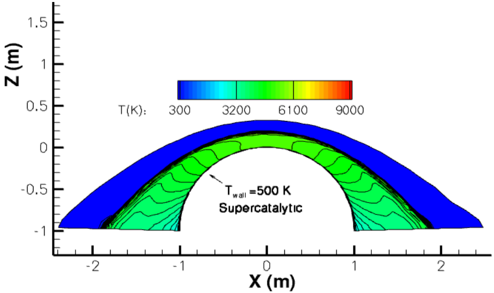
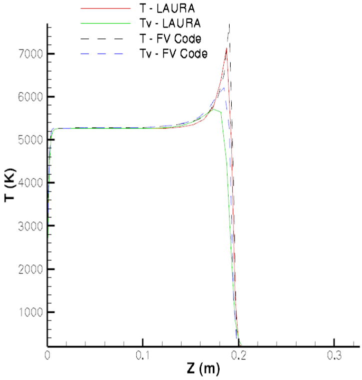


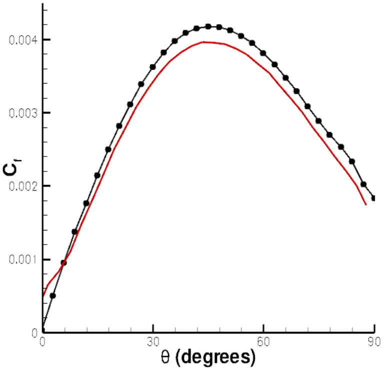
Table: Benchmark Flow Conditions

$V_\infty =$	5 km/s
$\rho_\infty =$	0.001 kg/m^3
$T_\infty =$	200 K
$T_{wall} =$	500 K
$M_\infty =$	17.605
$Re_\infty =$	376,930
$Pr_\infty =$	0.72

Flow Results



Temperature along Stagnation Streamline



Skin Friction Distribution

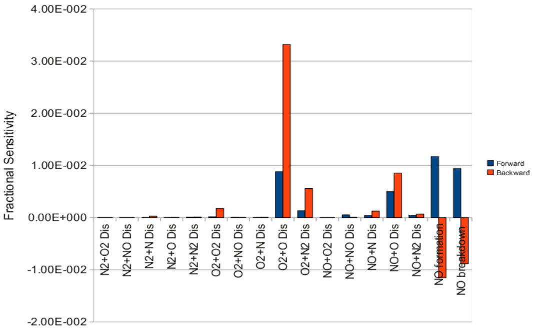
Real Gas Parameter Sensitivity

- Sensitivity of Surface Heating to Arrhenius Coefficients (34 Total):

$$K_f = C_f T_a^{\eta_f} e^{-\frac{E_{a,f}}{kT_a}} \quad (16)$$

$$K_b = C_b T_a^{\eta_b} e^{-\frac{E_{a,b}}{kT_a}} \quad (17)$$

- Sensitivities Expressed as fractional changes (i.e. $\frac{dL/L}{dD/D}$)



Uncertainty Quantification using Surrogates

- With Sensitivity derivatives calculated, attempt to reduce cost of Uncertainty Quantification
  - Dimension reduction to focus on highly sensitive parameters
  - Gradient Enhancement of Surrogate Model
- Need to Quantify Uncertainty in Output due to Uncertain Model Parameters
- Monte Carlo typically used due to ease of implementation and Nonlinear nature of most problems
- Monte Carlo Drawbacks:
  - Slow Convergence of Statistics
  - Requires Large number of samples (code evaluations)
  - (Prohibitively) Large computational cost

Perfect Gas Case Study

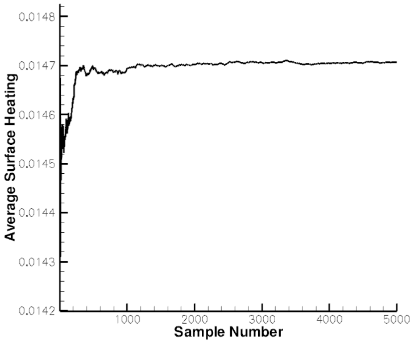
- Uncertainty in Surface Heating based on Freestream Conditions
- Using Perfect Gas Model, Five variables required (Incoming Flow Conditions):

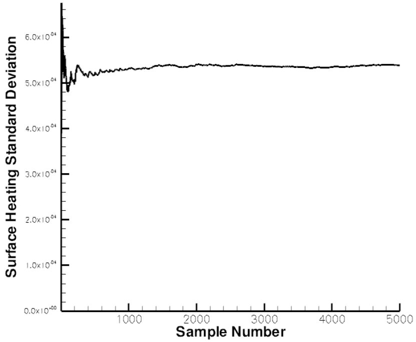
Variable	Mean Value	Standard Deviation
$V_\infty =$	5 km/s	15.42 m/s
$\rho_\infty =$	$0.001\ kg/m^3$	$5 \times 10^{-5}\ kg/m^3$
$T_\infty =$	200 K	10 K
$\mu_\infty =$	$1.3265 \times 10^{-5} kg/(m-s)$	$6.6325 \times 10^{-7} kg/(m-s)$
$k_\infty =$	$1.8576 \times 10^{-2} W/(m-K)$	$9.2880 \times 10^{-4} W/(m-K)$

- 5000 Samples generated via Latin Hyper Cube assuming Aleatory Uncertainty

Mean (μ)	1.47069×10^{-2}
Standard Deviation (σ)	5.38407×10^{-4}
95% Confidence Interval	$\pm 7.3218\%$

Monte Carlo Convergence





Linear Based Models

- For Small Uncertainty, Linear Extrapolation about Mean can be used:
- First Order Moment Method: (Aleatory)

$$\mu_{\mathcal{J}}^{(1)} = \mathcal{J}(D_0)$$
$$\sigma_{\mathcal{J}}^{(1)} = \sqrt{\sum_{j=1}^{M} \left(\left. \frac{d\mathcal{J}}{dD_j} \right|_{D_0} \sigma_{D_j} \right)^2}, \quad (18)$$

- Comparison with Monte Carlo:

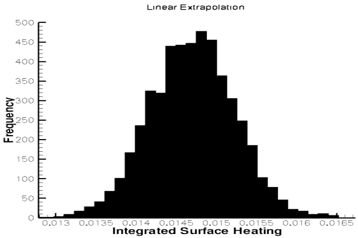
	Moment Method	Nonlinear Monte Carlo
Mean (μ)	1.46917×10^{-2}	1.47069×10^{-2}
Standard Deviation (σ)	5.32578×10^{-4}	5.38407×10^{-4}
95% Confidence Interval	$\pm 7.2501\%$	$\pm 7.3218\%$

Linear Extrapolation

- Extrapolation about Mean gives Linear representation of design space
- Straight-Forward Linear Extrapolation:

$$\mathcal{J}_{\text{Lin}} = \mathcal{J}\Big(D_0, q(D_0)\Big) + \left.\frac{d\mathcal{J}}{dD}\right|_{D_0} \cdot (D - D_0), \tag{19}$$

- Inexpensive Monte Carlo Sampling from Surrogate gives PDF



Kriging Surrogate Model

- Kriging Models borrowed from Geostatistics
- Create Model of Design Space based on assumption of Gaussian Process:

$$L(D) = N(m(D), K(D, D')) \tag{20}$$

- Ordinary Kriging: $m(D) = \mu_o$
- Gives Model Prediction with associated variance
- Can incorporate derivative observations to increase accuracy (Gradient Enhancement/Co-Kriging)
- Mean Kriging Prediction used to replace code evaluations
- Can also be expanded to include second order derivatives (Yamazaki and Mavriplis, 2010)

Kriging Results

- Monte Carlo Results

Mean	Standard Deviation	95% CI
1.47069×10^{-2}	5.38407×10^{-4}	$\pm 7.3218\%$

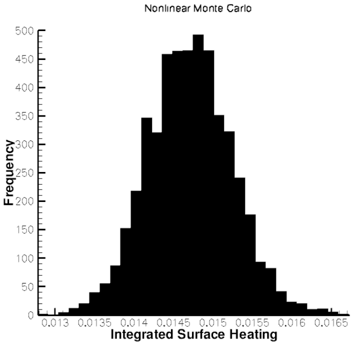
- Statistics Based on Kriging Surface:

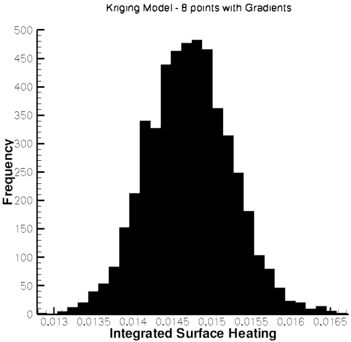
Sample Points	Mean	Standard Deviation	95% CI
10	1.47550×10^{-2}	5.48708×10^{-4}	7.4376%
20	1.47090×10^{-2}	5.39907×10^{-4}	7.3412%
30	1.47150×10^{-2}	5.46086×10^{-4}	7.4222%
50	1.47070×10^{-2}	5.38767×10^{-4}	7.3267%

- Statistics Based on Gradient Enhanced Kriging Model:

Sample Points	Mean	Standard Deviation	95% CI
4	1.47070×10^{-2}	5.38544×10^{-4}	7.3236%
8	1.47090×10^{-2}	5.39268×10^{-4}	7.3325%
50	1.47070×10^{-2}	5.38424×10^{-4}	7.3220%

Kriging PDF


Nonlinear Monte Carlo
Frequency
0
50
100
150
200
250
300
350
400
450
500
0.013
0.0135
0.014
0.0145
0.015
0.0155
0.016
0.0165
Integrated Surface Heating


Kriging Model - 8 points with Gradients
Frequency
0
50
100
150
200
250
300
350
400
450
500
0.013
0.0135
0.014
0.0145
0.015
0.0155
0.016
0.0165
Integrated Surface Heating

Epistemic Uncertainty

- Parameters lie within intervals, no associated distributions.
- Input Parameter Intervals for Perfect Gas Problem

Variable	Lower Bound	Upper Bound
$V_\infty(m/s) =$	4969.16	5030.84
$\rho_\infty\ (kg/m^3)=$	0.0009	0.0011
$T_\infty(K) =$	180	220
$\mu_\infty(kg/(m-s)) =$	1.19385×10^{-5}	1.45915×10^{-5}
$k_\infty(W/(m-K)) =$	1.6718×10^{-2}	2.0434×10^{-2}

- Output interval estimated using interval addition:

$$\Delta_J^{(1)} = \sum_{j=1}^{M} \left| \left.\frac{dJ}{dD_j}\right|_{D_0} \Delta_{D_j} \right| \tag{21}$$

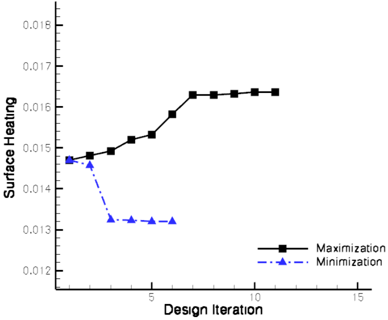
- Constrained Optimization used to determine actual output interval (using L-BFGS due to availability of gradient)

Epistemic Uncertainty

- Comparison of Linear to Optimization

Method	Lower Bound	Upper Bound	Interval Width
Linear	1.3121×10^{-2}	1.6262×10^{-2}	21.38%
Optimization	1.3201×10^{-2}	1.6359×10^{-2}	21.49%

- Optimization Convergence



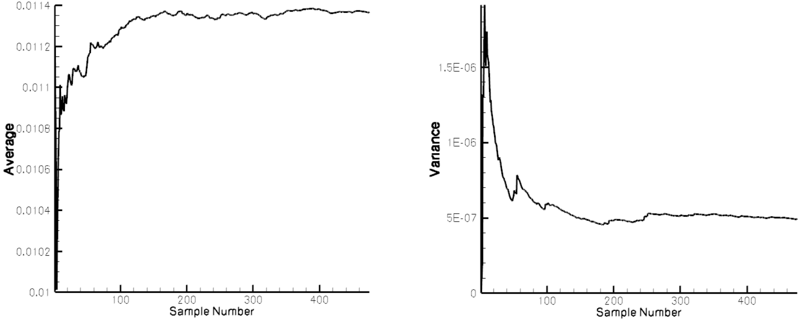
Real Gas Test Case

- 15 parameters treated as uncertain (distributed by normal distribution)
- Table of Variables with Standard deviations:

Number	Variable	Standard Deviations
1	$\rho_\infty \; (kg/m^3)$	5%
2	$V_\infty (m/s)$	15.42
3-4	$\Omega^{1,1}_{N2-N2}, \Omega^{2,2}_{N2-N2}$	10%
5-6	$\Omega^{1,1}_{N2-N}, \Omega^{2,2}_{N2-N}$	10%
7-8	$\Omega^{1,1}_{N2-O}, \Omega^{2,2}_{N2-O}$	10%
9-10	$\Omega^{1,1}_{N2-O2}, \Omega^{2,2}_{N2-O2}$	10%
11	$log_{10}(C_{b-O2+O \leftrightharpoons 2O+O})$	0.5
12	$log_{10}(C_{f-N2+O \leftrightharpoons NO+N})$	0.5
13	$log_{10}(C_{b-N2+O \leftrightharpoons NO+N})$	0.5
14	$log_{10}(C_{f-NO+O \leftrightharpoons O2+N})$	0.5
15	$log_{10}(C_{b-NO+O \leftrightharpoons O2+N})$	0.5

Monte Carlo Results

- Monte Carlo with Latin Hypercube sampling used for validation (475 Total Samples)
- Convergence History for Average and Variance



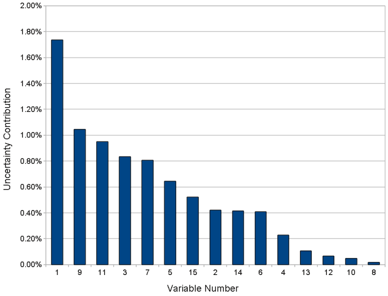
Monte Carlo Results

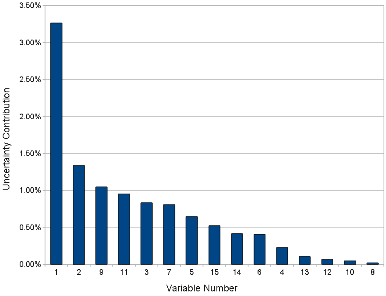
- Monte Carlo sample size determined by available computational budget
- Error bounds for average and confidence interval provided by sample variance and sample kurtosis
- Table for final MC statistics with 95% confidence bound estimate

Statistic	Value	Confidence Bound
Average	1.1368×10^{-2}	$\pm 6.46 \times 10^{-5}$
Variance	4.9562×10^{-7}	$\pm 5.10 \times 10^{-8}$
Standard Deviation	7.0400×10^{-4}	$\pm 3.63 \times 10^{-5}$
95% Confidence Interval	$\pm 12.385\%$	$\pm 0.637\%$

Linear Results

- Linear Representation used to estimate uncertainty contribution from each variable ($\frac{\partial L}{\partial D_i}\sigma_i$)
- Variable Ranking for Non-dimensional and Dimensional Surface heating:





- Rankings in general agreement with other works (e.g. Palmer 2007)

Linear Results

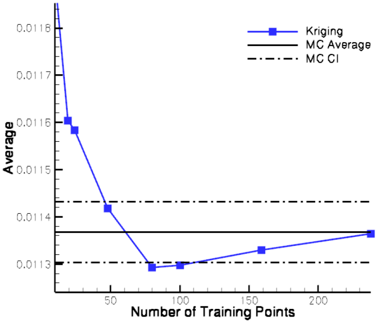
- Moment Method used to estimate total variance of Surface heating:

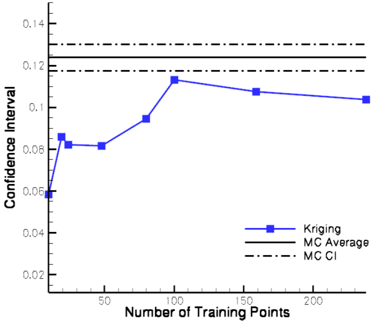
	Moment Method	Nonlinear Monte Carlo
Mean (μ)	1.1238×10^{-2}	1.1368×10^{-2}
Standard Deviation (σ)	3.1033×10^{-4}	7.0400×10^{-4}
95% Confidence Interval	$\pm 5.5231\%$	$\pm 12.385\%$

- Linear model underestimates average and variance
- May be valuable for situations only requiring rough variance estimate

Kriging Results

- Kriging model used to improve results
- Average and Confidence Interval Estimate vs. Training Points





- Kriging results provide reasonable statistics with approximately 100 samples
- Co-Kriging results unavailable due to adjoint solver robustness issues

Summary

Conclusions:

- Adjoint provides valuable information for hypersonic problems
- Addition of derivatives greatly reduces the required number of samples for a surrogate
- Linear and Kriging representations can effectively represent perfect gas design space
- Real gas design space requires more complex surrogate
- Linear analysis can provide estimates of individual contributions and rough approximations of statistics

Future Work:

- Adjoint solver robustness enhancements
- Epistemic Uncertainty propagation via optimization based on Kriging model
- Variable Fidelity Kriging Models