Uncertainty Quantification and Error Estimation in Scramjet Simulation

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The numerical prediction of scramjet in-flight performance is a landmark example in which current simulation capability is overwhelmed by abundant uncertainty and error. The aim of this work is to develop a decision-making tool for balancing the available computational resources in order to equally reduce the effects of all sources of uncertainty and error below a confidence threshold. To that end, a nested uncertainty quantification and error estimation loop is proposed that balances aleatoric uncertainty, epistemic uncertainty, and numerical error in an efficient way. Application to a nozzle flow problem shows a reduction of the confidence interval by three orders of magnitude. The framework applied to the HyShot II scramjet flight experiment validation simulation indicates that the epistemic uncertainty in the RANS turbulence model is the dominating contribution to the confidence interval.

I. Introduction

A scramjet engine is an airbreathing propulsion system in which the combustion takes place at supersonic speeds. This makes the development of reliable scramjets a critical prerequisite for establishing sustained hypersonic flight. However, the current simulation capability for the complex multi-physics scramjet flows is overwhelmed by abundant uncertainties and errors. This limited accuracy of the numerical prediction of in-flight performance seriously hampers scramjet design.

The objective of the Predictive Science Academic Alliance Program (PSAAP) at Stanford University is to improve the current predictive simulation capabilities for scramjet engine flows. We define a predictive simulation as a numerical simulation in which the effects of uncertainty and error on the output quantity of interest (QOI) are sufficiently reduced to use the results in a decision making process. The computational focus of Stanford’s PSAAP team is the validation of state-of-the-art modeling codes for the HyShot II scramjet flight experiment performed by the University of Queensland in Australia.

The HyShot II geometry, shown in Figure 1a, involves a series of oblique shock waves over the forebody and the inlet, which results in the creation of a shock train in the combustor. The hydrogen fuel injected in the combustor burns at supersonic speeds, which leads to the generation of thrust in the expansion nozzle. A sketch of the performance margins and uncertainties of the HyShot II, depicted in Figure 1b, shows the variation of the thrust between the critical no-thrust and unstart boundaries as function of the fuel injection rate in time. The current simulation capability represented in terms of the wide probability density function (PDF) at the right of the figure shows a too large spread of the prediction beyond the operability limits for the simulation results to be useful in the design process. The uncertainties and errors therefore need to be reduced until their effect is sufficiently small compared to the design margins, as shown by the PDF with smaller variance in Figure 1b. To this end, the objective of this work is to develop a decision-making tool for allocating resources to systematically balance and reduce the impact of all sources of uncertainty and error.

One can distinguish different types of uncertainty and error. Aleatoric uncertainties, or irreducible uncertainties, describe physical variations caused by intrinsic randomness in the system and its environment.6

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These uncertainties can be characterized in terms of probability distributions and covariance matrices. Epistemic uncertainty is a second type of uncertainty caused by a certain lack of knowledge, which is not probabilistic in nature and can better be described using intervals. The lack of knowledge can result from structural uncertainty in the model form or insufficient measurement data to quantify the value of an input parameter. An essential property of epistemic uncertainties is that they can be reduced either by increasing model fidelity or by performing additional experiments. Computer simulations are also inherently subjected to numerical error, such as mesh and time step discretization errors, iteration errors in nonlinear problems, and computer round-off errors.

Different methods for uncertainty propagation and error estimation are, therefore, necessary to quantify the effect of the different sources of uncertainty and error. The propagation of the aleatoric input uncertainties through the computational model requires probabilistic methods such as Polynomial Chaos\(^3,16\) (PC) and Stochastic Collocation\(^1,14,17\) (SC) approaches. The non-intrusive SC method is preferred in large-scale computational problems since it is based on performing a series of deterministic simulations for sampled values of the aleatoric parameters. Epistemic uncertainty quantification\(^4,10\) is based on resolving the upper and lower limits of the epistemic uncertainty interval for the QOI. Optimization algorithms can be used to find these extrema or multi-model approaches can be employed. The dominating source of numerical error is often the spatial and temporal discretization error. This contribution to the numerical error can rigorously be estimated using the adjoint equation approach.\(^15\) The proposed tool for balancing uncertainties and errors incorporates these separate methods for aleatoric uncertainty propagation, epistemic uncertainty quantification, and numerical error estimation.

The decision-making framework for balancing uncertainties and errors is introduced in Section II. The subcomponents that perform the aleatoric uncertainty propagation, epistemic uncertainty quantification, and numerical error estimation are discussed in Section III. In Section IV, the framework is tested in a quasi one-dimensional nozzle flow problem. The results of the application to the HyShot II scramjet flight experiment validation are presented in Section V. In that case are taken into account the aleatoric uncertainty in the flight conditions, epistemic uncertainty in the RANS model, and spatial numerical error. The main findings are summarized in the concluding section.

II. Balancing uncertainties and errors

In this section, the tool for managing the combined effect of aleatoric uncertainty, epistemic uncertainty, and numerical errors is presented. The conceptual framework is presented in terms of a block diagram and the underlying error estimates are discussed.

II.A. Conceptual framework

In order to take into account the effect of all uncertainties and errors, a deterministic simulation is not sufficient because one needs to propagate aleatoric uncertainty, quantify epistemic uncertainty, and estimate
numerical errors, as shown in Figure 2a. Based on the results of these subcomponents, the decision-making tool then indicates whether to invest additional resources in either more aleatoric uncertainty sampling, model fidelity improvement, or spatial mesh refinement to reduce the aleatoric uncertainty propagation error, epistemic uncertainty, or numerical error, respectively. Model fidelity and discretization error are here used as examples of epistemic uncertainty and numerical error, respectively. Balancing the computational efforts in the three types of uncertainty and error is, therefore, equivalent to balancing the aleatoric uncertainty propagation error, the epistemic uncertainty, and the numerical error.

The present methodology is based on a non-intrusive approach to propagate aleatory uncertainty in which the aleatoric output uncertainty is computed by analyzing the results of multiple deterministic simulations for varying aleatoric parameter values in an aleatoric post-processing step. In these deterministic computations for the aleatoric samples, the effect of epistemic uncertainty and discretization error can also be evaluated. The aleatoric post-processing step is, therefore, the most suitable step in the UQ process in which to perform this decision making, since the aleatoric uncertainty samples are inputs to the post-processing as well as the epistemic uncertainty and the numerical error in these samples, see Figure 2b. The aleatoric post-processing computes then as usual the probability distribution and the statistical moments of the QOI. In addition, it is also in the position to compute the combined confidence level of the aleatoric uncertainty propagation error, the epistemic uncertainty interval, and the numerical error bar for these outputs.

These three components give rise to the nested three-layer uncertainty quantification and error estimation loop shown in Figure 3. In the first layer, \( n_s \) samples are drawn for the aleatoric uncertainty propagation in the space of the aleatoric uncertain input parameters. The location of the sampling points depends on the aleatoric uncertainty quantification method used, which is further discussed in Section III.A. In order to compute the effect of epistemic uncertainty, an epistemic uncertainty quantification is performed for each aleatoric sample. One approach to quantify epistemic uncertainty is to propagate epistemic input intervals to the output using optimization over the space of the epistemic parameters. The contribution of spatial discretization to the numerical error can be estimated by solving, for example, an adjoint problem for each simulation performed in the epistemic optimization loop. Recombining the numerical error estimation with the epistemic uncertainty quantification and the aleatoric uncertainty propagation yields an estimate of the impact of all sources of uncertainty and error on the QOI. The result is then a cumulative probability distribution function (CDF) superimposed by an confidence interval that accounts for the aleatoric uncertainty propagation error, the epistemic uncertainty, and the numerical error. As a consequence, confidence intervals for statistical moments and percentiles are also obtained. Second order effects, for instance, of the error in the epistemic uncertainty quantification are neglected.

II.B. Error estimates

Since the magnitude of the aleatoric uncertainty propagation error caused by the finite number of aleatoric samples \( n_s \) is not known, error estimates form the basis for balancing the aleatoric error with the epistemic
uncertainty and the numerical error. The aleatoric propagation is here performed using the Simplex Stochastic Collocation (SSC) method, which is discussed further in Section III.A. This non-intrusive approach based on a multi-element discretization of the aleatoric parameter space $\Xi$ based on simplex subdomains leads to the following error estimate for the absolute aleatoric propagation error $\varepsilon_\mu$ in the mean $\mu_u$ of an output QOI $u$

$$\varepsilon_\mu \leqslant \sum_{j=1}^{n_e} \bar{\Omega}_j \varepsilon_{AUQ_j},$$  \hspace{1cm} (1)

with $n_e$ the number of simplex elements, $\varepsilon_{AUQ_j}$ the local absolute error estimate in simplex $\Xi_j$, and $\bar{\Omega}_j$ the probability contained in $\Xi_j$

$$\bar{\Omega}_j = \int_{\Xi_j} f_\xi(\xi) d\xi,$$  \hspace{1cm} (2)

with $\sum_{j=1}^{n_e} \bar{\Omega}_j = 1$. The vector of aleatoric parameters is here given by $\xi$, $f_\xi(\xi)$ is their probability density, and for the disjoint elements $\Xi_j$ holds $\Xi = \bigcup_{j=1}^{n_e} \Xi_j$. Taking into account also the absolute epistemic uncertainty $\varepsilon_{EUQ_j}$ in the subdomains $\Xi_j$ gives for $\varepsilon_\mu$

$$\varepsilon_\mu \leqslant \sum_{j=1}^{n_e} \bar{\Omega}_j (\varepsilon_{AUQ_j} + \varepsilon_{EUQ_j}).$$  \hspace{1cm} (3)

This expression leads to the important observation that while reducing the local aleatoric uncertainty propagation errors $\varepsilon_{AUQ_j}$ by increasing the number of aleatoric samples, $\lim_{n_e \to \infty} \varepsilon_{AUQ_j} = 0$, the epistemic uncertainty leads to a minimum residual error $\varepsilon_{\mu\text{min}}$ for $\varepsilon_\mu$ equal to

$$\varepsilon_{\mu\text{min}} \leqslant \sum_{j=1}^{n_e} \bar{\Omega}_j \varepsilon_{EUQ_j}. \hspace{1cm} (4)$$

Based on this estimate it can be concluded that, if the minimum obtainable error $\varepsilon_{\mu\text{min}}$ for $n_e \to \infty$ is larger than an accuracy requirement, then this threshold cannot be reached by performing aleatoric sampling alone according to estimate (4). First, the epistemic uncertainty needs to be reduced, for example, by improving the fidelity of the model description of the physical problem. Further including the effect of absolute numerical discretization error $\varepsilon_{\Delta x_j}$ leads to the following equivalent relations for the error estimate

$$\varepsilon_\mu \leqslant \sum_{j=1}^{n_e} \bar{\Omega}_j (\varepsilon_{AUQ_j} + \varepsilon_{EUQ_j} + \varepsilon_{\Delta x_j}),$$  \hspace{1cm} (5)

and the minimum error

$$\varepsilon_{\mu\text{min}} \leqslant \sum_{j=1}^{n_e} \bar{\Omega}_j (\varepsilon_{EUQ_j} + \varepsilon_{\Delta x_j}). \hspace{1cm} (6)$$

Figure 3. Nested uncertainty quantification and error estimation loop.
For deciding whether to allocate additional resources to reduce either the epistemic uncertainty or the numerical error in this case, their separate contributions to the minimum error $\varepsilon_{\mu_{\min}}$ can be estimated as follows:

$$
\varepsilon_{\mu_{\min,EUQ}} \lesssim \sum_{j=1}^{n_a} \bar{\Omega}_j \varepsilon_{EUQ_j},
$$

(7)

$$
\varepsilon_{\mu_{\min,\Delta x}} \lesssim \sum_{j=1}^{n_a} \bar{\Omega}_j \varepsilon_{\Delta x_j}.
$$

(8)

The estimates of the epistemic uncertainty $\varepsilon_{EUQ_j}$ and the numerical error $\varepsilon_{\Delta x_j}$ are obtained from the obtained from the epistemic uncertainty quantification and numerical error estimation layers in the nested loop of Figure 3, respectively. Equivalent error estimates for other statistical moments or, for example, the root mean square (RMS) error norm can be derived.

II.C. Block diagram

Based on the preceding sections, the presented framework for balancing uncertainties and errors can be summarized in the form of the block diagram in Figure 4. It is assumed that at the start of the process the aleatoric input uncertainty is sufficiently characterized and quantified. An initial model fidelity and spatial discretization are also selected. This initial numerical description can be based on a low fidelity model and a coarse mesh.

![Figure 4](image-url)

**Figure 4.** Uncertainty quantification and error estimation decision-making framework.

The first step is then to perform the smallest number of aleatoric samples $n_a$, in the sense of Figure 3, to obtain the error estimates (5) to (8). This number is, for example, $n_a = 5$ in case of one aleatoric uncertain
parameter and SSC as aleatoric propagation method. If the estimate (6) of the minimum obtainable error \( \varepsilon_{\mu_{\text{min}}} \) is smaller than an accuracy requirement \( \varepsilon \), then the aleatoric sampling loop of Figure 3 is performed until \( \varepsilon_{\mu} \) (1) reaches the threshold. The minimum error estimate \( \varepsilon_{\mu_{\text{min}}} \) can change slightly with increasing numbers of samples, because of the potential dependence of \( \varepsilon_{\text{EUQ}} \) and \( \varepsilon_{\Delta x_j} \) on the location in the aleatoric probability space \( \Xi \). Therefore, \( \varepsilon_{\mu_{\text{min}}} \) has to be smaller than \( \varepsilon \) with some margin to avoid \( \varepsilon_{\mu_{\text{min}}} \) becoming larger than \( \varepsilon \) after adding more samples.

On the other hand, if \( \varepsilon_{\mu_{\text{min}}} \) is larger than the threshold \( \varepsilon \), then the largest contribution to \( \varepsilon_{\mu_{\text{min}}} \) is reduced by comparing \( \varepsilon_{\mu_{\text{min}},\text{EUQ}} \) (7) and \( \varepsilon_{\mu_{\text{min}},\Delta x} \) (8). In order to reduce the largest contribution, either the model fidelity needs to be improved or the spatial mesh needs to be refined. The updated model or discretization is used to perform a new set of computations for the initial aleatoric samples. The resulting \( \varepsilon_{\mu_{\text{min}}} \) is then compared to the threshold \( \varepsilon \), and so on until \( \varepsilon_{\mu_{\text{min}}} \) is small enough. This process results in a validation simulation analogous to a validation experiment, where all sources of uncertainty and error are taken into account and sufficiently reduced below a tolerance \( \varepsilon \) in an efficient way. It can eventually also lead to the conclusion that the confidence requirement \( \varepsilon \) cannot be met within the available computational budget.

The advantage of the framework is that computational resources are invested in performing highly accurate aleatoric uncertainty propagation only, if the balanced contributions of epistemic uncertainty and numerical error are estimated to be small enough. To further minimize the number of cycles in the process, it is important to determine the improvement of model fidelity or spatial mesh refinement that is required in each step. Based on the order of convergence of the spatial discretization, the required mesh size can be estimated. In contrast, the reduction of epistemic uncertainty resulting from an improvement in model fidelity is more difficult to predict. Finding a higher fidelity model also requires detailed insight into the relevant physical processes, which makes it a highly problem-dependent step.

III. Subcomponents of the framework

The separate methods for aleatoric uncertainty propagation, epistemic uncertainty quantification, and numerical error estimation, that are incorporated in the combined framework and applied to the problems in the next sections, are briefly described below.

III.A. Aleatoric uncertainty propagation

For the non-intrusive aleatoric uncertainty propagation here the Simplex Stochastic Collocation\(^{13,14} \) (SSC) method is used, since it results in the error estimates from Section II.B which form the basis of the framework for balancing uncertainties and errors. An example of the simplex elements discretization of a two-dimensional probability space \( \Xi \) by SSC based on a Delaunay triangulation of \( n_s = 17 \) sampling points \( \xi_k \) is shown in Figure 5a with \( k = 1, \ldots, n_s \). The simplexes are subsequently refined from the initial discretization by adding a random sample in a subdomain of the element with the highest value of the refinement measure. The mean \( \mu_u \) and higher moments \( \mu_{u_i} \) of \( u(\xi) \) are then computed as summations of integrals over the simplexes

\[
\mu_{u_i} = \int_{\Xi} u(\xi)^i f_{\xi}(\xi) d\xi = \sum_{j=1}^{n_s} \int_{\Xi_j} u(\xi)^i f_{\xi}(\xi) d\xi.
\] (9)

To that end, the response surface \( u(\xi) \) is approximated by a piecewise polynomial approximation \( w(\xi) \) in the form of a local polynomial chaos expansion \( w_j(\xi) \) in the simplexes

\[
u(\xi) \approx w(\xi) = w_j(\xi) = \sum_{i=0}^{n_j} c_{ij} \Psi_{ij}(\xi),
\] (10)

with \( \xi \in \Xi_j \), basis polynomials \( \Psi_{ij}(\xi) \), coefficients \( c_{ij} \), and \( n_j + 1 \) the number of expansion terms. The coefficients \( c_{ij} \) are computed by constructing \( w_j(\xi) \) as an interpolation of a higher-degree stencil \( S_j \) of samples \( v_j \) in surrounding simplexes. In Figure 5b an example of such a two-dimensional stencil is given for polynomial degree \( p_j = 4 \). Limiters for the local polynomial degree \( p_j \) are used to achieve a robust approximation of discontinuities, which is consistent with the discretization in physical space. SSC also combines the effectiveness of random sampling in higher dimensions with the accuracy of higher-degree polynomial interpolation. The error estimate (1) is derived from the hierarchical surplus, which is the difference between the sampled value \( v_k = u(\xi_k) \) in a new sampling point \( \xi_k \) and the interpolated value.
\( w(\xi_k) \) at the previous approximation level. It represents the aleatoric uncertainty propagation error in the response surface approximation \( w(\xi) \) with respect to the exact response \( u(\xi) \) due to the finite number of samples \( n_s \).

III.B. Epistemic uncertainty quantification

There are several different approaches for computing the epistemic uncertainty interval for the output QOI. The upper and lower values of the interval can, for example, be determined by applying an optimization method in the space of the epistemic uncertain parameters. This involves solving two optimization problems for finding the extrema of the epistemic response surface. This approach is used in the nozzle flow problem, where the response surface is a monotonic function, such that only the extrema of the input interval need to be sampled.

Another technique to find the epistemic spread in the output is to solve the problem with different models in a multi-model approach. The different results give an indication of the uncertainty in the prediction caused by the modeling decisions. In the HyShot II scramjet simulations two different RANS turbulence models are used to assess the effect of the choice of the turbulence model. The minimum and maximum of the two results is then used as the local epistemic uncertainty interval. This approach does obviously not take into account the effect of the RANS modeling simplifications themselves. It can, therefore, be considered as the minimum uncertainty that can be expected from the choice of the model in RANS simulations.

III.C. Numerical error estimation

The adjoint method for the numerical error estimation of the spatial discretization error in integral outputs, or functionals, is based on a two-grid approach.\(^\text{15}\) Consider in physical space a baseline coarse grid \( \Omega_H \) and a fine grid \( \Omega_h \) which can be obtained, for instance, by isotropically refining the baseline mesh. The goal of this approach is to obtain an accurate estimate of some functional \( f_h(U_h) \) on the fine grid based on the flow and adjoint solutions on the coarse grid. To enable this estimation, the flow and adjoint solutions computed on the coarse grid have to be interpolated onto the fine grid. These interpolations are represented by \( U_h^H \) and \( I_h^H \Psi^H \), respectively. Assuming linearity and expanding the functional and residual about \( U_h^H \), and defining the adjoint solution \( \Psi^H \) as

\[
\left\{ \frac{\partial R^H}{\partial U^H} \right\}^T \Psi^H = - \left\{ \frac{\partial f^H}{\partial U^H} \right\}^T,
\]

the following expression was derived by Venditti and Darmofal\(^\text{15}\) for the estimate of the numerical error:

\[
f_h(U_h) = f_h(U_h^H) + \{I_h^H \Psi^H\}^T R_h(U_h^H) + R_h^k(I_h^H \Psi^H)^T (U_h - U_h^H)
\]

\[
= f_h(U_h^H) + \varepsilon_{cc} + \varepsilon_{re}
\]
In the above equation, the first two terms on the right hand side can be evaluated by post-processing the coarse grid flow and adjoint solutions while the third term is not computable. For the error estimation to be accurate, it would be desirable for $|\varepsilon_{re}|$ to be small relative to $|\varepsilon_{cc}|$. A possible way of achieving this could be to target the reduction of $|R^\Psi_h(I^H h \Psi_H)|$ via mesh adaptation.

IV. Quasi one-dimensional nozzle flow

The proposed framework is first tested on a quasi one-dimensional nozzle flow problem as a simplified model for a scramjet engine. The aleatoric and epistemic uncertainty is introduced in the boundary conditions and the numerical error estimation focuses on the discretization error caused by the spatial mesh size.

The flow through the quasi one-dimensional nozzle is modeled by the steady Euler equations. The spatial discretization is performed using a cell centered MUSCL scheme on a uniformly spaced mesh. The adjoint solution is obtained by the automatic differentiation software package Tapenade. The area variation of the nozzle is modeled as a source term in the one-dimensional Euler equations under quasi one-dimensional assumptions.

The area $A(x)$ of the diverging nozzle is taken to be a linear function of the longitudinal coordinate $x$ and is given by $A(x) = 1.0512 + 0.07x$, with $x = [0, 10]$, see Figure 6. The flow Mach number $M$ is assumed to be an aleatoric input parameter with a beta distribution in the range $[1.48; 1.52]$ with beta distribution parameters $\beta_1 = \beta_2 = 4$. The epistemic uncertainty is treated as a lack of knowledge of the value of the pressure ratio $p_{rat}$, because of, for example, limited available measurement data, in contrast to epistemic uncertainty due to structural model fidelity uncertainty. This lack of knowledge is expressed in terms of an initial interval of $p_{rat} = 2.45 \pm \Delta EUQ$, with $\Delta EUQ = 10^{-1}$. This type of epistemic uncertainty can be reduced by, for example, performing more experiments to determine the value of $p_{rat}$ more exactly. These settings for the boundary conditions induce a standing shock wave in the interior of the nozzle. The initial number of spatial cells is $n_x = 10$. The objective function is taken to be the integral of the pressure between $x = [4, 10]$. The target confidence in the prediction of this value is $10^{-3}$. Here the root mean square (RMS) error norm $\varepsilon_{rms}$ is used instead of the mean $\varepsilon_{\mu}$ of Section II.B, since the RMS norm converges more smoothly than an integral quantity such as the mean.

![Figure 6. Sketch of the nozzle flow problem geometry, boundary conditions, and objective pressure integral.](image)

The results of the application of the decision-making framework of Figure 4 to the nozzle flow problem are summarized in Table 1. The first row shows the results for the initial epistemic uncertainty of $\Delta EUQ = 10^{-1}$ and the initial discretization with $n_x = 10$ spatial cells. The number of aleatoric samples $n_s = 5$ is the minimum to obtain an estimate of the aleatoric uncertainty propagation error in this case. The minimum obtainable error $\varepsilon_{rms_{min}} = 6.45 \cdot 10^{-1}$, which contains the contributions of the epistemic uncertainty and numerical error, highlighted in the table is larger than the threshold of $10^{-3}$. It is, therefore, not useful to perform additional aleatoric samples, since the error $\varepsilon_{rms} = 6.50 \cdot 10^{-1}$ for $n_s = 5$ is already close to the minimum error.

In Figure 7a it is verified that increasing the number of aleatoric samples to $n_s = 15$ does indeed not decrease the error $\varepsilon_{rms}$ significantly. The figure illustrates that the error estimate $\varepsilon_{rms}$ approaches the minimum error $\varepsilon_{rms_{min}}$ from above. The estimates of $\varepsilon_{rms_{min}}$ shows a slight variation with $n_s$, since the effects of epistemic uncertainty and numerical error can depend on the sampling location in the space of aleatoric parameters. The decomposition of $\varepsilon_{rms_{min}}$ into the epistemic uncertainty $\varepsilon_{rms_{min,EUQ}}$ and numerical
shows that \( \varepsilon \) forms the largest contribution to the minimum discretization error \( \varepsilon_{\text{rms}, \Delta x} \) contributions is also given. The minimum discretization error \( \varepsilon_{\text{rms}, \Delta x} = 1.53 \cdot 10^{-2} \) falls outside the range of the vertical axis. The resulting large size of the confidence interval for the mean \( \mu \) in Figure 7b does also not decrease with an increasing number of aleatoric samples. Here the aleatoric approximation for the mean \( \mu \) is already available for the initial number of \( n_s = 3 \) samples. The estimate of the aleatoric uncertainty propagation error, and thus the combined effect of the three contributions, is only available after \( n_s = 5 \) samples. It can be concluded that the large confidence bars are not caused by aleatoric uncertainty propagation error, but by either epistemic uncertainty or numerical error.

*Figure 7. Nozzle flow problem for \( \Delta EUQ = 10^{-1} \) and \( n_s = 10 \).*

The data in Table 1 shows that \( \varepsilon_{\text{rms}, \Delta x} = 6.31 \cdot 10^{-1} \) forms the largest contribution to the minimum error \( \varepsilon_{\text{rms}, \Delta x} \). In the second row of the table, the epistemic uncertainty is, therefore, reduced with an order of magnitude to \( \Delta EUQ = 10^{-2} \). This can correspond, for example, to performing additional experiments to determine the true value of pressure ratio \( p_{\text{rat}} \) more accurately. The results show that for \( \Delta EUQ = 10^{-2} \) the minimum error \( \varepsilon_{\text{rms}, \Delta x} = 1.04 \cdot 10^{-1} \) and the epistemic contribution \( \varepsilon_{\text{rms}, \Delta x} = 7.83 \cdot 10^{-2} \) have decreased, but that \( \varepsilon_{\text{rms}, \Delta x} \) is still larger than \( 10^{-3} \). Further reducing \( \Delta EUQ \) to \( 10^{-3} \) results in the situation that the numerical error \( \varepsilon_{\text{rms}, \Delta x} = 2.34 \cdot 10^{-2} \) starts to dominate. As a next step, the number of cells in the spatial mesh \( n_s \) is increased to 25. This process can systematically be continued until \( \Delta EUQ = 10^{-5} \) and \( n_s = 100 \), which results in a minimum error \( \varepsilon_{\text{rms}, \Delta x} = 1.47 \cdot 10^{-4} \) smaller than \( 10^{-3} \) with a margin. Also the contributions of the epistemic uncertainty \( \varepsilon_{\text{rms}, \Delta x} = 9.88 \cdot 10^{-5} \) and the numerical error \( \varepsilon_{\text{rms}, \Delta x} = 4.83 \cdot 10^{-5} \) are then well balanced.

Only in the last row the number of aleatoric samples is increased to \( n_s = 11 \) to converge the actual error estimate to \( \varepsilon_{\text{rms}} = 9.80 \cdot 10^{-4} \) as shown in Figure 8a. The aleatoric refinement is automatically terminated when \( \varepsilon_{\text{rms}} \) reaches the accuracy threshold \( 10^{-3} \). Figure 8b illustrates that both the confidence interval and the mean converge in this case with an increasing number of aleatoric samples. It can be observed that not all confidence bars contain the converged solution for the mean, since the intervals are based on error estimates, instead of strict bounds. Error bounds are difficult or even impossible to obtain for non-intrusive aleatoric uncertainty propagation methods and adjoint numerical error estimation for general strongly nonlinear systems. It has been verified that further increasing \( n_s \) does not improve the results.

![Table 1. Reducing and balancing uncertainties and errors for the quasi one-dimensional nozzle flow.](image)

<table>
<thead>
<tr>
<th>( n_s )</th>
<th>( \Delta EUQ )</th>
<th>( n_s )</th>
<th>( \varepsilon_{\text{rms}} )</th>
<th>( \varepsilon_{\text{rms}, \Delta x} )</th>
<th>( \varepsilon_{\text{rms}, \Delta x} )</th>
<th>( \varepsilon_{\text{rms}, \Delta x} )</th>
<th>( \varepsilon_{\text{rms}, \Delta x} )</th>
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<tr>
<td>5</td>
<td>10^{-1}</td>
<td>10</td>
<td>6.50 \cdot 10^{-1}</td>
<td>6.45 \cdot 10^{-1}</td>
<td>6.31 \cdot 10^{-1}</td>
<td>1.53 \cdot 10^{-2}</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>10^{-2}</td>
<td>10</td>
<td>1.08 \cdot 10^{-1}</td>
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<tr>
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significantly.

It is illustrated in Figure 9 by comparing the initial and final results that the confidence in the numerical prediction is significantly improved using the decision-making framework. The size of the confidence interval has been reduced by three order of magnitude. This results also in a significant shift of the center of the interval. The final solution for the mean including the confidence in the prediction is \( \mu = 0.86985 \pm 7.77 \cdot 10^{-4} \).

The aleatoric uncertainty in the QOI and the confidence in the result can also be expressed in terms of an interval superimposed on a cumulative probability distribution function (CDF) as shown in Figure 10. It can be seen from the small confidence interval that the the CDF is known up to a high level of accuracy. From this information also the 95% percentile can, for example, be derived to be 1.22261 with a confidence interval of [1.22234; 1.22288].

In Table 1, the reduction of the epistemic uncertainty and numerical error has been performed in a number of smaller steps for illustrative purposes. The process could be completed in 1 step by using a linear estimate of the necessary epistemic uncertainty and using the spatial order of convergence for predicting the required mesh size. Further, if the aleatoric uncertainty propagation error is not of interest in the first step, but only \( \varepsilon_{\text{rms,min}} \), then 3 aleatoric samples would already be sufficient initially. This reduces the total computational costs of the framework to 6 simulations and adjoints on the initial coarse mesh and 22 for the fine discretization.
V. HyShot II flight experiment validation

The framework is here used for comparing the impact of the aleatoric uncertainty, epistemic uncertainty, and numerical error in the HyShot II flight experiment simulation. To that end, the aleatoric uncertainty in the flight conditions is first propagated separately. Next the aleatoric uncertainty is compared with the epistemic uncertainty in the RANS turbulence model and the numerical discretization error. The RANS equations are solved using an in-house flow solver with a second order spatial discretization on a mesh of $175 \cdot 10^3$ hexahedral cells.

V.A. Aleatoric flight conditions

The flow conditions of the HyShot II flight are uncertain due to the failure of the radar tracking system during the experiment. Therefore, the free stream conditions were inferred from pressure measurements in the unfueled side of the combustor in a previous study using Bayesian inversion. The result of the Bayesian inference analysis, in terms of the Markov Chain Monte Carlo (MCMC) sample density, is shown in Figure 11a for the angle of attack $\alpha$ and flight altitude $h$ for test case 2 at $t=538.172s$. The probability distribution of the flow conditions shows a highly correlated structure with a coefficient of variation (CV) of 2.1\% for the angle of attack and 0.2\% for flight altitude. The flight conditions can, therefore, be considered to be aleatoric uncertainties, in the sense that they are described by a probability distribution and a correlation. The variability also includes uncertainty caused by the pressure measurements and the ill-posedness of the inverse problem. In this case the Mach number is kept constant at 7.831.

![Bayesian inference results](image1)

(a) Bayesian inference results

![SSC discretization](image2)

(b) SSC discretization with $n_s = 11$ samples denoted by circles

Figure 11. Probability distribution of the aleatoric angle of attack and the flight altitude for the HyShot II flight experiment.

The SSC discretization of the aleatoric HyShot II flight conditions is shown in Figure 11b for $n_s = 11$. 

11 of 17

American Institute of Aeronautics and Astronautics
samples and \( n_e = 16 \) elements. The initial discretization consists of \( n_e = 4 \) triangular elements with samples at the four corners of the probability space and one in the center. The refined discretization leads to more samples in regions of higher probability in combination with a good spread of the sampling points for accurate interpolation. That shows that SSC is effective in discretizing the correlated inputs of the HyShot II case given by the MCMC data points. At \( n_s = 11 \) samples the first estimate of the aleatoric uncertainty propagation error is obtained.

The mean pressure field and standard deviation in the cold combustor are given in Figure 12 for the 11 aleatoric samples. These results are based on two-dimensional steady Reynolds Averaged Navier Stokes (RANS) simulations, with the Spalart-Allmaras turbulence model at constant specific heat ratio \( \gamma \). The relative value of the energy residual is converged up to \( 10^{-4} \). In the mean pressure field, the shock train in the combustor can be recognized. The standard deviation is highest near the shocks, particularly at the shock wave/boundary layer interactions (SWBLI) where the shock train reflects from the combustor walls. The magnitude of the standard deviation is approximately 1\% of that of the mean pressure, compared to a 2.1\% and 0.2\% input CV for the angle of attack and the altitude, respectively.

![Figure 12. SSC results for the mean pressure and standard deviation fields for the cold HyShot II combustor with aleatoric flight conditions: Top figure denotes mean and bottom figure denotes standard deviation.](image)

Wall pressure at the transducer locations is shown in Figure 13 in terms of the predicted mean, and the 99\% computational and experimental confidence intervals. Thus aleatoric uncertainty alone does not fully account for the discrepancy with the experiments or with the size of the experimental uncertainty bar.

V.B. Epistemic turbulence model

In addition to aleatoric uncertainty in the flight conditions, epistemic uncertainty in the choice of the RANS turbulence model is also considered here. An interval description is used to represent this type of model form uncertainty. The interval is determined using a multi-model approach by performing the simulations for both the the Spalart–Allmaras and the Menter \( k-\omega \) SST turbulence models. In Figure 14, the results for the two models are shown in terms of the wall pressure for the first aleatoric sample at \( \alpha = 3.98^\circ \) and \( h = 34.1 \) km. It shows the pressure jumps due to the reflecting shock train and the pressure drop in the nozzle. The models lead to a significant difference in predicting of the pressure, with a maximum of 20\% over all 11 aleatoric samples. The local difference between the minimum and maximum of the two predictions is used as the local epistemic uncertainty interval for wall pressure. Since only two turbulence models are considered, the interval is an estimate of the minimum uncertainty involved with the choice of model. This is a first step to quantify epistemic uncertainty in the HyShot II case. The total epistemic uncertainty is larger since, for example, the effect of the RANS assumptions is not taken into account here. The non-reacting case is considered here to eliminate additional epistemic uncertainty stemming from mixing and combustion models.
Figure 13. SSC results for the mean and 99% confidence intervals of the combustor wall pressure of the cold HyShot II combustor with aleatoric flight conditions compared to the experimental uncertainty bars.

Figure 14. Epistemic uncertainty due to the choice of the RANS Spalart–Allmaras or Menter $k-\omega$ SST turbulence model for the first aleatoric sample of the cold HyShot II combustor.
The prediction of wall pressure including the effect of both aleatoric and epistemic uncertainty is compared to the measurements in Figure 15 in terms of the 99% confidence intervals. The computational interval accounts for the aleatoric uncertainty, the aleatoric uncertainty propagation error, and epistemic uncertainty. The new predicted intervals show significant improvement over using only aleatoric uncertainty, in the sense that they overlap to a larger extent with the experiments.

![Figure 15. Mean and 99% confidence intervals of the combustor wall pressure of the cold HyShot II combustor with aleatoric flight conditions and epistemic RANS turbulence model compared to the experimental uncertainty bars.](image)

The confidence bars are derived from the cumulative probability distribution functions (CDF). A example of such a CDF for the first pressure transducer is shown in Figure 16. Because of the combined effect of aleatoric and epistemic uncertainty, the probability distribution is given in terms of a confidence band. The CDF accounts for the probabilistic character of aleatoric uncertainty, whereas the interval represents epistemic uncertainty and aleatoric propagation error. The 99% confidence bar of Figure 15 is then given by the 99% percentiles of the CDF, denoted by the circles in Figure 16.

![Figure 16. Confidence interval of the cumulative probability distribution function (CDF) for the first wall pressure transducer of the cold HyShot II combustor with aleatoric flight conditions and epistemic RANS turbulence model.](image)

The balance of aleatoric and epistemic uncertainty is given in Table 2 for the x-locations of the pressure transducers. The mean is shown together with the confidence interval and the contributions of the aleatoric propagation error and the epistemic uncertainty to the interval. The confidence interval is largest for the 7th pressure transducer at \( x = 0.591 \) m with a mean of \( \mu = 37,200 \) Pa and an interval of \( \varepsilon_\mu = \pm 2990 \) Pa which is 8.026%. The contribution of the aleatoric propagation error is only 70.4 Pa compared to 2910 Pa for
the epistemic uncertainty. The conclusion of the first step of the framework of Figure 4 is that epistemic uncertainty is dominating the confidence bar. The minimum of $n_s = 11$ aleatoric samples is, therefore, already sufficient in this case. If it is necessary to further improve the predictive capability of the simulation beyond the 8.026% confidence, then this analysis points out that the epistemic uncertainty needs to be reduced. This reduction can be achieved by replacing the RANS computations by Large Eddy Simulations (LES) or by calibrating the RANS model using experimental data for the HyShot II case.

Table 2. Mean and confidence intervals of the combustor wall pressure of the cold HyShot II combustor with aleatoric flight conditions and epistemic RANS turbulence model.

<table>
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<tr>
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V.C. Numerical discretization error

Finally the combination of aleatoric uncertainty and numerical error is considered. The numerical error in the prediction of the pressure transducer measurements is estimated by solving an adjoint problem for each of the transducers and each of the $n_s = 11$ aleatoric samples. The 99% confidence intervals in Figure 17 contain the effect of the aleatoric uncertainty, the aleatoric propagation error, and the numerical error. The prediction is similar to Figure 13, in which only aleatoric uncertainty was considered, which indicates that the numerical error is relatively small.

In Table 3 the contributions of the aleatoric propagation error and the numerical error to the confidence interval are given. Both errors are approximately of the same order of magnitude over the whole range of x-locations. The largest confidence interval of 251Pa also at $x = 0.591m$, which is 0.734% of the mean 3420Pa, is an order of magnitude smaller than the effect of the epistemic uncertainty. In conclusion, also the spatial mesh is fine enough such that the aleatoric and numerical error are well-balanced and significantly smaller than the effect of the epistemic uncertainty.

VI. Conclusions

A framework for combining the effect of aleatoric uncertainty, epistemic uncertainty, and numerical error is presented and applied to scramjet engine models for hypersonic flight vehicles. The proposed tool reduces the impact of uncertainty and error by balancing all sources of uncertainty and error. The process is performed in the nested uncertainty quantification and error estimation loop. The result is a simulation in which all sources of uncertainty and error are taken into account and balanced in an efficient way.

The framework is successfully tested on a quasi one-dimensional nozzle flow problem with aleatoric and epistemic uncertainty in the boundary conditions, and spatial discretization error estimation. In that case, it achieves a reduction of the size of the confidence intervals by three orders of magnitude, which also leads to a significant shift of the center of the interval.

In the simulation of the HyShot II scramjet flight experiment, aleatoric uncertainty in the flight conditions, epistemic uncertainty in RANS turbulence model, and spatial discretization error estimation are considered. The combination of aleatoric and epistemic uncertainty leads to a maximum confidence interval of 8.026%.
Figure 17. Mean and 99% confidence intervals of the combustor wall pressure of the cold HyShot II combustor with aleatoric flight conditions and numerical error estimation compared to the experimental uncertainty bars.

Table 3. Mean and confidence intervals of the combustor wall pressure of the cold HyShot II combustor with aleatoric flight conditions and numerical error estimation.

<table>
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<tr>
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The epistemic uncertainty forms the dominant contribution to the confidence interval with 2910Pa compared to the mean pressure of $\mu = 37,200$Pa and 70.4Pa of the aleatoric uncertainty propagation error. The combined effect of aleatoric uncertainty and numerical error leads to a confidence interval of only 0.734%. Therefore, the initial number of aleatoric samples of $n_s = 11$ and the initial spatial mesh of $175 \cdot 10^3$ cells are sufficient compared to the epistemic uncertainty. In order to balance the epistemic uncertainty with the aleatoric uncertainty propagation error and the numerical error, the epistemic uncertainty can be reduced, for example, by replacing the RANS computations by Large Eddy Simulations (LES) or by calibrating the RANS model using experimental and LES data for simplified unit problems.

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