Design and Analysis of Computer Experiments (DACE)
An Introduction

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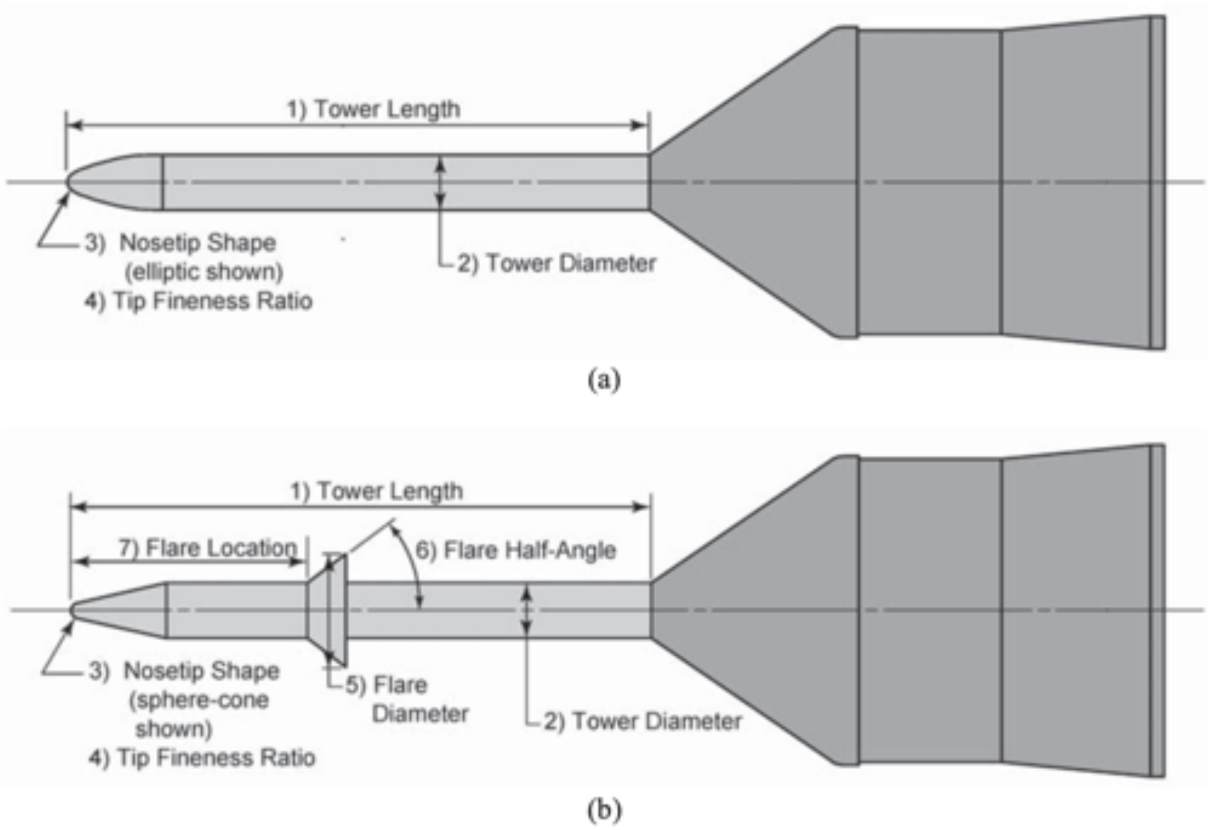
Motivating Example – Launch Abort System (LAS) Study

- Study the effects of 7 LAS Tower Design Parameters on Drag through the ascent trajectory

1. Tower length
2. Tower diameter
3. Tip fineness ratio
4. Tip shape
5. Flare diameter
6. Flare angle
7. Flare location

Continuous and Categorical Factors

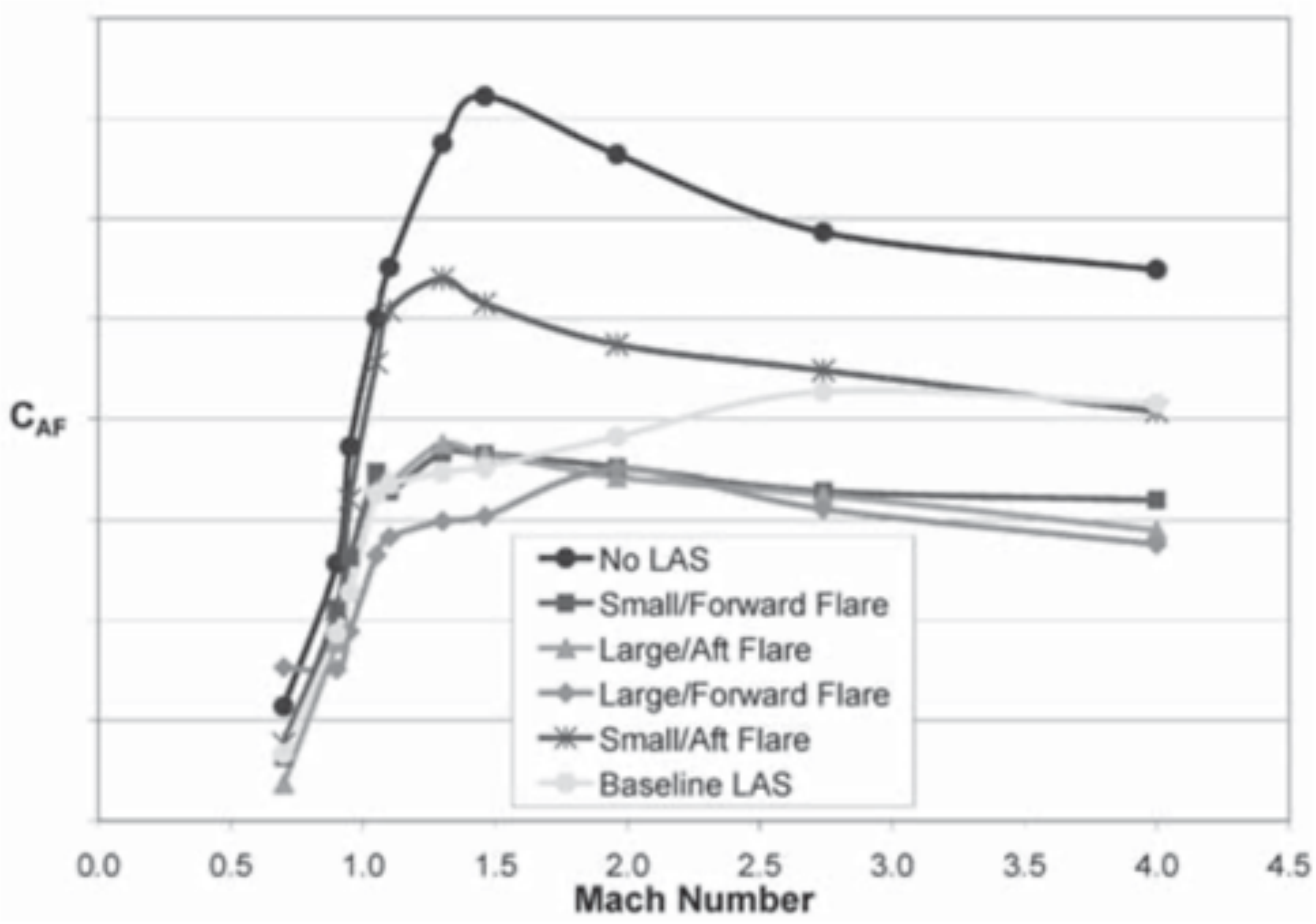


- Reduction in drag can increase vehicle payload capability

Huebner et al. (2008) “Status, Plans, and Initial Results for Ares I Crew Launch Vehicle Dynamics,” Journal of the British Interplanetary Society, Vol. 61.
Rhew and Parker (2007) “A Parametric Geometry Computational Fluid Dynamics Study Utilizing Design of Experiments,” AIAA-2007-1615

Response of Interest

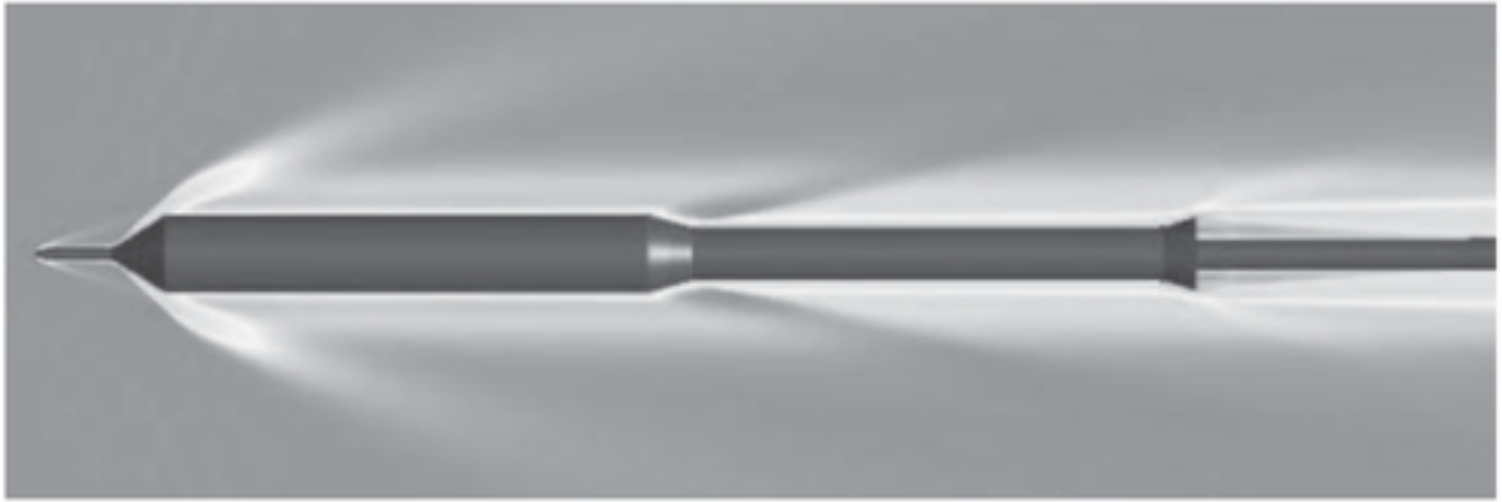
- Profile response of drag at discrete Mach numbers during the ascent trajectory of the vehicle
- Compressed to a weighted average "integrated drag" for each factor combination (design point)



Multiple CFD codes utilized across the flow regimes

Why Design a Computer Experiment?

- CFD was computationally expensive to run across all of the speed regimes for each case to develop integrated drag, therefore computational resources needed to be reduced/optimized.
- To improve subsequent wind tunnel validation efficiency and inform/simplify the article design
- Why build an empirical model, when we have the underlying physics-based functions in the CFD?
  - Study relatively “local” behavior in a region of the full design space for this vehicle
  - Surrogate models provide insights on the relationships among factors, i.e. interactions



Designing the Computer Experiment

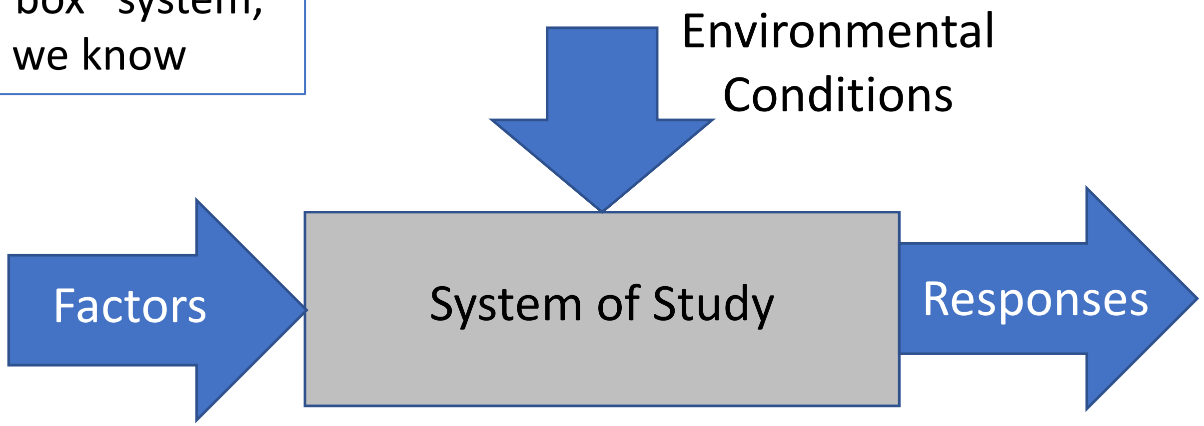
Need to specify which design configurations (design points) to run in CFD

- Running one-factor-at-a-time, while holding the other factors constant, was performed as a pilot study, however this approach lacked important insights on the factor combinations (interactions)
- The initial, intuitive approach was to specify a fine, exhaustive grid of factor combinations
    - 10 levels of each of the 7 factors -> 10^7 combinations, 10 million CFD cases
    - Approach ”broke the supercomputer bank”
    - Alternative approaches were sought to efficiently capture multi-dimensional relationships
- The philosophy of **Response Surface Methodology offers a powerful strategy** to design computer experiments, however **there are differences in application compared to physical experiments**

Traditional RSM Similarity – It's Still an Experiment, just not Physical

- **RSM is a science** of efficiently discovering and characterizing factor-response relationships, if they exist, for product and process optimization
- Purposely changing the factors and measuring responses to determine factor-response relationships, if they exist or not – **a virtual experiment**
- **Starting with the objective and research questions**, we specify the design points and acquisition process/sequence to efficiently answer the research questions in a defensible, rigorous manner
- **Subject-matter expertise is critical** to inform the experiment design, so a RSM practitioner needs to ask lots of questions about the context – very critical skill and discipline

Often, DACE involves "grey box" system, which we can exploit what we know



Key Differences Between Physical and Computational Experiments

- **Can usually obtain responses faster than physical experiments**
  - Relative time comparison, but typically true in aerospace applications
  - Recall DOE history of moving from agricultural to industrial applications, faster responses
  - Can exploit sequential experimentation, even more than physical experiments
    - Careful to not get lost in unguided iteration on an unchartered path
- **Random errors may or may not be included in a computational experiment**
  - **Stochastic simulation**, with random error, less common in aerospace applications
    - Often can apply physical experiment techniques directly
  - **Deterministic simulation**, most common
    - Running the same combination of factors produces the same responses, within numerical roundoff or variations in the initial random seed
- **With no random error, model residuals need to be interpreted carefully**
  - Residuals are all model lack-of-fit, model misspecification, bias
  - An interpolating model, not an approximating, smoothing function may be more appropriate

Response Surface Modeling Approaches

	Approximating, Fitting Functions	Interpolating Representations
Model Form	Taylor series expansion, graduating Polynomials, Parametric functions	Splines, Gaussian Process Models, Non-Parametric smoothing
Modeling Features and Errors	Does not go-through every point, results in residual/model errors	Goes-through every point, it "connects the dots," no residual/model errors, prediction accuracy is a focus
Model Parameters	Estimate parameters that have a physical interpretation relative to factors	Estimated parameters represent weighted average and correlation of all design points, no physical interpretation
Measures of Design Sufficiency	Assuming a model form allows for design optimality/efficiency based on estimation and prediction variance before execution	Coverage across the design space, less emphasis on optimality, prediction quality from cross-validation after execution
Design Characteristics	Sparse, design points spread apart, geometric, points at boundaries, edges, centroids, face-centers, few factor levels	Dense, space-filling, points are distributed across the design space/dimensions, many unique levels of each factor

Which Modeling Approach is Best for Computer Experiments?

- **It depends on the objectives - “All models are wrong, but some are useful”**
  - In the LAS example, we want to understand factor-response relationships to guide the design and make subsequent wind tunnel testing more efficient –> Approximating model
  - If our objective is to produce an empirical, surrogate model of a complex physics-based model to support efficient subsequent simulations to quantify uncertainty in the model parameters or environmental conditions -> Interpolating model
- **Both modeling approaches have their place in DACE** and could be employed in different phases of the same application, for example,
  - In early phases, small designs can support simple models and provide efficient diagnostics of the computational virtual apparatus
  - Simple models (sensitivity studies) can more efficiently focus our attention of the most promising portions of the design space, maybe help reduce the dimensionality
  - Once we have identified regions of interest, we might consider moving to comprehensive designs and more complex models in local regions of the response surface

Choice of Modeling Approach Influences (Drives) the Design

- The **modeling approach should drive the design strategy** (not always true in practice) to be efficient in the usage of experimental resources, true for physical and virtual experiments
  - This is consistent with the foundations of RSM
  - Computer experiments are not free, in fact they can be very expensive
  - Said another way, **given a design, it may limit the modeling approach**
- **A strong modeling assumption (prior knowledge) leads to a relatively small designs**
  - We are seeking to confirm/refine what we think we already know
- **A weak model assumption (little prior knowledge) leads to a larger design**
  - We are exploring the design space to learn something new
- In practice, there's a mixture, often implicit, and the designer needs to decide how strongly to let prior knowledge influence the design.

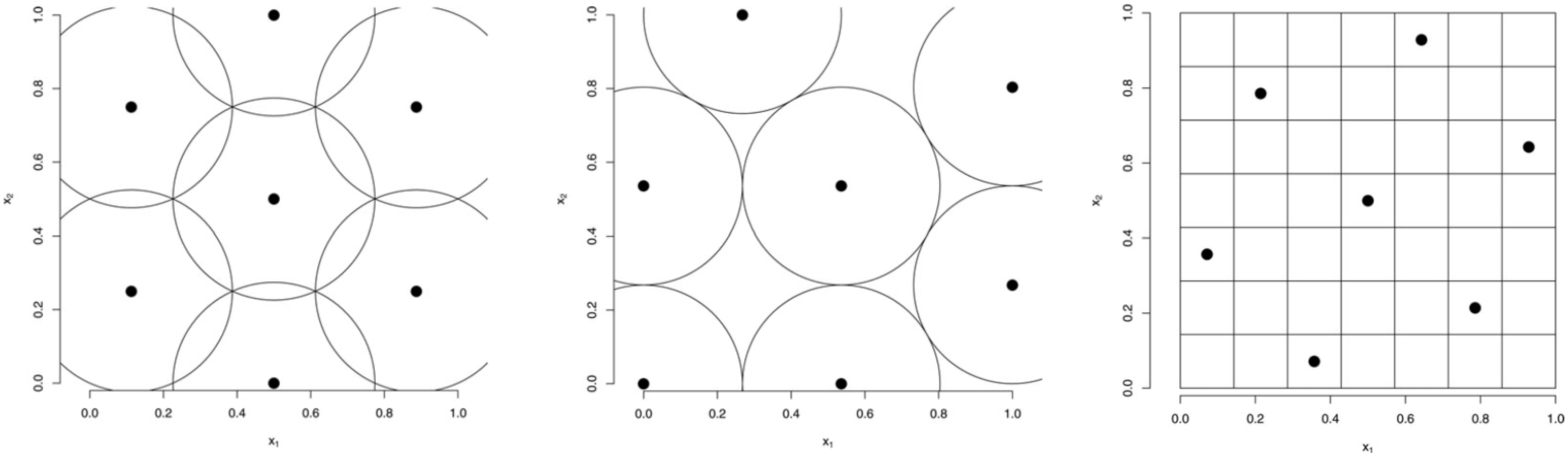
Classes of Experimental Designs for Computer Experiments

- **Geometric Designs**
  - Factorial design
  - Response surface designs (central composite)
  - Computer-generated optimal designs
- **Space Filling Designs**
  - Uniform grid, simplest case
  - Latin hypercube, most popular
  - Computer-generated consider factor constraints and response surface characteristics
- **Dimensionality (number of factors) can be a challenge** for both types of designs
- **Combining design and modeling types can be a powerful strategy**
  - One design could be used for model building, and one design for confirmation points
  - Start with a space filling design and augment it with computer-generated optimal points

Johnson, Montgomery, Jones, Parker, (2010) "Comparing Computer Experiments for Fitting High Order Polynomial Metamodels," Journal of Quality Technology, 42, pp. 86–102.

Space-Filling Design Concepts

- Many optimization criteria: Latin Hypercube, Sphere Packing, Uniform Distribution, Minimum Potential, Maximum Entropy, Gaussian Process integrated Mean Squared Error, Fast Flexible Filling



Minimax Design

Maximin Design (Sphere Packing)

Maximin Latin Hypercube Design

Joseph (2016) “Space-Filling Designs for Computer Experiments: a Review,” Quality Engineering
Parker (2016) “Discussion of “Space Filling Designs for Computer Experiments: a Review”,” Quality Engineering

Hypersonic Air-Breathing Propulsion Demonstration

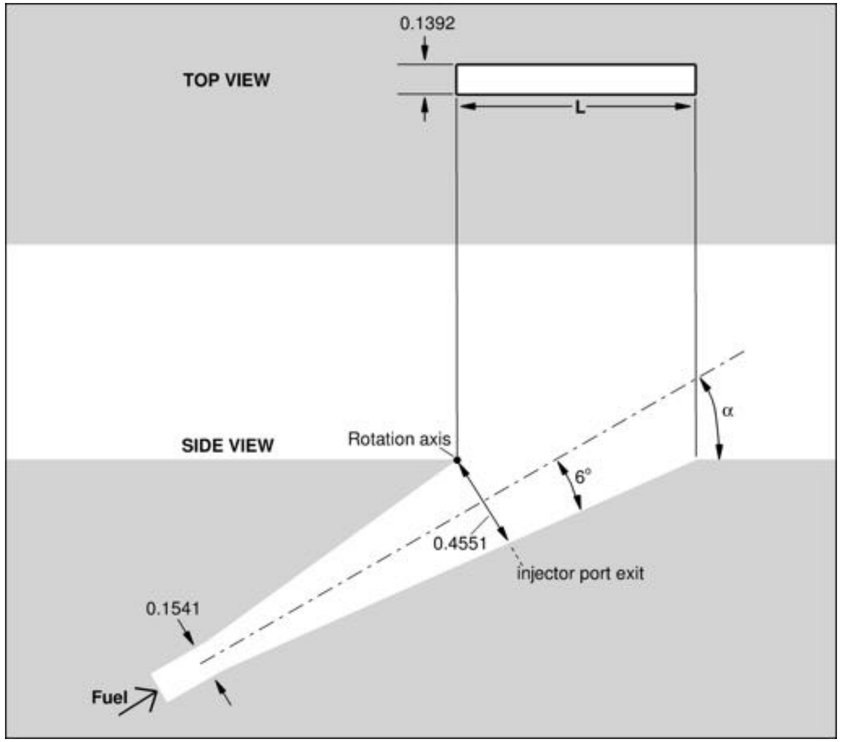
- Reynolds-averaged simulations (RAS) may be used for design optimization. However, when generating a dense database of response values, RAS can become prohibitively expensive for even a few design variables.
- Therefore, researchers rely on surrogate model based optimization
    - Efficiently sample the design space to perform RAS
    - Fit surrogate models to approximate objective function responses
    - Utilize the surrogate models to optimize the design

Shenoy, Drozda, Baurle, Parker (2019) “Surrogate Modeling and Optimization of a Combustor with Interdigitated Flushwall Injector,” JANNAF

Factors and Responses

Factors (4)

Mach, Duct Height, Spacing Width, Injection Angle



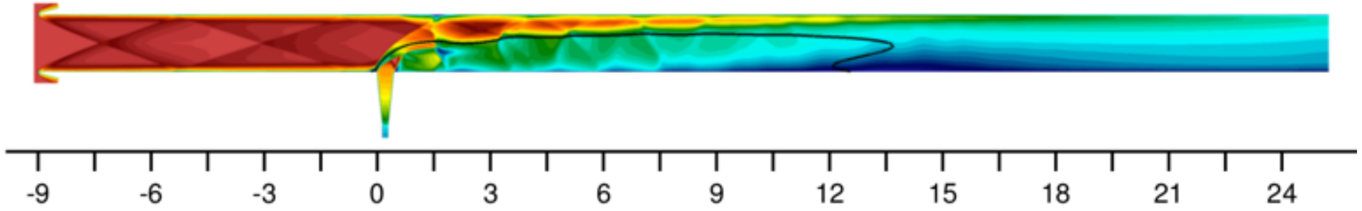
Flushwall injector port's exit interface based on Ogawa, H., J. Propul. Power, Vol. 31, No. 6, 2015, pp. 1505–1523.

Responses (2)

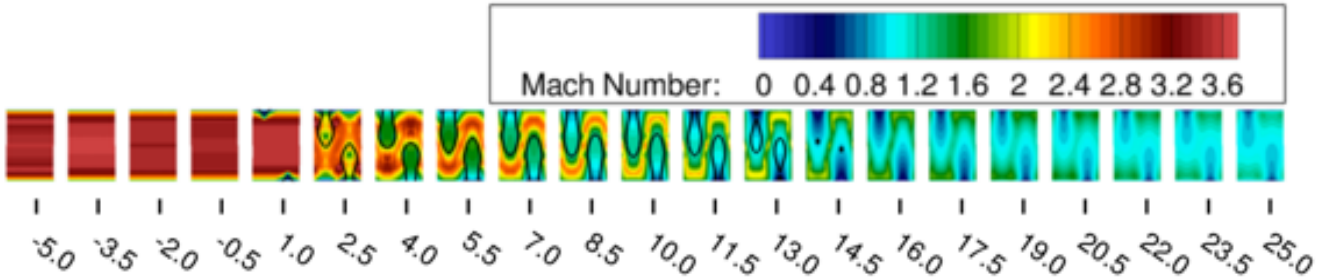
Thrust potential: TP_m

Combustion efficiency: η_c

Obtain a value for each response at combustor exit for every factor combination, want to maximize both



Cross-stream planes shown below



Study of Various Experimental Design Approaches

Original: One-Shot, Space-Filling + Geometric Design

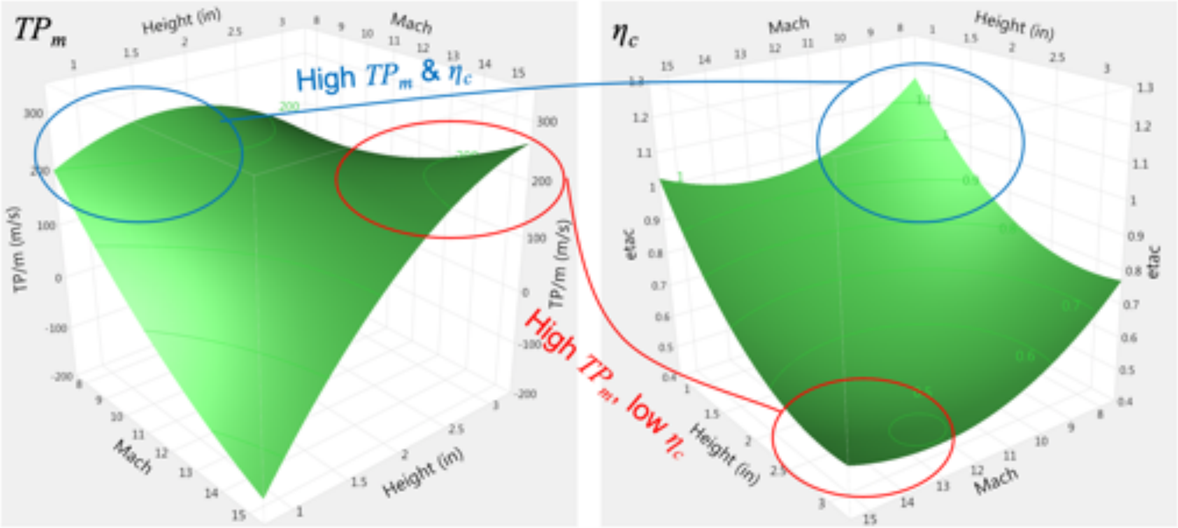
- Training data composed of **66 design points**
  - Generated a Latin hypercube sampling specifying 50 design points
  - Augmented with 16 corners of the 4D hypercube
  - 3 additional confirmation (challenge) points

Proposed: Sequential, Geometric Design

- Full Factorial Design with a Center-Point, **17 design points**
  - 16 corner-points were used from the space-filling design above
  - Allows estimation of 4 main effects, all interactions, test for curvature
  - Indicated second-order would be beneficial
- Augmented the FF Design with 8 Axial Points, **25 design points (total)**
  - Cuboidal central composite design
  - Allows for a full second order model in 4 factors, and some mixed cubic terms

Employed a Sequential Design Approach

- Developed response surfaces for both responses (thrust potential and efficiency)
- **Multiple response optimization** using desirability function, and a multiobjective genetic algorithm generating a pareto front of nondominated solutions
- **Width factor had a small effect**, and the design was projected to 3 factors
- **Two regions of the 3-factor design space were identified for further study**, zoomed-in



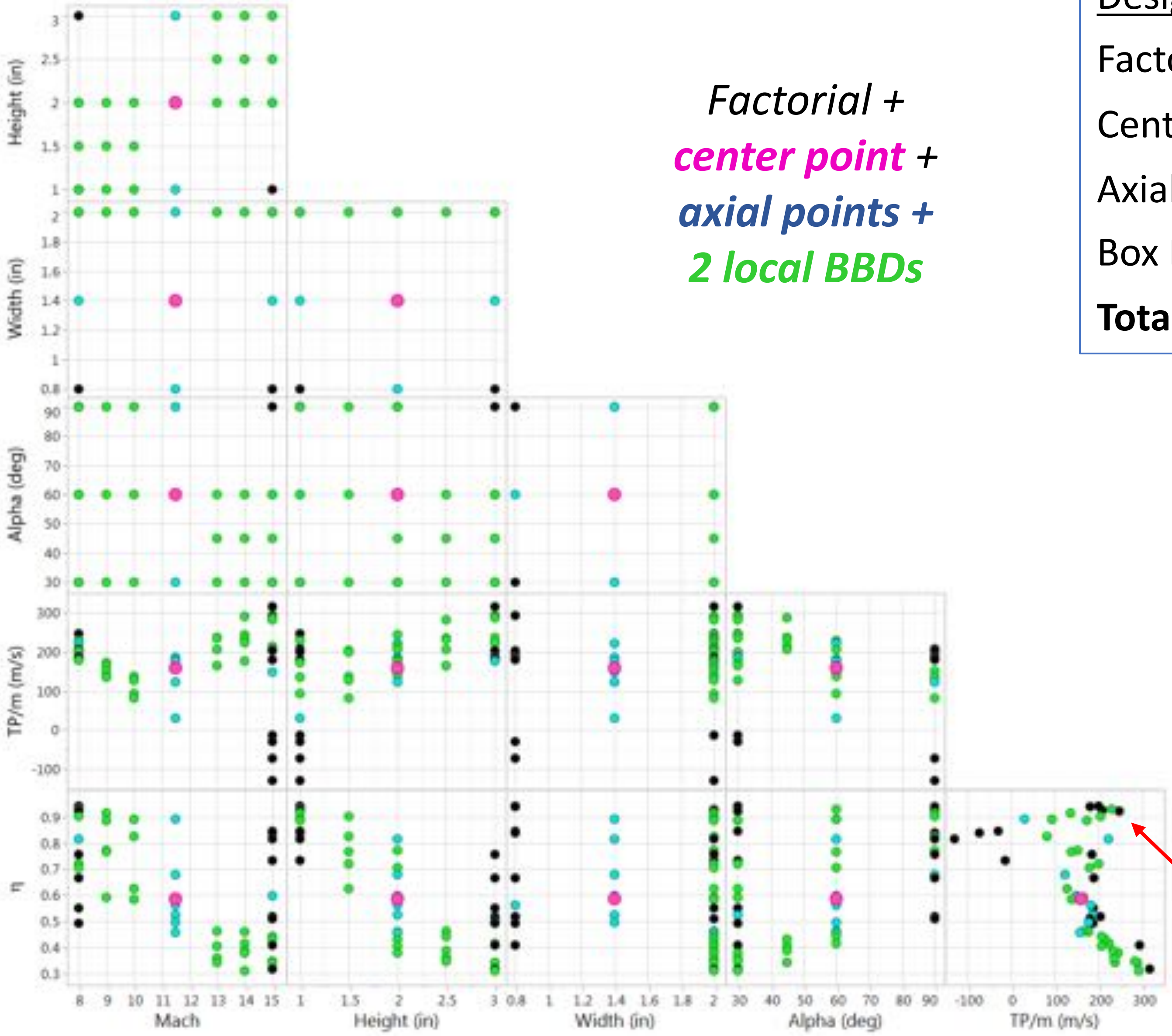
Augmented with Geometric Design in Focused Areas

- Box-Behnken design in each local region of joint optima, 13 design points each region

Combined Designs and Responses

Design Factors

Responses



Factorial +
center point *+*
axial points +
2 local BBDs

<u>Design Point Allocation</u>

Factorial = 16

Center Point = 1

Axial Points = 8

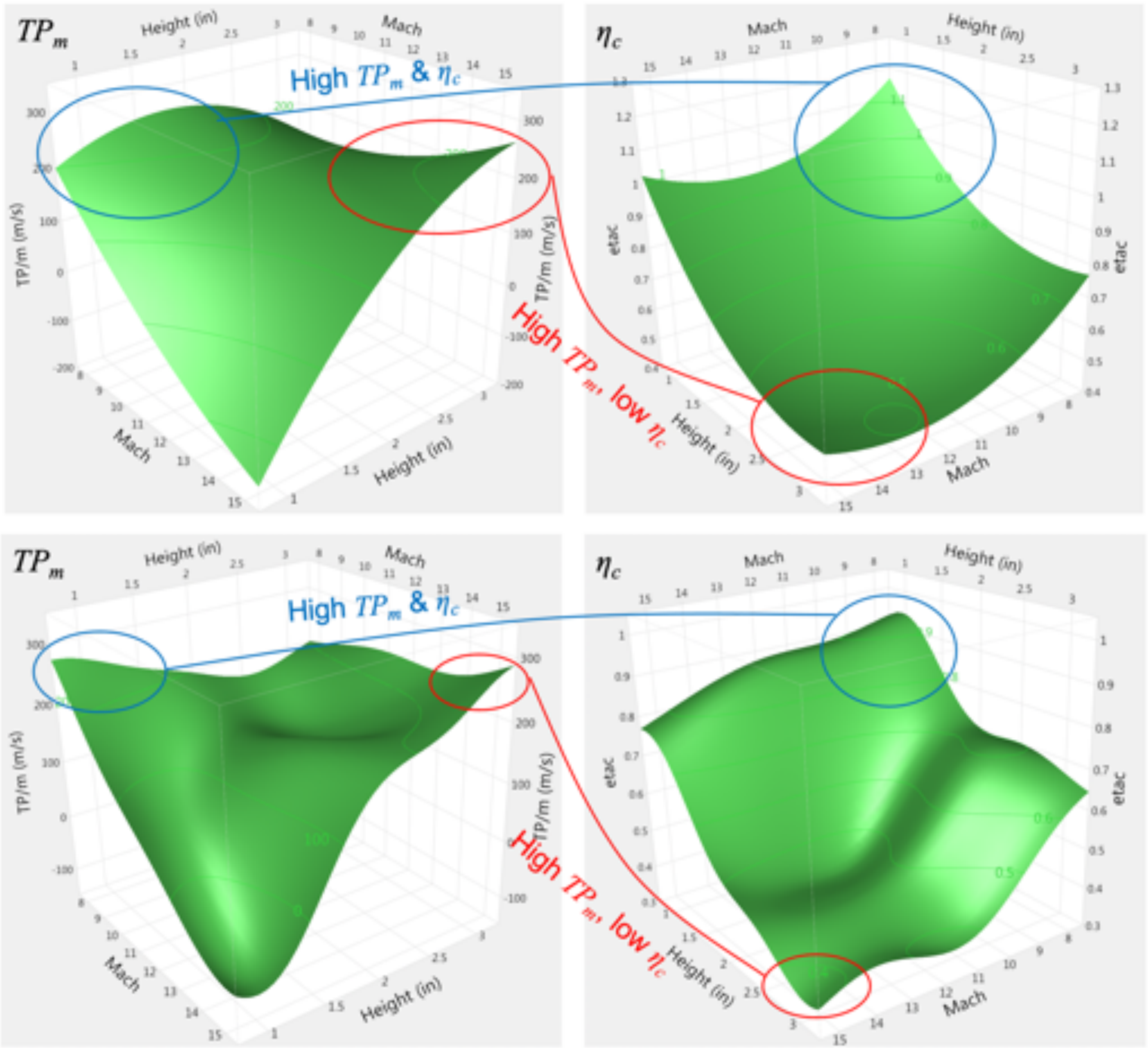
Box Behnken = 13 each

Total Number of Design Points = 51

Design approaches combines an overall (global) perspective and a refined, focused view in regions of local optima

Objective: maximum efficiency and maximum thrust

Comparing Modeling Approaches



2nd-order Taylor series (classical RSM model)

Which one is better?

Gaussian Process Model

Modeling Errors and Prediction Accuracy in Computer Experiments

Modeling Error – using the model, predict at the data points collected, this is the deviation between the model predictions and actual values ($\hat{y} - y$)

- For approximating models, modeling errors result from model misspecification (form and/or order). Model errors are expected/accepted when approximating the true underlying relationship
  - Need to be careful/diligent in explaining what this error represents. For example, they are not drawn from a distribution (Normal) and they have no probabilistic interpretation
- For interpolating models, there is usually no modeling error.
  - Once again, careful in explaining the lack of modeling error. For example, it does not imply that the model accurately represents the underlying true model, rather it matches the data

Prediction Accuracy – using the derived model, predict responses at factor combinations that were not collected/observed during the computer experiment, aka Uncertainty Quantification

- Can be inferred from the modeling error and/or based on cross-validation approaches
- Physics of the simulation model must be considered, e.g., grid refinement
- In high-dimensional space, interpolation versus extrapolation can be difficult to determine
- May involve test conditions that cannot be validated with experiments, e.g. nuclear tests

Uncertainty Quantification


Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification

ASSESSING THE RELIABILITY OF COMPLEX MODELS

MATHEMATICAL AND STATISTICAL FOUNDATIONS OF VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION

Committee on Mathematical Foundations of Verification, Validation, and Uncertainty Quantification

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- UQ - Often synonymous with computer experiments, many definitions and scopes, has become a popular topic
- “Uncertainty quantification (UQ) is the process of quantifying uncertainties associated with model calculations of true, physical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.”
- “Quantifying uncertainty in a prediction for a QOI means making a quantitative statement about the values that the QOI for the physical system may take, often in a new, unobserved setting.”
- Communication of uncertainty, what it includes and what it doesn’t is vital to decision makers

QOI – Quantity of Interest, a response or function of multiple responses

National Academy of Sciences (2012) “Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification”

Concluding Remarks

- The **philosophy of Response Surface Methodology provides a systematic, efficient, and rigorous approach to the design and analysis of computer experiments**
  - However, there are differences in design strategies and modeling/analysis approaches
  - Clearly understanding the experiment objectives is crucial in determining any approach
- Discussed **types of computer simulation** used in computer experiments
  - Deterministic (most common) versus Stochastic
- Described **modeling approaches**
  - Approximating (fitting) versus Interpolating
- Explained **design building strategies**, influenced by the modeling approach and utility
  - Geometric versus Space-Filling
- **Motivated and illustrated concepts with examples**

I hope that when you review an article on a computer experiment, you'll be able to discern the aspects discussed, and when you design a computer experiment, you'll appreciate the choices available and their consequences.