QUANTIFYING AND IMPROVING CONFIDENCE IN
MODEL PREDICTIONS FOR HYPersonic aircraft
STRUCTURES

Benjamin P. Smarslok
Hypersonic Sciences Branch
High Speed Systems Division

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5. AUTHOR(S)
Benjamin P. Smarslok

6. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Hypersonic Sciences Branch (AFRL/RQHF)
High Speed System Division
Air Force Research Laboratory, Aerospace Systems Directorate
Wright-Patterson Air Force Base, OH 45433-7542
Air Force Materiel Command, United States Air Force

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10. ABSTRACT
The current lack of confidence in structural response and life predictions of a vehicle exposed to combined extreme environments for extended durations prevents the USAF from fielding affordable, reliable, and reusable hypersonic platforms. The prohibitive computational cost of high-fidelity, coupled, aeroelastic simulation and the inability to fully replicate the high, in-flight, aerodynamic, thermal, and acoustic loads through ground tests poses a significant challenge for assuring the needed confidence in model predictions. The first objective is to enable the quantification uncertainty in coupled multi-physics interactions for fluid-thermal-structural computational models of hypersonic aircraft. The next objective is to propagate and analyze uncertainty for coupled aerothermal predictions to determine the most significant sources of model error. The final objective is to assess prediction confidence for hypersonic aircraft structures, focusing on optimal data collection methods for uncertainty reduction.

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ABSTRACT

The current lack of confidence in structural response and life predictions of a vehicle exposed to combined extreme environments for extended durations prevents the USAF from fielding affordable, reliable, and reusable hypersonic platforms. The prohibitive computational cost of high-fidelity, coupled, aerothermoelastic simulation and the inability to fully replicate the high, in-flight, aerodynamic, thermal, and acoustic loads through ground tests poses a significant challenge for assuring the needed confidence in model predictions. The first objective is to enable the quantification uncertainty in coupled multi-physics interactions for fluid-thermal-structural computational models of hypersonic aircraft. The next objective is to propagate and analyze uncertainty for coupled aerothermoelastic predictions to determine the most significant sources of model error. The final objective is to assess prediction confidence for hypersonic aircraft structures, focusing on optimal data collection methods for uncertainty reduction.

**Laboratory Task Manager:** Dr. Benjamin P. Smarslok, AFRL/RQHF

**AFOSR Program Managers:** Dr. Jean-Luc Cambier, Computational Mathematics/RSL
Dr. Jay Tiley, Structural Mechanics/RSA

**Collaborators:**
Dr. Greg Bartram, AFRL/UTC, Postdoctoral Researcher
Dr. Diane Villanueva, AFRL/UTC, Postdoctoral Researcher
Dr. Zach Riley, AFRL/UTC, Postdoctoral Researcher
Dr. Ricardo Perez, AFRL/UTC, Postdoctoral Researcher
Erin DeCarlo, Vanderbilt University, Graduate Research Assistant
Prof. Sankaran Mahadevan, Vanderbilt University
Dr. Ravi Chona, AFRL/RQHF, Structural Sciences Center Director
1 PROJECT OVERVIEW

Uncertainty is inherent in all computational model predictions due to imperfect knowledge, physical variability in the system, model order reduction, assumptions and approximations, and limited experimental data available for model calibration and validation [1]. This is especially the case for compliant structures in hypersonic environments due to the complex and poorly-understood loading and the coupled multi-physics nature of the fluid-thermal-structural interaction. This FY15-17 in-house research project focused on developing the necessary methods in a framework to quantify and improve model prediction confidence for coupled multidisciplinary systems using experimental data and multi-fidelity simulations. The three research objectives are:


2. **Propagation and Analysis of Uncertainty for Coupled Aerothermoelastic Predictions** - Investigate computationally efficient: (a) propagation of model uncertainty throughout the coupled system; and (b) sensitivity analysis for the various quantities of interest in aerothermoelastic predictions. Additionally, develop the scientific insights to interpret this uncertainty and sensitivity information for model selection to achieve a desired level of fidelity, determine the most significant contributors to model error, and suggest where best to focus limited resources to reduce uncertainty and improve prediction confidence.

3. **Prediction Confidence Assessment for Hypersonic Aircraft Structures** - Develop optimal data collection methods that can be employed in a notional validation plan to reduce model uncertainty by integrating experimental observations of coupled aerothermoelastic response into the model selection and improvement process.

Previous in-house research (FY12-14) [2] led to novel approaches that were further investigated in FY15-17 for quantifying model uncertainty for coupled multidisciplinary models using Bayesian model calibration, including: (1) segmented Bayesian model calibration [3]; and (2) the incremental calibration strategy for coupled models with time-dependent data [4]. Segmented calibration differs from traditional, simultaneous calibration for multidisciplinary models by isolating the error for each constituent model and strategically integrating the data into the Bayesian network in a segmented way. Segmented Bayesian model calibration resulted in fewer model evaluations than necessary for simultaneous calibration, while yielding equivalent posterior distributions for model discrepancy based on the Kullback-Leibler distance [3]. Historic aerothermal data was further used as the basis for an investigation using time-dependent temperature data for calibrating the model errors of coupled aerodynamic heating and heat transfer [4]. A coupled, input-dependent error model was developed for aerodynamic heating and heat transfer using time dependent aerothermal data. In addition, the coupled model error was calibrated using an incremental Bayesian calibration procedure, rather than the traditional, global approach. The incremental calibration approach quantifies and corrects the error at each time step, which improves confidence in model extrapolation.

The design of hypersonic air vehicles involves coupled, multi-physics interactions, which are predicted through computational models of various levels of fidelity and accuracy. To reduce...
uncertainty and improve predictive capability, these models must be calibrated with experimental data. Since wind tunnel test data is so limited and costly for high-speed structures, the FY15-17 research effort developed an optimal experimental design method by calculating the maximum expected information gain (i.e., the expected difference between the prior and posterior distributions) to determine the test conditions that would most inform and improve the coupled models [5-7]. An optimal data collection approach was developed to maximize uncertainty reduction and achieve a globally accurate model through experimental design, while still ensuring accurate prediction of targeted events, such as high temperatures or structural failure [8]. This is especially important due to the significant cost of high-fidelity aerothermoelastic simulations and limited aero-thermal-structural test data. This research on optimal experimental design to was extended to explore the expected information gain and experimental cost tradeoff. Notional cost models for wind tunnel specimen complexity and instrumentation were formulated in a bi-objective optimization problem to maximize the expected information gain and minimize the cost of the experiment. Further details on this optimal experimental design research is presented in Section 2 and [9].

Uncertainty in boundary-layer transition remains a major obstacle in aerothermodynamic load characterization and life prediction for hypersonic structures. A global sensitivity analysis was performed for uncertainty in transitional aerothermodynamic loading on an aerothermoelastic panel [10-12]. This study identified sources of uncertainty related to boundary-layer transition and quantifies their importance for accurate structural response prediction. The uncertain input include the transitional $N$ factor (i.e., onset location), transition length, and the potential for overshoot in the aerothermodynamic loads. The transition onset location is found to have a predominant influence on the maximum displacement and average surface temperature of the panel. However, the location of the peak displacement is dependent on the interaction between the onset location and length of transition. Transitional aerothermodynamic loading that accounts for overshoot and becomes turbulent prior to the mid-panel results in displacements and average temperatures that exceed the fully turbulent prediction. Section 3 summarizes this research on identifying significant sources of model uncertainty in boundary-layer transitional loading and quantifying their impact on the structural response.

Global sensitivity methods were also investigated by DeCarlo et al. [13-14] to develop an efficient approach for calculating sensitivity indices of correlated variables. This global sensitivity methodology is particularly valuable in the context of a comprehensive uncertainty quantification framework since it enables efficient post-calibration sensitivity analyses using existing input-output samples obtained directly from Bayesian calibration.

In addition to quantifying model uncertainty and sensitivity analysis, another research thrust explored data-driven modeling techniques of full-field dynamic response data. Full-field measurement techniques, such as 3-D digital image correlation (DIC) and pressure sensitive paint (PSP), collect spatially dense data using high-speed cameras, resulting in large volumes of high-dimensional data. The approach investigated to represent this data combines singular value decomposition (SVD) and autoregressive moving average (ARMA) modeling into a SVD+ARMA model [15-17]. This approach has the potential to provide accurate modeling of spatio-temporal data and is summarized in Section 4.

This FY15-17 Lab Task effort contributed to longer-term research plan for developing a framework for integrating various sources of uncertainty in a coupled aerothermoelastic simulation and assessing the confidence in model predictions. Publications associated with this in-house research task included 1 journal paper, 9 conference papers, and 9 conference presentations,
including a best presentation award at the 12\textsuperscript{th} ASME Dayton Engineering Sciences Symposium [3-8, 10-22].
2 DESIGN OF EXPERIMENTS FOR MODEL CALIBRATION OF MULTI-PHYSICS SYSTEMS

Given the complexity of coupled multi-physics response, the limited number of tests, and the wide range of possible, combined loading conditions that can be explored, it is critical to concurrently develop methods that reduce the model uncertainty through experimental design, as well as use the valuable experimental data to improve the model predictive capability. Therefore, an optimal experimental design approach to determine panel geometry and instrumentation for high-speed wind tunnel specimens to achieve maximum uncertainty reduction in aero-thermal-structural predictions. Multiple observables can be measured in a wind tunnel test of this nature, namely aerodynamic pressure and heat flux. Related efforts [23-24] focusing on quantifying model uncertainty in aerothermal predictions followed the framework described by Kennedy and O’Hagan [25] that relates the measurement from the experiment $y$ to the model output $G$ through model discrepancy $\varepsilon_G$ (also referred to as model error or model inadequacy), and measurement error $\varepsilon_y$. This relationship is shown as

$$y = G(x, \theta) + \varepsilon_G(x) + \varepsilon_y(x)$$

(1)

Bayesian model calibration is a technique used to obtain the distributions of model inadequacy and uncertain model parameters $\theta$, given experimental observations of the quantities of interest, such as aerodynamic pressure $y_p$ and heating $y_Q$. Bayes’ theorem, written for the aerothermal models, where the prior distributions of the uncertain parameters are given by $\pi(\theta)$ takes the form:

$$\pi(\theta | y_p, y_Q) = \frac{\Pr[y_p, y_Q | \theta] \pi(\theta)}{\int \Pr[y_p, y_Q | \theta] \pi(\theta) d\theta}$$

(2)

Since the number of experiments is limited, it is imperative to be able to anticipate the benefit from conducting experiments and maximize the amount of information that is gained from an experiment. Information theory and decision theory approaches previously have been used extensively in experimental design, taking different approaches in measuring the information gained from an experiment in terms of reducing the uncertainty in model parameters. For nonlinear relationships between observables and models, which is typical of aerothermoelastic models for hypersonics, these approaches include the maximization of expected information gain [26-28], entropy [29], and mutual information [30]. Bryant and Terejanu [30] sought to find the optimal sequence of experimental designs by maximizing the mutual information. Maximization of the expected information gain (EIG) criterion is considered here to determine which design is optimal in terms of the specimen geometry and instrumentation. The expected information gain can be simply thought of as the expected change in prior-to-posterior distributions of uncertain parameters (measured by the Kullback-Leibler divergence) after an experiment is performed:

$$EIG(x) = \int \int_{\theta} \Pr(\theta | y, x) \ln \left[ \frac{\Pr(\theta | y, x)}{\Pr(\theta)} \right] d\theta \Pr(y | x) dy$$

(3)

where $\theta$ denotes the uncertain parameters, $y$ are the future experimental result, and $x$ are the design variables. This formulation can be interpreted intuitively by examining the possible effect of a
future result, \( y \). For example, let \( y \) decrease the entropy of \( \theta \) by a large amount (e.g., increasing \( \Pr(\theta | y, x) \) relative to the prior distribution of \( \Pr(\theta) \)). In this case, when the information gain is large, then it is more informative for inference or calibration. The expectation is taken over the possible experimental results \( y \) given a design \( x \), prior distributions \( \Pr(\theta) \), and measurement uncertainty \( \varepsilon_y \) of the experiment. A large expected information gain value would correspond to a large change in the distribution of the uncertain parameters, which indicates that the experimental design provided information that had a large effect on the uncertainty.

2.1 Budgeting Model Calibration Experiments with Expected Information Gain

Expected information gain can be used to compare the utility of data gathered from experiments or simulations of various fidelities. Additionally, it allows the design of experimental conditions under cost constraints (e.g., cost of experiment versus expected information gain). This cost applies for not only optimal design of the experimental specimen, but also the optimal instrumentation and measurement locations for the observables. For a given experimental budget, a natural trade-off exists between the expected information gained from the experiment and the cost itself. In this research, approximate costs were assumed for instrumentation (where \( Q \) measurements cost more than \( P \)) and manufacturing (cost is proportional to the magnitude of the structural mode shapes) of wind tunnel test panel specimens. First, assume that more complex geometries are more difficult to manufacture. Therefore, more complex geometries are penalized by forming a cost model that is a function of the mode scale factors \( a_1 \) and \( a_2 \) where \( A = [a_1, a_2]^T \). The cost of the specimen geometry for a test (\( C_A \)) is

\[
C_A(A) = 3\left( \frac{|a_1|}{5} + \frac{|a_2|}{2} \right) + 12
\]

Next, assume that heat flux measurements are 3 times more expensive than a pressure measurements. The instrumentation type is represented as a binary vector \( S \), where 0 represents a pressure measurement and 1 represents a heat flux measurement. Therefore, the instrumentation cost (\( C_S \)) is

\[
C_S(s) = \#\{S : s = 0\} + 3(\#\{S : s = 1\})
\]

Thus, the total cost of the experiment \( C_{total} \) is then the sum of the geometry and instrumentation costs, as shown in Eq. (6).

\[
C_{total}(X) = C_A(A) + C_S(S)
\]

To demonstrate this approach, random specimen geometries and instrumentation types were generated for candidate design, and three example cases (A, B, and C) are shown in Fig. 1. Specimens A, B, and C represent varying levels of cost and expected information gain (i.e., the anticipated reduction in the current model uncertainty for aerodynamic pressure and heat flux). Therefore, with increasing cost, the mode shapes become more complex and more resources have to be allocated to instrument for heat flux. For example, Design A is a shallow Mode 1 type deformation with a cost of 35.6 and EIG of 0.78 (i.e., low cost and small model uncertainty reduction). For Design B, increasing the cost by nearly 20% results in a design that has a larger
Mode 1 scale factor and four times the expected information gain of Design A. Finally, the most expensive design, Design C, is a combination of the two mode shapes with the largest magnitudes and more heat flux instrumentation locations.

![Figure 1. Specimen geometries and instrumentation locations for various costs and corresponding information gain.](image1)

All of the possible experimental designs for this example were constructed as a Pareto Front in Fig. 2, where the information gain was calculated by performing a test (using synthetic data from RANS for this demonstration) and Bayesian model calibration. That is, the expected information gain is the KL-divergence between the prior and posterior distributions of the uncertain model discrepancy parameters for low-fidelity aerodynamic pressure and heat flux models. Examining the three specimens shown in Fig. 2, the tradeoff is readily apparent when considering the type of instrumentation and geometric complexity. This research on budgeting experiments using expected information gain provides a foundation for aiding decision-making by considering resource allocation for model calibration data collection in a multi-physics system. For additional details on this research, refer to the interim technical report [9].

![Figure 2. Pareto Front of maximum expected information gain and minimum cost.](image2)

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2.2 Targeted Information Gain for Error Reduction (TIGER)

In the previous scenario, expected information gain was formulated for obtaining data to calibrate models with the goal of global accuracy (Eq. (3)). To ensure a reduction in uncertainty near specific events, such as structural failure or regions of high temperatures, optimal data collection methods can also aid in achieving models that also predict targeted events. The method developed by Villanueva and Smarslok called Targeted Information Gain for Error Reduction (TIGER) uses a weighted expected information gain formulation to balance the placement of exploration points in the design space and capturing a specific event of interest \[8,9\]. To target regions of the design space where an event of interest (EoI) occurs, EIG can be weighted by the probability of the event. This is achieved by introducing the probability into the Monte Carlo estimate of EIG, such that this weight is calculated for every realization of the set of \( \theta \). Therefore, if the probability of the EoI is small when EIG is large, the weighted criterion would drive optimal designs away from that area of the design space. The weighted expected information gain estimate \( EIG_W \) is shown in Eq. (7).

\[
EIG_W(x) \approx \Pr(\text{EoI}(x, \theta)) \frac{1}{N} \sum_{i=1}^{N} \left\{ \ln[\Pr(y(i) | \theta(i), x)] - \ln \left( \frac{1}{M} \sum_{j=1}^{M} \Pr(y(i) | \theta(j), x) \right) \right\} \\
\text{Note that } \Pr(\text{EoI}(x, \theta)) \text{ does not need to be the actually probability of the EoI itself. For example, if it is set as the probability of failure, the designs chosen by } EIG_W \text{ may be driven to areas where the estimated probability is 1. This may result in inaccurate estimation of the entire failure region, particularly if the failure region is large, because points are only placed where the probability approaches 1. Instead, this probability may be set as the probability of being near the limit state of the EoI. For example, for an EoI defined by } g \geq \tau, \text{ the term } \Pr(\text{EoI}(x, \theta)) \text{ can be replaced by } \Pr(g - 2\tau \leq \kappa \leq g + 2\tau) \text{ where } \tau \text{ defines an area about the limit state.}
\]

Using the \( EIG_W \) criterion alone as a measure of utility would drive the optimal design to areas of predicted high probability of the EoI. Therefore, we introduced a bi-objective formulation, the Targeted Information Gain for Error Reduction (TIGER) formulation, where the utility function consists of both \( EIG \) and \( EIG_W \). The optimization problem of Eq. (8) is used to find the optimal design \( x^* \), where \( \alpha \) weights the two objectives.

\[
\max_x U_{\text{TIGER}} = \alpha EIG(x) + (1 - \alpha) EIG_W(x) \\
\text{s.t. } x \in X
\]

The purpose of \( \alpha \) is to balance global accuracy through designs chosen with large \( EIG \) and local, near EoI accuracy through those with large \( EIG_W \). When only maximizing \( EIG_W \), there is a risk of missing other areas of the design space where the EoI might occur. This is possible if one or more of the models is inaccurate in the design space. A natural way to avoid the use of test points to determine model error is to use a cross-validation metric, here the partial prediction error sum of squares \( PRESS_{\text{RMS}} \). This is found by leaving out a design point, re-training with the remaining data, and measuring the error at that point to get \( e_{XY} \) at that point. The operation is repeated for \( p \) training points to form a vector of \( e_{XY} \). The \( PRESS_{\text{RMS}} \) is calculated by

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For each model, the $PRESS_{RMS}$ is used to determine the value of $\alpha$. The value of $\alpha$ is increasing with $PRESS_{RMS}$, such that a large $PRESS_{RMS}$ corresponds to a large value of $\alpha$. The exact form of $\alpha$ as a function of $PRESS_{RMS}$ is user-defined.

The process of calibration of the uncertain parameters proceeds in iterations. In each iteration, the optimal design is found and added to the data set, and the models are calibrated with the new data. The flowchart in Fig. 3 displays the sequential data collection process using the TIGER criterion for $n$ models.

![Flowchart of sequential data collection process using TIGER criterion.](image)

A comparison of global and local prediction errors for the different experimental objectives was analyzed for a two-dimensional example (i.e., modified camelback function), shown in Fig. 4. A Gaussian process surrogate model was sequentially trained (i.e., selected points to reduce model uncertainty) using three different experimental designs. The high-value regions in the contour plots indicate where failure is likely to occur, thus the three different sequential data collection strategies allocated tests points to inform the model at those conditions for $u$ and $v$: a) global accuracy, b) event targeting, and c) balanced exploration for global and local accuracy near a targeted event.
Figure 4. Optimal experimental designs for a) global accuracy, b) event targeting, and c) balanced exploration for global and local accuracy near a targeted event.

The TIGER method was also successful in a classification problem for flutter and critical limit cycle oscillation amplitude for a panel in hypersonic flow [8], and additional details and can be found in the interim technical report by Villanueva and Smarslok [9].
3 UNCERTAINTY IN AEROTHERMOELASTIC MODELS UNDER TRANSITIONAL FLUID LOADING IN HIGH-SPEED FLOW

Thin-gauge metallic aircraft panels provide a means to minimize the weight and improve the serviceability of reusable, long duration cruise hypersonic vehicles [31-33]. However, the compliant nature of these structures, in combination with the severe aerothermodynamic loading, results in a propensity for nonlinear fluid-structure interactions. Thus, hypersonic vehicle design necessitates the consideration of aerothermoelastic coupling. Accurate characterization of the aerothermodynamic loads is critical to predicting the response and life of structural components. This already challenging task is further complicated by the fact that aerodynamic heating varies significantly with the state of the boundary-layer. This is particularly important for air-breathing hypersonic vehicles which primarily fly at conditions where the flow is transitional [34]. Therefore, aerothermoelastic response prediction and boundary-layer transition are key challenges in the development of future hypersonic systems.

Boundary-layer stability is highly dependent on wall temperature [35, 36] and surface geometry [36-38], both of which vary during flight for hot structure hypersonic vehicles. Previous studies have examined how aerothermoelastic effects, such as thermally induced deformations, can augment aerothermal loads [39,40] and impact boundary-layer transition [41,42]. Aerothermodynamic loading with a fixed transition region can result in structural responses that exceed those predicted assuming turbulent conditions [43,44]. In a recent study, Riley and McNamara [45] examined the response of a simply-supported panel assuming a fixed transition region and one which varied as a function of the structural state. Neglecting the movement of the transition region resulted in a constant region of elevated heating which made the panel more susceptible to deformation at reduced pressure loading [45].

The uncertainty associated with boundary-layer transition prediction necessitates a nondeterministic analysis. Previous studies have attempted to quantify the uncertainty in \( e^N \) predicted transition onset for 2D incompressible flow using a derivative-based sensitivity measure that tracks the change in the transitional Reynolds number with \( N \) factor [46,47]. Sensitivity of the onset location to the transitional \( N \) factor was found to increase with the height of a subcritical isolated smooth hump on a flat plate [46]. Additionally, Masad and Malik [47] determined that while wall suction and increasing Mach number delay transition, the onset location becomes more sensitive to the \( N \) factor. Lamorte et al. [43] applied stochastic collocation to investigate how uncertainty in the transition onset location affects the aerothermoelastic stability of a representative hypersonic vehicle surface panel. The onset location was uniformly distributed between 0.2 and 1.0m upstream of the panel leading edge. Transition onset was prescribed as a uniform distribution of locations upstream of the panel. Transitional heat flux was obtained using an algebraic transition model in conjunction with a RANS-based CFD solver. Accounting for uncertainty in the transitional loading revealed a potential for earlier flutter onset.

The previous study by Lamorte et al. [43] indicates that the probability distributions of the uncertain input significantly affects the aerothermoelastic stability of a surface panel. Additionally, the parametric investigation of Riley et al. [44] determined that structural response is more sensitive to transition onset than length of transition. The objective of this research is to more rigorously quantify the uncertainty in the predicted structural response associated with transitional boundary-layer effects. Specifically, a global sensitivity analysis is performed on a fundamental 2-D aerothermoelastic model under the assumption of a simply-supported titanium panel. Probability distributions based on historical data and the advice of subject matter experts are used to characterize the transitional \( N \) factor, the length of transition, and the potential for overshoot in
the aerothermodynamic loads. Transitional loading configurations that result in structural responses in excess of the fully turbulent prediction are identified.

### 3.1 Transitional Aerothermodynamic Modeling

A schematic of the configuration examined in this study is provided in Fig. 5. It is assumed that a titanium panel is located 2m from the leading edge of a 2-D surface inclined 5deg to the freestream, representing the forebody of a supersonic/hypersonic vehicle. The freestream conditions and panel geometry considered are listed in Table 1. The flow the panel experiences corresponds to the post oblique shock conditions. The freestream conditions coincide with the proposed cruise velocity and altitude specified for the conceptual Mach 5-7 hypersonic cruise vehicle outlined in [33]. Based on the surface temperatures predicted at this cruise condition, titanium alloys could be employed as the outer mold line structure of the vehicle [33,38].

![Figure 5. Panel located on inclined surface subject to a transitional boundary layer](image_url)

**Table 1. Freestream conditions and panel geometry**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach number</td>
<td>5.20</td>
</tr>
<tr>
<td>Altitude</td>
<td>27.4 km</td>
</tr>
<tr>
<td>Unit Reynolds number</td>
<td>$2.85\times10^6$ m$^{-1}$</td>
</tr>
<tr>
<td>Turn angle</td>
<td>5.0 deg</td>
</tr>
<tr>
<td>Length</td>
<td>1.50 m</td>
</tr>
<tr>
<td>Thickness</td>
<td>5.00 mm</td>
</tr>
</tbody>
</table>

The aerothermoelastic model, depicted in Fig. 6, has three primary components: 1) aerothermodynamic loads, 2) structural dynamics, and 3) heat transfer. The aerothermodynamics drive the thermo-structural response through the application of a pressure load (composed as the summation of mean and fluctuating components) and a surface heat flux. The mean flow pressure is modeled using third-order piston theory [49] which accounts for changes in the mean pressure due to structural deformations. The fluctuating pressure load (FPL) is computed using the model presented in [44]. The surface heat flux accounts for both aerodynamic heating, modeled using Eckert’s reference enthalpy method [50], and radiation between the structure and the freestream. The FPL and heat flux are dependent on the boundary-layer edge properties, which are obtained from the mean flow pressure in conjunction with isentropic flow relations [51]. A recent comparison with RANS based aerothermodynamics indicates that the analytical models used here adequately capture the characteristic aerothermoelastic response [52]. This framework was
previously used to assess the impact of transitional loading on panel response, where the transition onset and length were parametrically varied along the panel [44].

The structure is modeled as cylindrical bending of an isotropic plate with the assumptions of von Karman moderate deflection plate theory [51]. The structural equation of motion is solved using Galerkin’s method where the transverse displacement is approximated as a series of 25 free-vibration mode shapes of the panel. The structural temperature is computed using a finite element formulation of the transient, 2-D heat transfer equation with temperature-dependent specific heat and thermal conductivity [53]. The 2-D formulation allows for heat conduction through both the thickness and length of the panel. An adiabatic wall condition is prescribed for each boundary of the panel, except the upper surface where the net heat flux (aerodynamic and radiation) is applied.

Figure 6. Aerothermoelastic Model

The aerothermal and aeroelastic solvers are advanced in a loosely-coupled partitioned manner using a predictor implicit time integration approach [54]. This approach is advantageous in terms of computational efficiency as the individual solvers can use different time steps and information is exchanged between the solvers only once per time step [54]. In this study, the aeroelastic time step is 12.5 µs whereas the aerothermal solution is updated at a coarser time step of 125 µs. Therefore, the panel temperature obtained from the heat transfer analysis is passed to the structural solver only on the coarser aerothermal time step. In-depth descriptions of the aerothermoelastic model formulation are provided in [51, 53]. The coupling procedure and numerical schemes implemented in the aerothermoelastic model are discussed in [54].

The aerothermodynamic loads acting on the panel are heat flux and an overall pressure load. Transitional boundary-layer effects are incorporated into the heat flux and fluctuating pressure through blending laminar and turbulent profiles in proportion to the intermittency $\gamma$, which represents the fraction of time any spatial location spends in turbulent flow [55]. The intermittency function in Eq. (10) is derived from Emmon’s probabilistic model [56, 57] with the assumption of a Dirac delta burst source-rate density function and the transition length defined as the spatial distance between intermittency values of 0.01 and 0.99.
Note that the intermittency is a function of the transition length $\Delta x_t$ and onset location $x_t$. A general expression for the transitional loading is:

$$\gamma(x) = 1 - \exp\left[-\frac{4.1850}{\Delta x_t^2} (x - x_t)^2\right]$$

(10)

where $F_{\text{tran}}$ is the spatial distribution of the heat flux or skin friction coefficient. The fluctuating pressure model accounts for transitional effects through the skin friction coefficient. As shown in Eq. (11) overshoot is modeled by specifying the turbulent boundary-layer to originate at $x_t$ instead of the leading edge (LE) of the geometry. This is controlled through a binary input parameter $OS$. Here the authors emphasize that for transition models similar to Eq. (11) the overshoot magnitude decreases with increasing $\Delta x_t$ due to the asymptotic nature of the loads (heat flux and skin friction) at the boundary-layer origin. Transitional loads are computed based on the underlying aerothermodynamic models and the input $x_t$, $\Delta x_t$, and $OS$. Further detail on the transitional heat flux and fluctuating pressure models is available in [44]. An example of the transitional heat flux and pressure fluctuation is provided in Fig. 7 for transition beginning at $x/L = 0.3$ and ending at $x/L = 0.5$. The results in Fig. 7 demonstrate how the intermittency-based blending can be used to account for ($OS = 1$), or neglect ($OS = 0$), the effect of transitional overshoot.

![Figure 7. Transitional aerothermodynamic loads $x_t/L = 0.30$ and $\Delta x_t/L = 0.20$](image)

Accounting for boundary-layer transition introduces additional sources of uncertainty into the aerothermoelastic response prediction of panels. This uncertainty can be attributed to the computation of the transitional aerothermodynamic loads which require $x_t$, $\Delta x_t$, and $OS$ as input. Each input represents a source of epistemic uncertainty. Characterizing the uncertainty in $x_t$ is difficult as the onset location is dependent on the geometry and flow conditions. This study relates the onset location to a transitional $N$ factor ($N_{tr}$) obtained using the linear Parabolized Stability Equations (LPSE) and semi-empirical $e^N$ correlation method implemented in STABL [28].
Specifically, the LPSE are used to assess the stability of fixed-frequency (13400 kHz) perturbations imposed on a base flow that corresponds to the initial (undeformed, unheated) panel configuration. The $e^N$ method relates transition onset to the spatial amplification of fixed-frequency perturbations. Once a certain level of amplification is achieved (i.e., $N \geq N_{tr}$) the flow is assumed to be transitional.

The aerothermoelastic framework in Fig. 6 is rearranged in Fig. 8 to depict how the uncertain transitional input ($N_{tr}$, $\Delta x_t$, and OS) propagate through the model. At each time step, the transitional heat flux $Q$ and fluctuation pressure $P$ are computed based off the specified transitional input. These loads are passed as boundary conditions to the thermo-structural (TS) panel solver which computes the temperature field $T$ and displacement $w$ of the panel.

**Figure 8. Propagation of uncertain transitional input through the aerothermoelastic model**

The transitional $N$ factor is broadly divided into two categories: low-disturbance and noisy environments. Low-disturbance environments result in larger $N_{tr}$ and include smooth bodies in flight and quiet wind tunnel experiments. Noisy environments lead to lower $N_{tr}$ and correspond with rough geometries in flight and conventional wind-tunnel tests. Thus, the variability in $N$ at transition can be reduced through characterization of the freestream disturbance environment and surface conditions. Uncertainty in the transitional $N$ factor is characterized using the beta distribution $\text{Beta}(\alpha = 10, \beta = 7)$ in Table 2. This $N$ factor range accounts for transition occurring in both low disturbance and noisy environments.

Characterizing the length of transition requires an understanding of the formation, growth, and propagation of turbulent spots. As the first detailed experimental measurements of the internal pressure structure of turbulent spots in a hypersonic boundary-layer were made by Casper et al. in 2014 [59], this remains an area of active research. However, past experimental investigations of boundary-layer transition have examined transition length by computing the ratio of completed transition distance (or Reynolds number) to the distance from the model leading edge to onset $x_{te}/x_t$. A lognormal distribution $\text{lnN}(\mu = 0.99, \sigma = 0.88)$ is found to adequately capture the collected data [10].

Heat flux and surface pressure fluctuations peak near the end of transition. Overshoot refers to the fact that the magnitude of these peak loads is often underpredicted by fully turbulent models. Numerous experiments have demonstrated the overshoot phenomenon for heat flux [60-62] and surface pressure fluctuations [63-66]. Peak heating and fluctuating pressure RMS values have been reported as high as 1.5 [61] and 3.3 [65] times the fully turbulent predictions, respectively. The ability to predict the heating overshoot (i.e., location and magnitude) associated with transition is a critical design factor for air-breathing hypersonic cruise vehicles. Identification of the mechanisms that lead to overshoot in the aerothermodynamic loads during transition will help to
bound its likelihood and magnitude. As previously discussed, the transitional aerothermodynamic load models account for overshoot through a binary input parameter that alters the origin of the turbulent boundary-layer. Due to this modeling constraint uncertainty in the transitional overshoot is characterized with a binomial distribution $B(n=1500, p=0.5)$. The distribution specifies that for 1500 observations, 50% will exhibit overshoot during transition. Recall that the overshoot magnitude is dependent on the length of transition.

The uncertain input and their assumed probability distributions are summarized in Table 2 and 7500 samples taken from a Sobol sequence.

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
<th>Distribution Type</th>
<th>Parameter 1</th>
<th>Parameter 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transitional $N$ factor</td>
<td>$N_{tr}$</td>
<td>Beta: Beta($\alpha,\beta$)</td>
<td>10.0</td>
<td>7.0</td>
</tr>
<tr>
<td>Transition length</td>
<td>$\Delta x_t$</td>
<td>Lognormal: $\ln N(\mu,\sigma)$</td>
<td>0.99</td>
<td>0.88</td>
</tr>
<tr>
<td>Overshoot</td>
<td>$OS$</td>
<td>Binomial: $B(N,P)$</td>
<td>1500</td>
<td>0.5</td>
</tr>
</tbody>
</table>

### 3.2 Sensitivity Analysis and Probability of Exceeding Turbulent Loading

For conservative vehicle design, the assumption of fully turbulent flow is typically considered for the aerothermodynamic loading. However, the transitional overshoot phenomenon can result in loading which locally exceeds turbulent predictions. To quantify the importance of accounting for boundary-layer transition the probability of exceeding the turbulent prediction is computed for the applied loads (Fig. 9a) and response of the panel (Fig. 9b). Nearly a quarter of the cases exceed the turbulent RMS pressure whereas 11.3% result in larger peak heat flux. Approximately 15% of the panel responses have a larger maximum surface temperature. However, less than 3% of the responses result in greater maximum displacement and average temperature.

Further insight into the panel responses that exceed the turbulent conditions can be gained by examining the scatter plots in Fig. 10. Each scatter plot displays a horizontal banding caused by panel responses with laminar or fully turbulent loading. In Fig. 10 the turbulent banding occurs at average (Fig. 10a) and maximum temperatures (Fig. 10b) of 355 K and 382 K, respectively. The cases which exceed the average turbulent temperature in Fig. 10a have an $N_{tr}$ of 6.6 to 8.8 with a corresponding onset location range of 39% $L$ upstream and 12% $L$ downstream of the panel leading edge. Additionally, for each response the boundary-layer is fully turbulent by 47% $L$ with $\Delta x_t/x_t$ ranging from 0.03 to 0.83. In Fig. 10b, the maximum temperature is color contoured by its location along the panel. The peak temperature for the laminar and turbulent responses occur at the leading edge of the panel ($x/L = 0$). As anticipated, the largest maximum temperature of 448 K coincides with the shortest transition length of $\Delta x_t/x_t = 0.02$. 
The transitional cases with similar peak displacement locations to the laminar and turbulent responses ($0.54 \leq x/L \leq 0.57$) exceed the turbulent prediction of average panel temperature and maximum displacement. This is demonstrated by the displacement profile labeled “A” in Fig. 11, which corresponds to the transitional loading ($x_t = 1.94$ m, $\Delta x_t/x_t = 6.3\%$, $OS=1$) resulting in the largest displacement and average temperature. Recall the panel leading edge is at $x = 2.0$ m. The “B” displacement profile coincides with the transitional loading ($x_t = 2.90$ m, $\Delta x_t/x_t = 5.6\%$, $OS=1$) leading to the maximum surface temperature. Finally, “C” illustrates the variability in the panel response as the transitional loading ($x_t = 2.35$ m, $\Delta x_t/x_t = 2.0\%$, $OS=1$) results in the most downstream peak displacement.
Figure 11. Panel displacement predictions at 10s for various transitional loading

The sensitivity of the aerothermodynamic loading and response of a representative hypersonic vehicle panel to boundary-layer transition was examined. Uncertainty in the transitional $N$ factor, length of transition, and potential for overshoot was characterized using probability density functions based on experimental data and the advice of subject matter experts. The global sensitivity analysis revealed that the maximum overall pressure, panel displacement, and average heat flux are most sensitivity to the transition onset location. The maximum heat flux and RMS of the surface pressure fluctuation are dependent on both the onset and length of transition. Surface temperature sensitivities are consistent with those corresponding to heat flux. Transition with onset occurring upstream or near the panel leading edge and length less than the extent of laminar flow results in displacements and average surface temperatures that exceed values predicted based on the turbulent flow assumption.
4 DATA-DRIVEN MODELING OF FULL-FIELD DYNAMIC RESPONSE

To study fluid-structure interactions in high-speed flow, recent advances in full-field measurement techniques such as high-speed 3D digital image correlation (DIC) and fast-reacting pressure sensitive paint (PSP) have been implemented in related aero-structures research by Perez et al. [67]. These techniques collect spatially dense data using high speed cameras, resulting in large volumes of high-dimensional data (i.e., 1-sec ~ 10 GB). Models of such data enable simulation of experimental conditions, potential extrapolation to new conditions, and deeper study of the problem domain. However, integrating this high-dimensional, time-dependent data directly with the coupled aerothermoelastic models is cumbersome and imposes prohibitive memory requirements. For example, the pressure sensitive paint (PSP) data from the RC-19 experiments yielded a 526 x 654 node grid that has 344,004 correlated variables, corresponding to each pixel in the images [17]. Building models is a key way to extract useful knowledge from the high-dimensional data. Models mathematically encode the relationships between system variables and parameters, allowing the system to be simulated, at a fraction of the cost of performing an equivalent experiment. However, as the data increases in dimensionality, the benefits of modeling become increasingly challenging to attain as computational complexity drastically increases costs. Efficient modeling approaches must be explored to accommodate data of ever increasing dimension.

Turbulent boundary layer models are typically empirical formulations [68-70], the most prominent being the Corcos model [71,72]. In practice, it has been difficult to obtain good models with empirical formulations [73,74]. While direct numeric simulation (DNS) or large eddy simulation (LES) are possible, they are prohibitively expensive, especially for long-duration fluid-thermal-structural interaction simulations. Thus, it is reasonable to pursue data-driven approaches, especially in the presence of full-field measurement data. Data-driven techniques have underlying organizational structures and assumptions with abstract interpretations, but allow the features of the data to shine. They can be costly to train, but are generally inexpensive to evaluate. Examples include neural networks, Gaussian processes, random field models, support vector machines and relevance vector machines, random forests, and autoregressive integrated moving average models. Such a model must accurately reproduce the frequency response of the pressure field (particularly under 1000 Hz), and have sufficient spatial resolution to capture the localized behavior of the field, all while being computationally tractable.

An option for overcoming challenges with high-dimensionality is the spatial Markov-assumption, which enforces sparsity in the covariance matrix. However, it was discovered that the slow decay of spatial correlations in the RC-19 pressure data set make this technique inaccurate when coupled with structural response prediction and capturing spectral features. Gaussian processes can model the spatial correlation effectively, but typically model a white noise spectrum and are not suitable for very large $n$ as they have computational complexity $O(n^3)$. Vector autoregressive (VAR) models can accurately model the spatial correlations the frequency spectrum of the data, but have many parameters and require prohibitive amounts of data to train.

To efficiently model turbulent boundary layer noise from PSP measurements, a data-driven modeling approach is employed based on Devathi et al. [75] and da Silva et al. [76], which combines singular value decomposition (SVD) and autoregressive moving average (ARMA) modeling into a SVD+ARMA model. Here, this approach is called SVD+ARMA to distinguish it from the SVD-ARMA method for selecting ARMA model orders [77-79]. Singular value decomposition (SVD) transforms the data into many uncorrelated variables, changing the modeling task from training one high dimensional model to making many univariate models.
Autoregressive (AR) models are then fit to the transformed data due to their ability to efficiently and accurately model the time and frequency components of the data without requiring any knowledge of the physics. Data simulated by the AR models is easily rotated back to the original problem space. The SVD+ARMA approach (or PCA+ARMA when principal component analysis is used instead) has previously been used for multivariate signal modeling. Da Silva et al. [75] compressed multivariate signals with PCA and built ARMA models of them for structural health monitoring, and Devathi et al. [76] compressed a spatio-temporal loading with SVD and built ARMA models of the significant principal components for reliability analysis. Current quantitative validation results using SVD+ARMA demonstrate agreement in the time, space, and frequency domains. This indicates that the SVD+AR approach is capable of scaling from modeling tens of variables [75,76] to the thousands of variables of the PSP data.

In SVD+ARMA, SVD transforms the data into many uncorrelated variables, then ARMA models are fit to the transformed data. An ARMA model is of the form:

\[
x_t = c + \varepsilon_t - p \sum_{i=1}^{p} x_{t-i} \varphi_i + \sum_{i=1}^{q} \varepsilon_{t-i} \theta_i
\]

where \(x_t\) is the value of the signal at time \(t\), \(p\) and \(q\) are respectively the AR and MA orders, \(\varphi_i\) are the AR coefficients, \(\theta_i\) are the MA coefficients, \(\varepsilon_t\) are the errors (or innovations), and \(c\) is a constant. Additionally, \(\varphi_0 = \theta_0 = 1\). If \(q = 0\) and \(p \geq 1\), the model is simply an AR model, meaning that \(x_t\) is a function of itself at previous times. A special case of this is when \(p = 1\), yielding a random walk. If \(p = 0\) and \(q \geq 1\), the model is a MA model. SVD provides two important benefits for modeling a high dimensional dataset. The first is the orthonormal nature of the principal components. This allows the use of many independent single output models as opposed to one high dimensional multivariate model of the data, which is required when building a model in the original problem space. The second benefit of SVD is dimensionality reduction, which, in addition to reducing storage requirements and file transfer times, reduces the training and simulation effort associated with the ARMA models. ARMA models are of particular use for modeling time series data that has important frequency components. This is in contrast to regression methods that treat all variations about the mean prediction as broadband (Gaussian) white noise. In fact, ARMA model coefficients in the time domain formulation have a dual purpose as filter coefficients in the frequency domain, defining a transfer function. Additional benefits of ARMA models are that they are relatively inexpensive to train and simulate, while being available in many popular software packages.

Figure 12 compares one dimension of pressure sensitive paint data by considering the empirical power spectral density (PSD), a PSD resulting from simulations of a VAR model, and the theoretical PSD resulting from an SVD-AR model. Both the SVD+AR method and VAR model track the empirical PSD well. The PSD of the VAR model closely matches the empirical PSD, while the theoretical PSD from an SVD+AR model is somewhat smoother. However, the data requirements for VAR model construction are prohibitive.
The results demonstrate agreement in the time, space, and frequency domains. This indicates that the SVD+ARMA approach has scaled up well, from its proven capability of modeling tens of variables to the case with thousands of variables, such as full-field data. This methodology has many potential uses, including simulating and extrapolating wind tunnel tests to longer durations, estimating natural frequencies, and determining the strength of the fluid-structure coupling. Further, SVD+ARMA is a flexible modeling framework. It can extend to handle exogenous inputs, necessary for two-way fluid-structure coupling and to handle nonstationary data, which is encountered in the necessarily short-duration extreme environment experiments that never reach a steady-state. Two challenges of the SVD+ARMA method are selection of the ARMA model orders \((p\) and \(q\)) and validation of high dimensional models in the space, time, and frequency domains. Various approaches exist for quantitative model comparisons, such as hypothesis tests, Bayes factor, and a model reliability metric [80]. However, model selection and validation with consideration of frequency domain features has received less attention. Other validation metrics are based on the cosine similarity between two vectors. The benefit of cosine similarity metrics is the simplicity of the method, and that they are intuitive by lying on \([-1,1]\). Two metrics based on the cosine similarity are the well-known modal assurance criterion (MAC) [81], used to compare modal vectors; and the frequency response assurance criterion (FRAC) [82], used when phase angle and PSD are both important. The FRAC compares the complex response (computed via Fourier transform) of a system with the complex response of some validation data. As it is complex, differences in the phase spectrum and power spectrum affect the value of the FRAC. The PAC, on the other hand, considers only the squared magnitudes, the power spectral densities (PSDs). Given signals \(x\) and \(y\), with power spectral densities \(P_{xx}\) and \(P_{yy}\), the PAC is:

\[
PAC = \frac{P_{xx} \cdot P_{yy}}{\sqrt{P_{xx} \cdot P_{xx}} \sqrt{P_{yy} \cdot P_{yy}}}
\]

where \((\cdot)\) indicates the dot product. While the PAC of the principal components may be sufficient for validation, it does not provide a great visual impact, particularly for spatial data. Thus, it is interesting to spatially compare the variances and PACs of the spectral densities response in the

Figure 12. Comparison of power spectral densities for turbulent boundary-layer noise from pressure sensitive paint data
original space. Such information helps to visualize where a model is performing well, and perhaps more importantly, where it is not.

Validation of a model in a single domain, (such as, an SVD+ARMA model of measured turbulent boundary layer noise) is an important step in solidifying confidence in a multi-physics simulation. However, it is also important to validate the combined performance of coupled models. An example of this is using pressure data simulated from an SVD+ARMA model as a load on a structural panel model. The panel response to simulated pressure should match the response to the validation pressure. Ideally, when experimental pressure and panel response measurements are available, the panel response to the simulated data should match the displacement measurements. Figure 13 shows a contour plot of the PAC for the dynamic response of the panel (modeled with a reduced order model) coupled directly with the pressure sensitive paint data, as well as a SVD+ARMA model representing the turbulent boundary layer noise. Observe that the PAC values indicate a high quality representation of the SVD+ARMA model to the PSP data, however there is some spatial variation.

Figure 13. PAC of panel ROM response, with PSD comparisons for pressure input from the validation data (PSP measurements from the rigid panel) and surrogate model (SVD+AR model)
5 REFERENCES


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