Comparison of Response Surface and Kriging Models for Multidisciplinary Design Optimization

Paper No. AIAA-98-4755

Timothy W. Simpson
Mech Engr & Ind Engr Depts
Penn State University
University Park, PA 16802

Timothy M. Mauery
Civil and Env Engr Dept
Brigham Young University
Provo, UT 84602

John J. Korte
Multidisciplinary Optimization Branch
NASA Langley Research Center
Mail Stop 159, Hampton, VA 23681

Farrokh Mistree
Woodruff School of Mech Engr
Georgia Institute of Technology
Atlanta, GA 30332-0405

This work has been supported by the National Aeronautics and Space Administration under NASA Contract NAS1-19480 while in residence at the Institute for Computer Applications in Science and Engineering (ICASE) at the NASA Langley Research Center in Hampton, Virginia.

PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering

Email: tws8@psu.edu

Presentation Outline

- Approximations in MDO
  - Motivation for using approximations
  - Approximation techniques and concerns
  - Overview of response surface and kriging models
- Multidisciplinary Design of an Aerospike Nozzle
  - Introduce example
  - Geometry and MDO decomposition
  - Approximation specifics
  - Graphical comparison and error analysis
  - Optimization study and results
- Closing Remarks and Ongoing Work

Why Use Approximations in MDO?

- Gain a better understanding of relationship between design variables, $\underline{X}$, and responses, $\underline{Y}$
- Facilitate integration of domain dependent analysis codes and simulations
- Provide surrogate approximations for rapid concept exploration and evaluation
- Find better solutions through improved convergence (smoothing of non-linearities and numerical noise)
- Identify important design variables through Analysis of Variance (ANOVA)

Approximation Techniques

EXPERIMENTAL DESIGN	MODEL CHOICE	MODEL FITTING	SAMPLE METAMODELING TECHNIQUES
(Fractional) Factorial	Polynomial (linear, quadratic)	Least Squares Regression	Response Surface * Methodology
Central Composite	Splines (linear, cubic)	Weighted Least Squares Regression	
Box-Behnken			
D-Optimal	Realization of a Stochastic Process	Best Linear Unbiased Predictor (BLUP)	Kriging *
G-Optimal			
Orthogonal Array	Kernel Smoothing		
Plackett-Burman	Radial Basis Functions	Best Linear Predictor (BLP)	
Hexagon			
Hybrid		Log-Likelihood	
Latin Hypercube	Network of Neurons	Backpropagation	Neural Networks
Select By Hand			
Random Selection	Rulebase or Decision Tree	Entropy (info.-theoretic)	Inductive Learning

PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

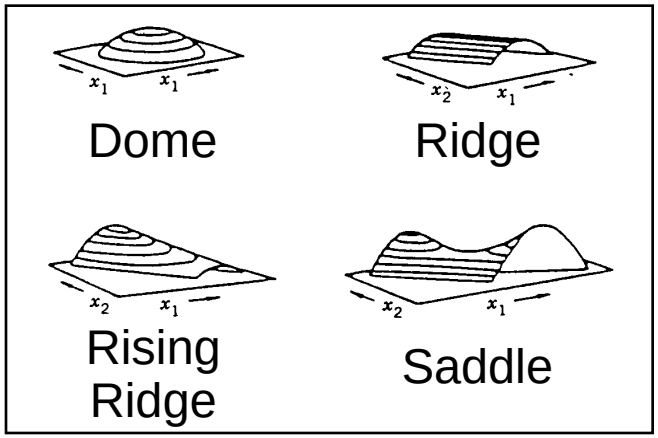
Response Surfaces (Myers and Montgomery, 1996)

- General form of a response surface:

$$y(\mathbf{x}) = f(\mathbf{x}) + \varepsilon$$

where:

- $y(\mathbf{x})$ is unknown function of interest
- $f(\mathbf{x})$ is a polynomial function of $\mathbf{x}$
- $\varepsilon \sim$ i.i.d. $N(\mu=0, \sigma^2 \neq 0, Cov=0)$



Example Response Surfaces (Box and Draper, 1987)

- Remarks:
  - $f(\mathbf{x})$ dictates "global" behavior of model
  - $f(\mathbf{x})$ is often first- or second-order polynomial
  - statistical measures (e.g., t-statistic and F-test) for validation may not be applicable when computer codes are deterministic

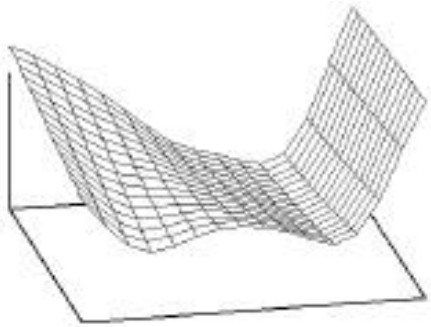
Overview of Kriging (Sacks, et al., 1989)

- General form of a kriging model:

$$y(\mathbf{x}) = f(\mathbf{x}) + Z(\mathbf{x})$$

where:

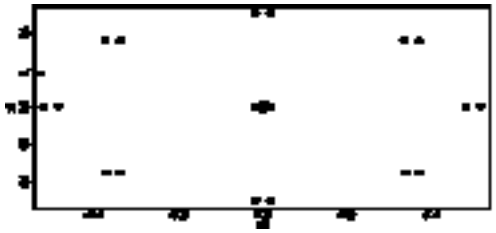
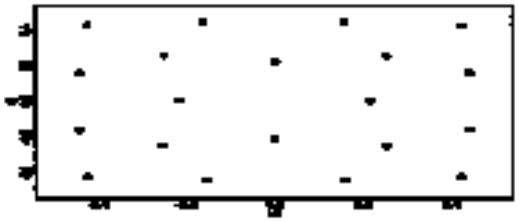
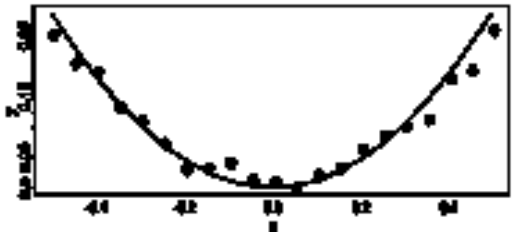
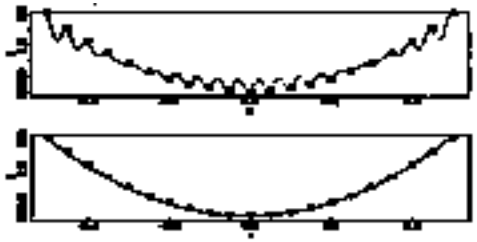
  - $y(\mathbf{x})$ is unknown function of interest
  - $f(\mathbf{x})$ is a known polynomial function of $\mathbf{x}$
  - $Z(\mathbf{x}) \sim N(\mu=0, \sigma^2 \neq 0, Cov \neq 0)$



Example
Kriging Model

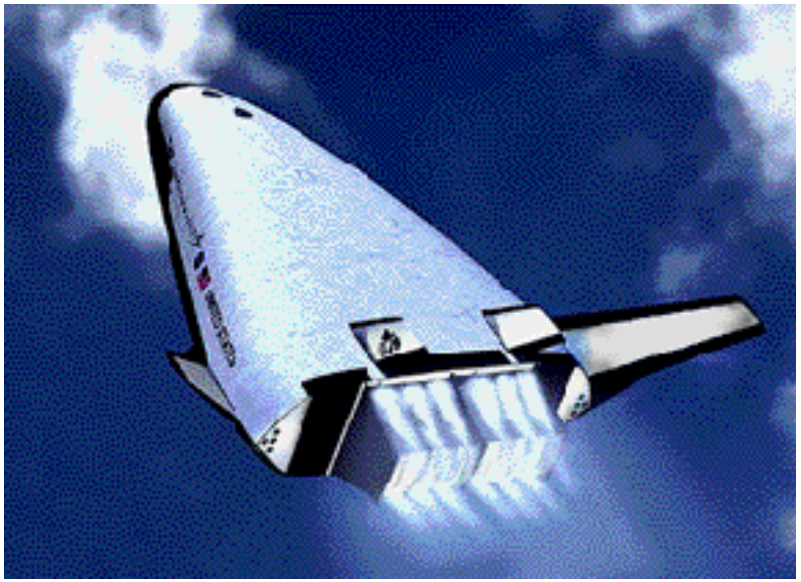
- Remarks:
  - kriging model interpolates the sampled data
  - $f(\mathbf{x})$ dictates "global" behavior of model in the design space
  - $f(\mathbf{x})$ is often taken as a constant term, β
  - $Z(\mathbf{x})$ dictates "local" behavior of the model

DOE/RSM versus DACE/Kriging (Booker, 1996)

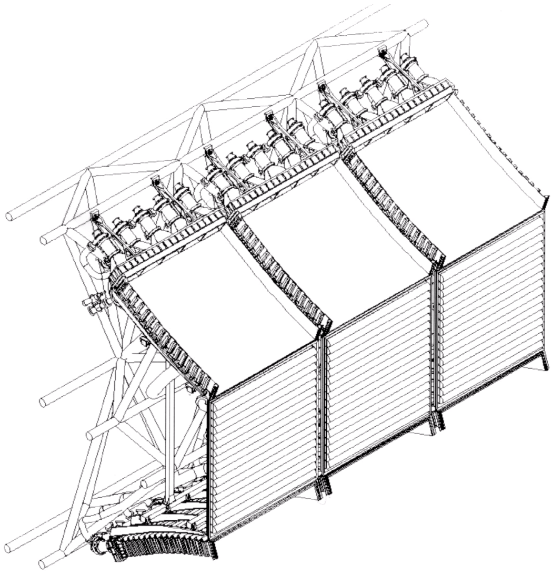
	DOE/RSM	DACE/Kriging
Experimental Design Input settings at which to obtain output	Account for variability 	Space filling 
Models Inexpensive model to estimate output at untried input	Least squares fit 	Maximum likelihood estimate 
Validation Determine adequacy of fit	t-tests and F-statistics R-square Residual plots	Cross validation Integrated mean square error

Aerospike Nozzle Example (Korte, et al., 1997)

- *Objective:* Compare and contrast the use of second-order response surface models and kriging models in the multidisciplinary design of an aerospike nozzle



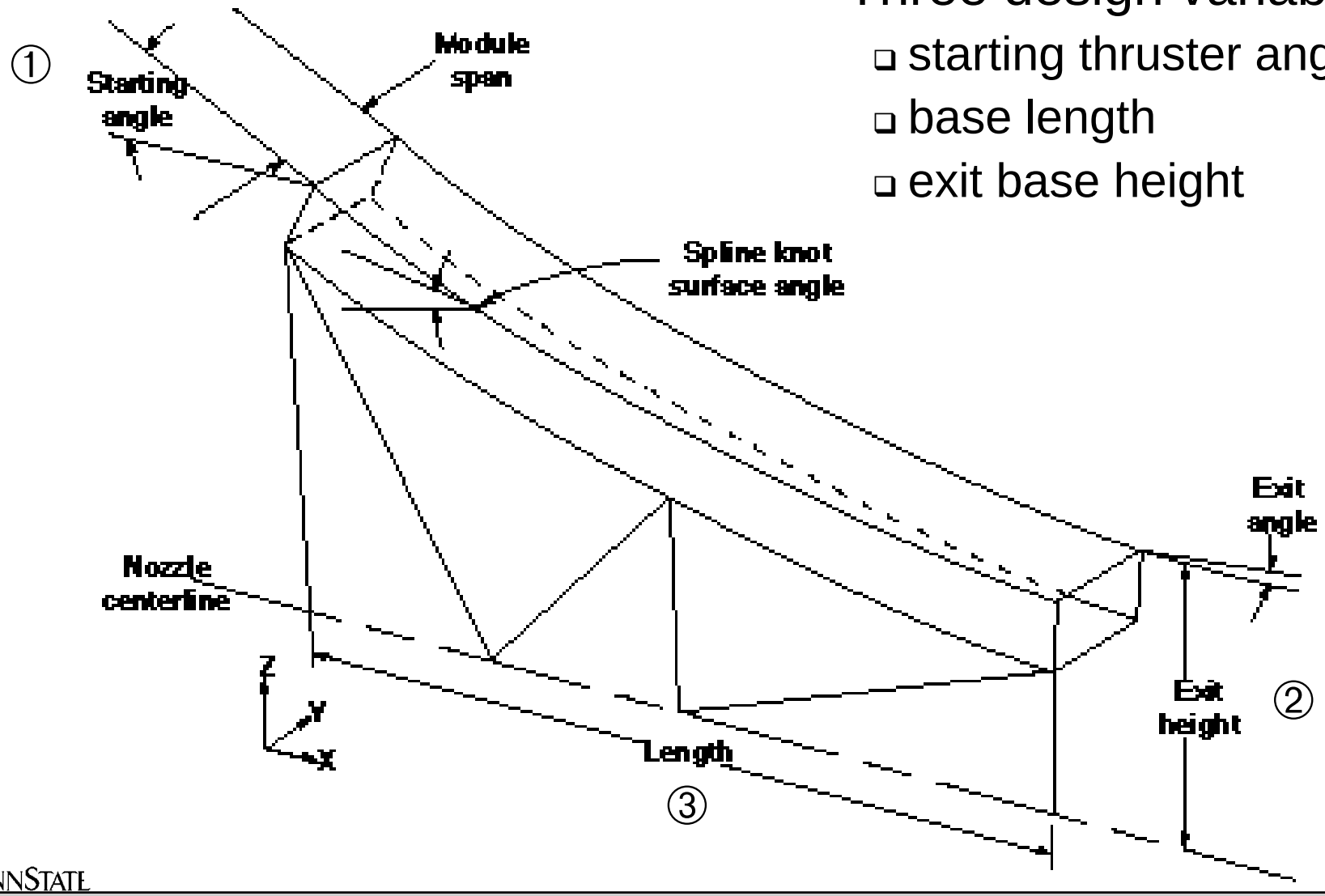
Venture Star RLV



Aerospike Nozzle

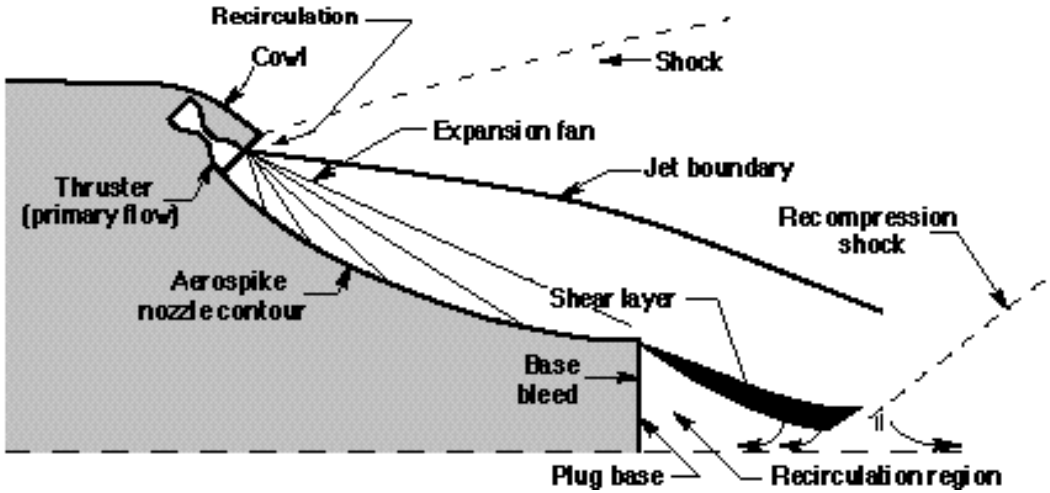
Aerospike Nozzle: Geometry

- Three design variables:
  - starting thruster angle
  - base length
  - exit base height



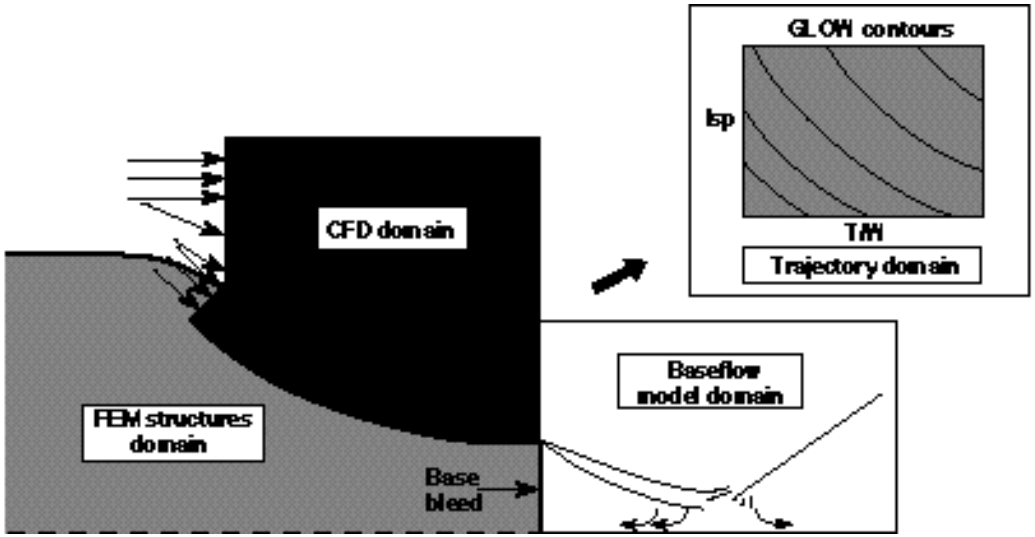
PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Aerospike Nozzle: MDO Decomposition



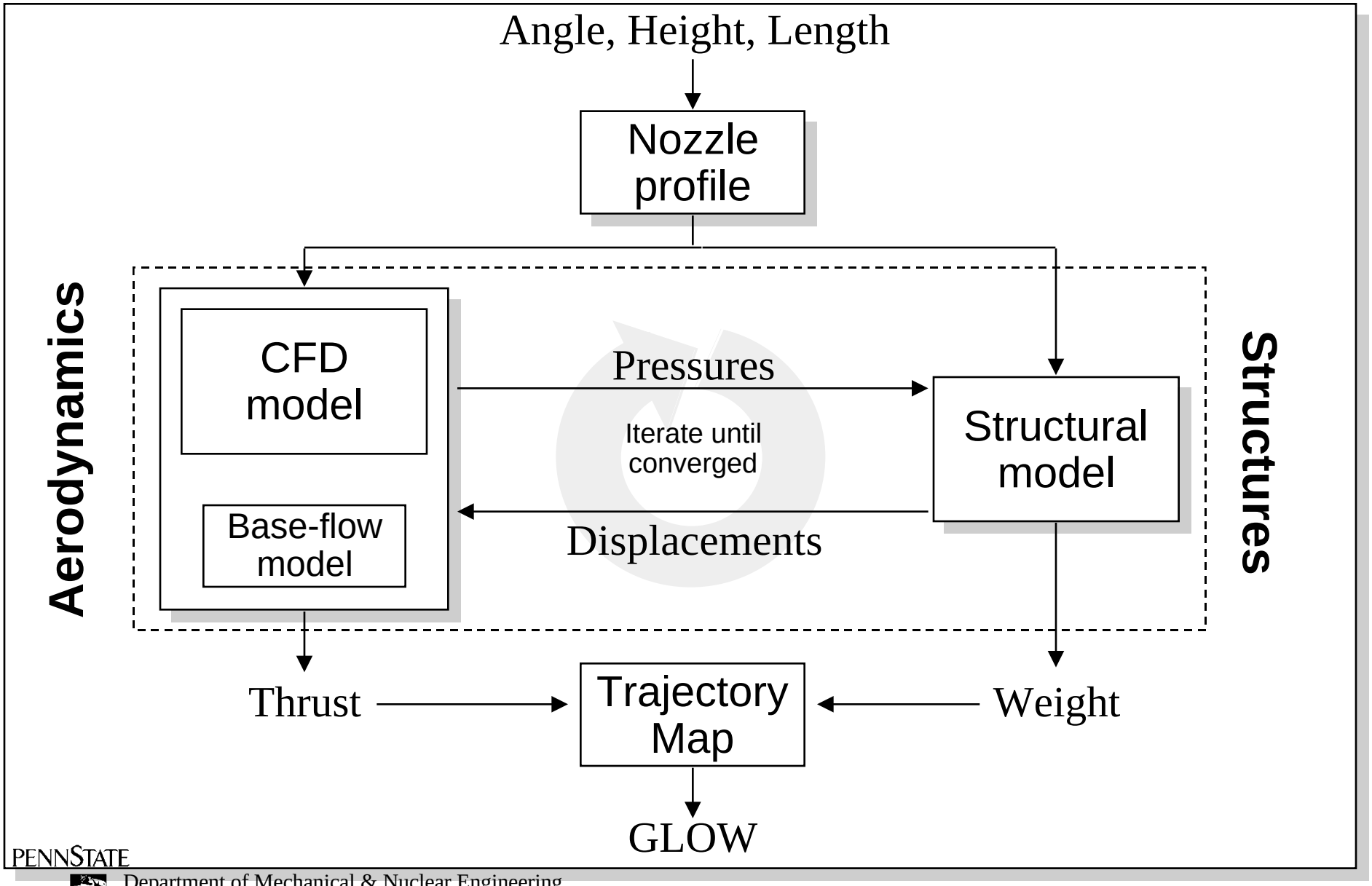
Aerospike Components and Flow-Field Characteristics

Multidisciplinary Domain Decomposition



PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Aerospike Nozzle: MDO Interactions

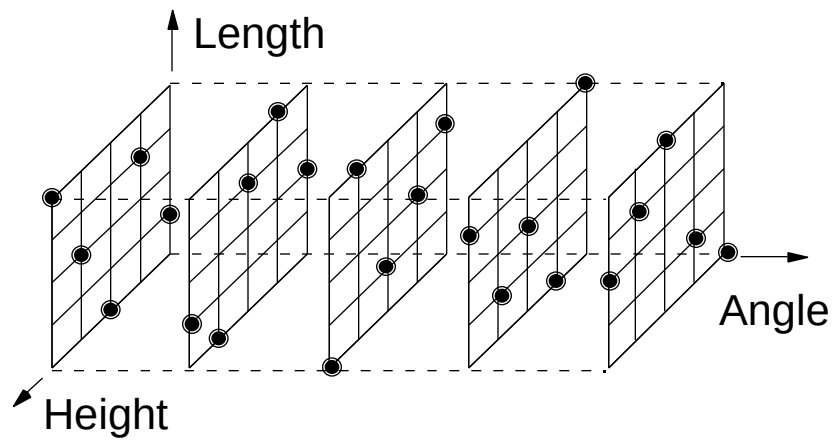


PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

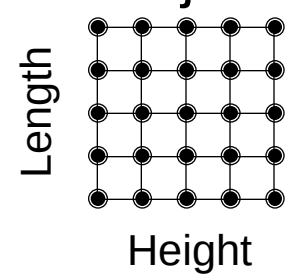
Aerospike Nozzle: Approximation Specifics

- Design variables (3):
  - Angle, height, length
- Sampling strategy:
  - 25 point randomized OA
- Model choice:
  - 2nd order response surface
  - Kriging : β + Gaussian corr. fcn.
- Responses of interest (3):
  - Thrust - output from CFD code
  - Weight - output from NASTRAN optimization
  - GLOW - tabulated as a function of thrust and weight

3-D View of Sample Points

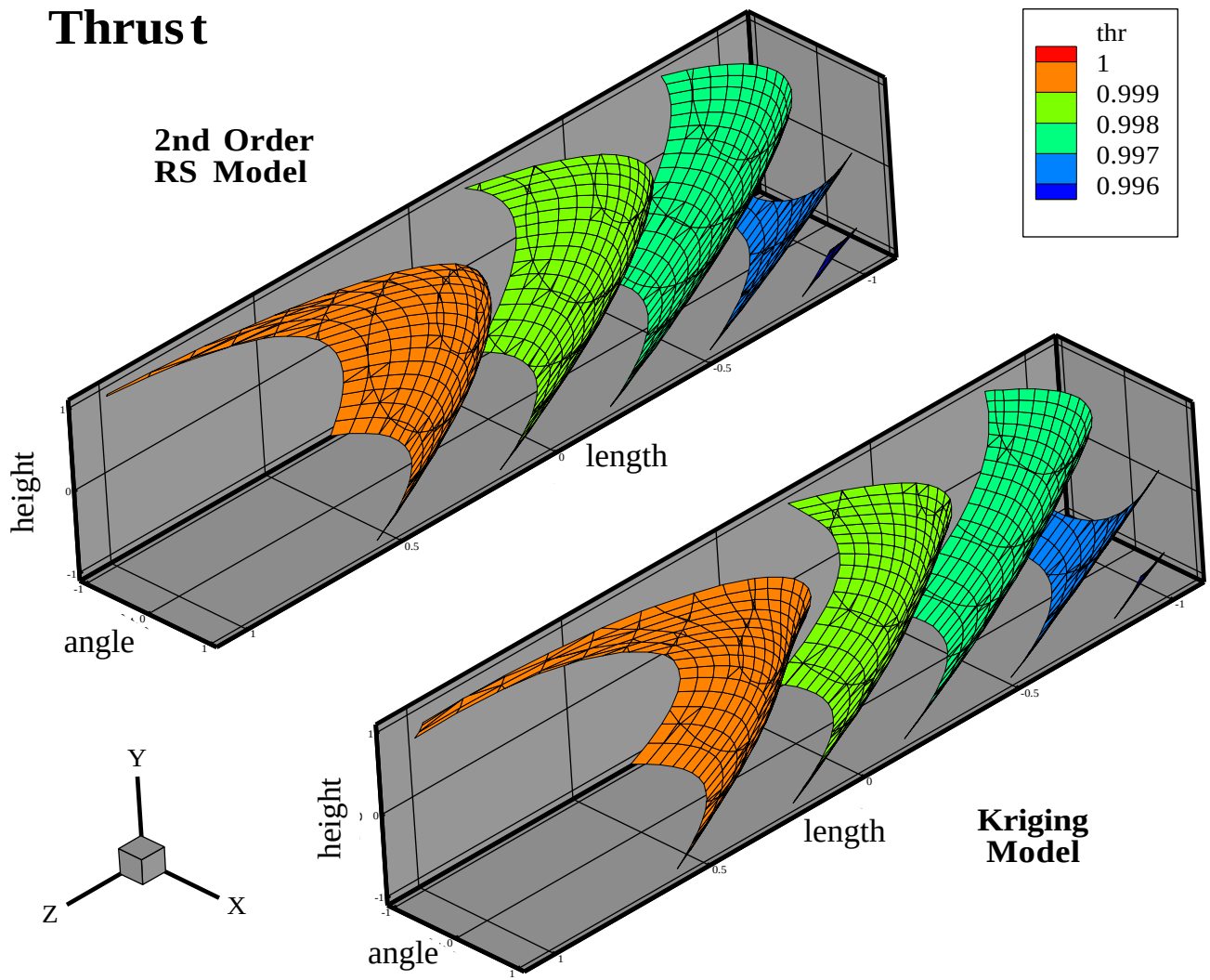


2-D Projection



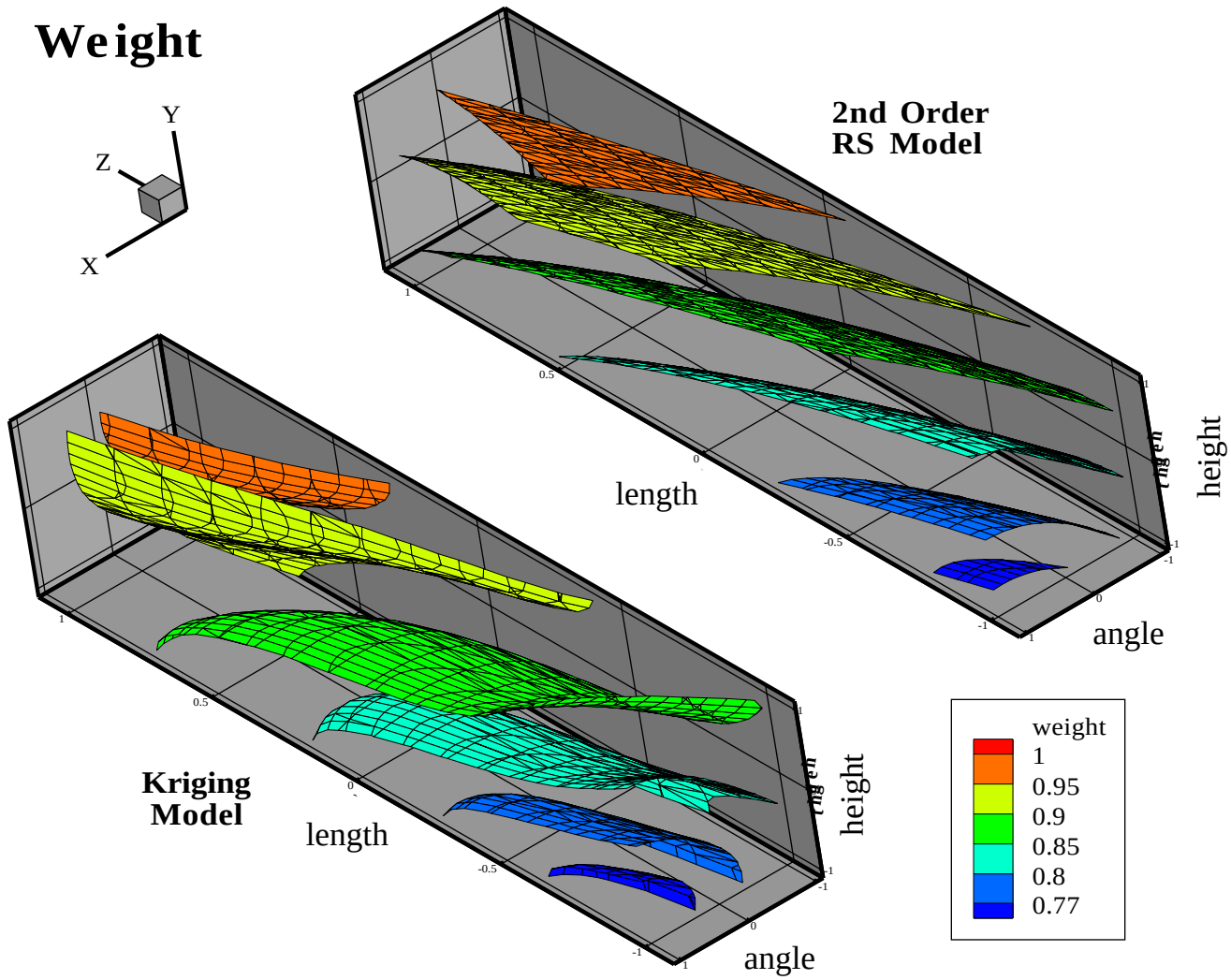
PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Thrust Model Contours



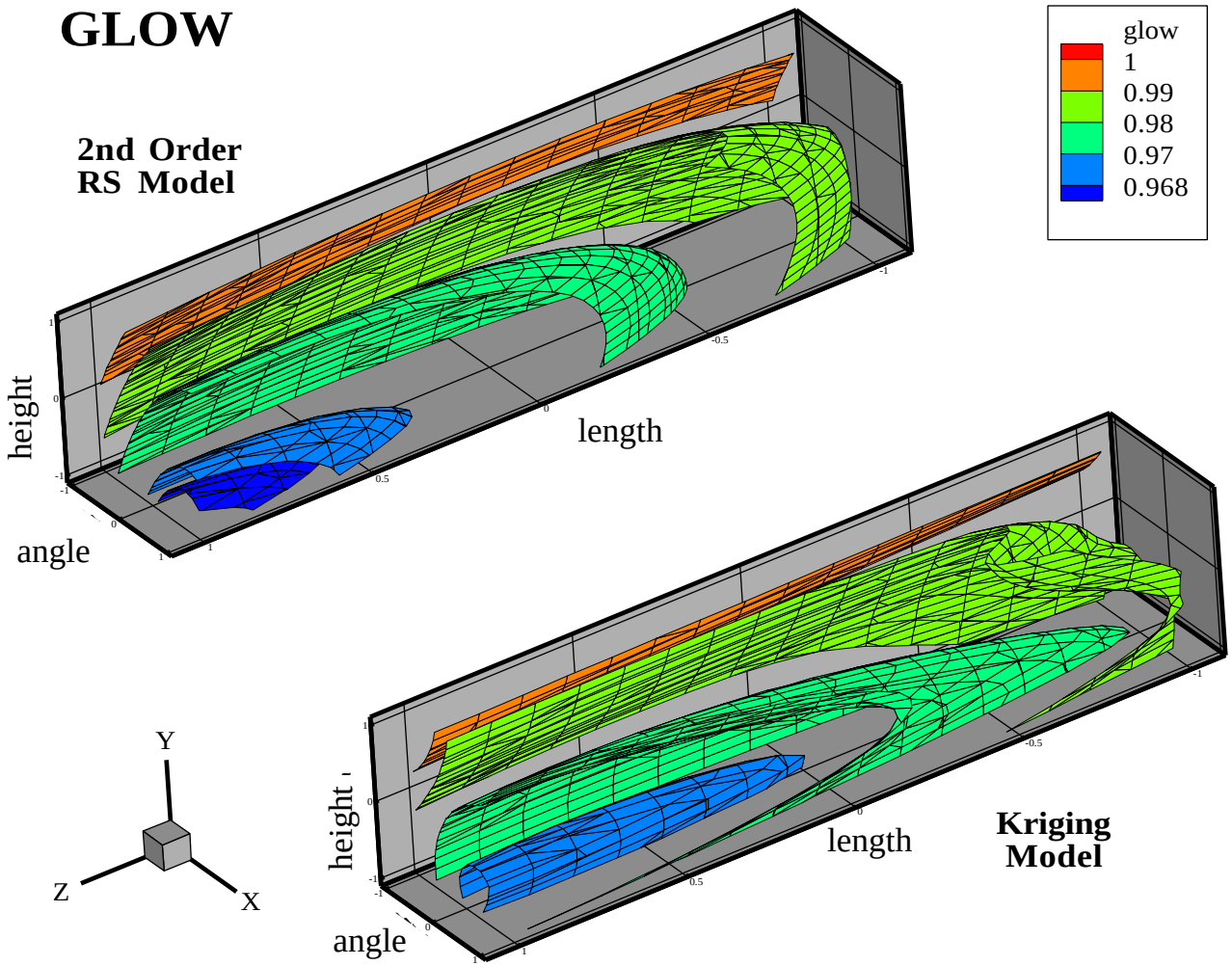
PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Weight Model Contours



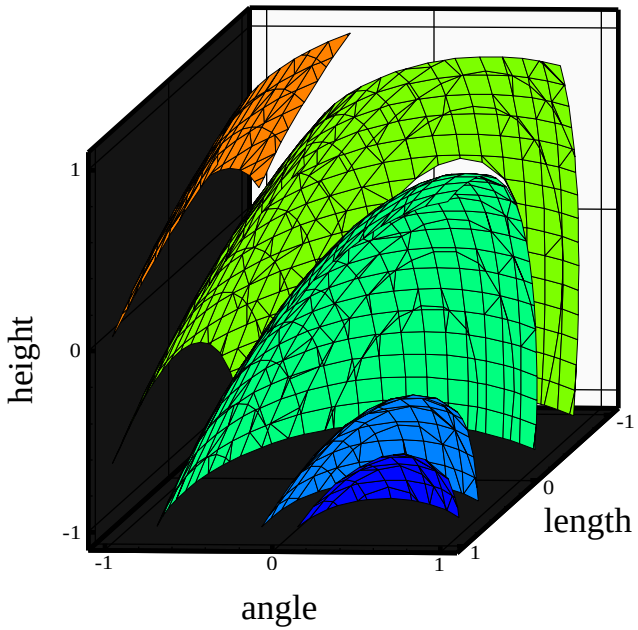
PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

GLOW Model Contours



PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

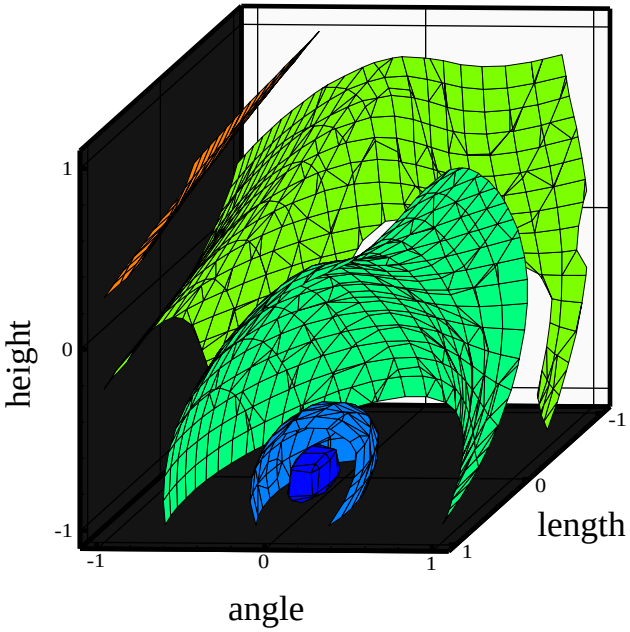
GLOW Model Contours–End View

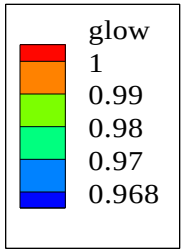


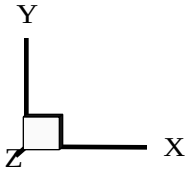
2nd Order RS Model

GLOW

Kriging Model







PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Approximation Model Validation

- Twenty-five (25) additional validation points are used to test the accuracy of the approximations

RS Model - 2nd order polynomial			
	weight	thrust	glow
Max ABS(error*)	19.57%	0.032%	3.68%
Min ABS(error)	0.32%	0.001%	0.05%
Average ABS(error)	2.44%	0.012%	0.53%
Root MSE**	4.54%	0.015%	0.90%
Kriging Model - constant term			
	weight	thrust	glow
Max ABS(error)	17.23%	0.048%	3.43%
Min ABS(error)	0.02%	0.001%	0.04%
Average ABS(error)	2.51%	0.012%	0.59%
Root MSE	4.37%	0.018%	0.89%

$$*\text{error} = y - \hat{y} \qquad **\text{rootMSE} = \sqrt{\sum_{i=1}^{n_e} \left(\frac{y - \hat{y}}{n_e}\right)^2}$$

PENNSTATE
Department of Mechanical & Nuclear Engineering
Department of Industrial & Manufacturing Engineering
Email: tws8@psu.edu

Aerospike Nozzle: Optimization Study

- Four (4) optimization problems are formulated and solved to compare further approximation accuracy

Find: *angle, height,* and *length* of the nozzle

Satisfy:

- Bounds: -1 ≤ angle, height, length ≤ 1
- Constraint limits on responses not in objective function

Objective:

Single discipline	*Multiple disciplines*
1. Maximize Thrust	3. Maximize Thrust/Weight Ratio
2. Minimize Weight	4. Minimize Gross Lift-Off Weight

- GRG algorithm in OptdesX; three (3) starting points

Optimization Results: Minimize GLOW

Approx. Model	Avg. # Analysis Calls	Avg. # Gradient Calls	Design Variable		Response	Predicted Optimum	Verified Optimum	% Error
			Angle	0.616	Thrust	1.0013	0.9957	0.56%
RS	30.67	3.33	Height	-1.000	Weight	0.8969	0.8617	4.09%
Models			Length	1.000	Thr/Wt	1.0251	1.0286	-0.34%
					GLOW	0.966	1.0146	-4.79%
			Angle	0.764	Thrust	1.0009	1.0006	0.04%
Kriging	57.67	6.33	Height	-0.833	Weight	0.906	0.8732	3.75%
Models			Length	0.676	Thr/Wt	1.0228	1.0302	-0.72%
					GLOW	0.9675	0.968	-0.05%

- Kriging models typically require
  - 1-3 more gradient calls
  - 2-3 times more analysis calls

- However, predicted optimum design is more accurate, particularly in the multidisciplinary design cases

Closing Remarks

- Demonstrated usefulness of approximation models in a realistic, engineering application

- Second-order response surface models and kriging models yield comparable results in this example as verified through:
  - graphical comparison
  - additional validation points
  - optimization study

- *Kriging model with constant "global" model and "local" Gaussian correlation function is as accurate as a full second-order response surface model*

Ongoing and Future Work

- Additional testing of the utility of kriging approximations
  - Which correlation function is best?
  - Should a linear or quadratic “global” model be employed?
- Usefulness of different experimental designs
  - “Classical” DOE (2): central composite; Box-Behnken
  - “Space-filling” DOE (9): random, minimax, maximin, IMSE optimal, orthogonal, and orthogonal-array based Latin hypercubes; orthogonal arrays; Hammersley sampling sequences; uniform designs
- Aerospike Nozzle Example
  - Decompose disciplines, build separate approximations for each, and then optimize using different MDO formulations
  - Numerical noise in the data