Progress in Scramjet Design Optimization Under Uncertainty Using Simulations of the HIFiRE Direct Connect Rig

Gianluca Geraci∗
Sandia National Laboratories, Albuquerque, New Mexico 87123, USA

Friedrich Menhorn†
Technical University of Munich, Garching, Germany

Xun Huan‡ and Cosmin Safta§
Sandia National Laboratories, Livermore, California 94550, USA

Youssef M. Marzouk¶
Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Habib N. Najm†
Sandia National Laboratories, Livermore, California 94550, USA

Michael S. Eldred∗∗
Sandia National Laboratories, Albuquerque, New Mexico 87123, USA

We present an overview of optimization under uncertainty efforts under the DARPA Enabling Quantification of Uncertainty in Physical Systems (EQUiPS) ScramjetUQ project. We introduce the mathematical frameworks and computational tools employed for performing this task. In particular, we provide details in the optimization and multilevel uncertainty quantification algorithms, which are available through the SNOWPAC and DAKOTA software packages. The overall workflow is first demonstrated on a simplified model design problem with non-reacting inviscid supersonic flows. Preliminary results and updates are then reported for an in-progress, highly computationally intensive scramjet design optimization case using large-eddy simulations of supersonic reactive flows inside the HIFiRE Direct Connect Rig.

I. Introduction

Supersonic combustion ramjet (scramjet) engines are propulsion systems for hypersonic flight that aim to directly utilize atmospheric air for stable combustion while maintaining supersonic airflow. When attained, this technology obviates the need to carry on-board oxidizer and sidesteps the losses from slowing flows to subsonic speeds. Therefore, scramjets can potentially reach much higher efficiencies in hypersonic conditions compared to traditional systems such as rockets or turbojets. However, the design for well-performing scramjet engines is still in its early stages [1,2]. One of several major challenges [3] is in characterizing and predicting combustion properties for multiscale and multiphysical turbulent flows under these extreme environments. Whereas designing an optimal engine typically involves maximizing combustion efficiency while minimizing pressure losses, thermal loading, and the risk of unstart and flame blow-out, achieving this while also producing designs that are robust and reliable against uncertainty and noise presents an extremely demanding undertaking. Advancing scramjet design thus requires a combination of accurate flow simulations together with mathematical structures that are capable of quantifying uncertainty, such as the framework of design optimization under uncertainty (OUU).

∗Limited Term Employee, Optimization and Uncertainty Estimation, MS1318. Member AIAA.
†PhD Candidate, Department of Informatics.
‡Currently Assistant Professor, Mechanical Engineering, University of Michigan, Ann Arbor, Michigan 48109. Portions of this research were conducted as Postdoctoral Appointee, Combustion Research Facility, Sandia National Laboratories. Member AIAA.
§Principal Member of Technical Staff, Quantitative Modeling and Analysis, MS9159. Senior Member AIAA.
¶Associate Professor, Department of Aeronautics and Astronautics.
†Distinguished Member of Technical Staff, Combustion Research Facility, MS9051. Member AIAA.
∗∗Distinguished Member of Technical Staff, Optimization and Uncertainty Estimation, MS1318. Associate Fellow AIAA.
Research for scramjet with uncertainty quantification (UQ) has been gaining traction in recent years\textsuperscript{[4–11]}. Notably, several of these papers have demonstrated the maturing computational methods, as well as standing difficulties, for performing UQ assessment to large-eddy simulations (LES). Indeed, a comprehensive integration of uncertainty in these models has been prohibitive due to the high cost of simulating turbulent reacting flows compounded with the multi-query, exploratory nature of UQ procedures, and is recognized as a grand challenge for high-fidelity scramjet simulations\textsuperscript{[2]}. OUU, which requires repeating the UQ analysis at different candidate design configurations and concurrently searching for good and optimal design regions, is considerably much more challenging. With such demanding tasks only now coming into the realm of possibility owing to advances in both computational power and numerical algorithms, we are not aware of any OUU attempts with LES for scramjet in the public domain. In this paper, we present a brief overview of our OUU efforts for a preliminary scramjet application focusing on the HIFiRE Direct Connect Rig (HDCR) combustor, with details in Section\textsuperscript{[II]}.

We carry out the optimization procedure by leveraging SNOWPAC (Stochastic Nonlinear Optimization With Path-Augmented Constraints)\textsuperscript{[12,13]} and DAKOTA\textsuperscript{[14]} software packages. SNOWPAC accommodates stochastic nonlinear constrained derivative-free optimization, and extends the path-augmented constraints framework introduced by its deterministic counterpart NOWPAC (Nonlinear Optimization With Path-Augmented Constraints) using a noise-adapted trust region approach with Gaussian processes for noise reduction. The method showed promising results in benchmark cases, outperforming prominent optimization algorithms like COBYLA\textsuperscript{[15]} and Nomad\textsuperscript{[16]}. Additionally, its derivative-free approach and robust optimization formulation are well-suited for our application where we treat the model as a black-box. Recently, SNOWPAC has been made available in the DAKOTA framework, which offers a highly flexible interface to couple the optimizer with different sampling strategies and surrogate models. In order to accelerate the convergence of statistics, we utilize the multilevel Monte Carlo (MLMC) estimator\textsuperscript{[17]} currently implemented in DAKOTA. As such, an integration between SNOWPAC and DAKOTA also required algorithmic development in order to extract error measures from MLMC to accelerate SNOWPAC. A brief description of SNOWPAC and demonstration of its coupling with DAKOTA will be presented in Section\textsuperscript{[III]}.

We showcase the overall method through two design problems. The first involves a test problem, where we optimize the shape of an entry obstacle in a two-dimensional inviscid supersonic duct in the presence of uncertain inlet conditions without reaction. This test problem furnishes a simplified environment with low simulation costs that imitates features also found in the HDCR LES application—such as the formation of a shock train in the duct—while providing a convenient platform for testing our algorithms. This problem also allows us to demonstrate the added efficiency attained by MLMC which relies on the availability of different mesh densities. We then present some preliminary results regarding our main demonstration involving the OUU formulation and results for the HDCR, where we design injector locations and angles, and fuel equivalence ratios in the presence of uncertain inlet, fuel, and turbulence model parameters.

This paper is structured as follows. Section\textsuperscript{[II]} introduces the physical application with the HDCR and the deterministic code used for carrying out LES. Section\textsuperscript{[III]} describes the main algorithmic components of our OUU framework. In particular, Section\textsuperscript{[III.A]} introduces the SNOWPAC algorithm, while Section\textsuperscript{[III.B]} presents the MLMC error estimator developed for informing SNOWPAC. OUU results are then reported in Section\textsuperscript{[IV]} for both the test problem involving two-dimensional supersonic inviscid duct (Section\textsuperscript{[IV.A]}) as well as the reactive flow inside the HDCR combustor (Section\textsuperscript{[IV.B]}). The paper ends with conclusions in Section\textsuperscript{[V]}.

II. Large-Eddy Simulations of the HIFiRE Direct Connect Rig

We focus on a cavity-based hydrocarbon-fueled dual-mode scramjet configuration studied under the HIFiRE (Hypersonic International Flight Research and Experimentation) program\textsuperscript{[18,19]}. The payload from its HIFiRE Flight 2 testing\textsuperscript{[20,22]} is depicted in Figure\textsuperscript{[I(a)]} and a ground test rig known as the HDCR was built to duplicate the isolator/combustor section. Since the HDCR offers publicly accessible data from its ground-based experiments\textsuperscript{[23,24]}, our investigations in this paper target numerical simulations of reactive flows inside the HDCR so that experimental datasets may be used for future modeling development and verification.

The computational domain for the HDCR is highlighted by red lines in Figure\textsuperscript{[I(b)]}. The rig consists of a constant-area isolator (planar duct) attached to a combustion chamber. Primary injectors are mounted upstream of flame stabilization cavities on both the top and bottom walls, and secondary injectors are similarly placed downstream of the cavities. Air enters the isolator from the left and travels to the right in the $x$ (streamwise) direction. The geometry is symmetric about the centerline in the $y$ (wall-normal) direction, and we take advantage of this symmetry by considering a domain that covers only the bottom half of the rig. The fuel supplied through the injectors is a gaseous mixture containing 36%
methane and 64% ethylene by volume, and possesses similar combustion properties as JP-7 \cite{25}. A reduced, three-step mechanism \cite{26, 27} is initially employed to characterize the combustion process. Arrhenius formulations of the kinetic reaction rates are adopted, and the parameters are fixed at values that retain robust and stable combustion in the current simulations. LES calculations are carried out using the RAPTOR code framework developed by Oefelein \cite{28, 29}. The code solves the fully coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow, and can handle high Reynolds number, real-gas conditions over a wide range of Mach numbers. The implementation employs non-dissipative, discretely conservative, and staggered finite-volume schemes, that are capable of preventing numerical contamination from subfilter models.

In our numerical studies, we designate five input scalars as design parameters that we can directly control during the optimization process. These design parameters are the global equivalence ratio (\(\phi_G\)), ratio of primary to secondary injector equivalence ratios (\(\phi_R\)), location of the primary injector (\(x_1\)), location of the secondary injector (\(x_2\)), and angle of the primary injector (\(a_1\)). Specifically, if \(\phi_1\) and \(\phi_2\) denote equivalence ratios of mixtures inserted at the primary and secondary injectors, respectively, then \(\phi_G = \phi_1 + \phi_2\) and \(\phi_R = \phi_1 / \phi_2\). The feasible ranges for design parameters can be found in Table 4. We further allow a total of 11 model parameters to be uncertain, reflecting uncertainty in inlet and fuel inflow boundary conditions as well as turbulence model parameters for the LES sub-grid scale model. Uncertain parameters are endowed with uninformative uniform distributions, summarized in Table 5.

The data utilized in the current analysis are two-dimensional simulations of flows inside the HDCR, using grid resolutions where cell sizes are 1/8, 1/16, and 1/32 of the injector diameter \(d = 3.175\) mm (respectively denoted by “\(d/8\)”, “\(d/16\)”, and “\(d/32\)” cases in this paper), corresponding to respectively around 63 thousand, 250 thousand, and 1 million grid points. The number of time steps for each run at different grid resolutions are selected to maintain approximately equal simulated physical times. While the timestep sizes are determined adaptively based on the Courant-Friedrichs-Lewy (CFL) criterion, their values are approximately proportional to the grid spacing. The simulations are warm-started on solutions engineered from a quasi-steady state nominal condition run, and take around \(1.7 \times 10^3\), \(1.1 \times 10^4\), and \(7.3 \times 10^4\) CPU hours per run in practice for \(d/8\), \(d/16\), and \(d/32\), respectively (their theoretical relative computational costs differ by a factor of 8 between resolutions, and are shown in Table 11). Figure 2 provides example solution fields for Mach number \(M\), and carbon monoxide mass fraction \(Y_{CO}\), simulated at a randomly sampled input setting using the three different grids. Qualitative differences can be observed, cautioning that even finer grid...
resolutions may be required to reach the grid converging regime. However, simulations using finer grids are impractical given our current computational budget, and will be a target for future work. These observations also imply that correlations across these resolution levels may be lower than desired, which could decrease the benefits from the MLMC framework. Several QoIs enter the OUU formulation in this paper and are detailed below. All QoIs are time-averaged variables, where the instantaneous solutions corresponding to the second half for each run are time-averaged to generate one solution per run.

- **Combustion efficiency** ($\eta_{comb}$), a critical performance indicator for engines, is defined based on static enthalpy quantities [24][30]:

$$\eta_{comb} = \frac{H(T_{ref}, Y_e) - H(T_{ref}, Y_{ref})}{H(T_{ref}, Y_{e,ideal}) - H(T_{ref}, Y_{ref})}$$

Here $H$ is the total static enthalpy, the “ref” subscript indicates a reference condition derived from the inputs, the “e” subscript is for the exit, and the “ideal” subscript is for the ideal condition where all fuel is burnt to completion. The reference condition corresponds to that of a hypothetical non-reacting mixture of all inlet air and fuel at thermal equilibrium. The numerator, $H(T_{ref}, Y_e) - H(T_{ref}, Y_{ref})$, thus reflects the global heat released during the combustion, while the denominator represents the total heat release available in the fuel-air mixture.

- **Burned equivalence ratio** ($\phi_{burn}$) is defined to be equal to $\phi_{burn} = \phi_G \eta_{comb}$. It represents the air excess, and high values of $\phi_{burn}$ results from a combination of high thermal efficiencies and stoichiometric to rich equivalence ratios, and are associated with conditions away from blowout regimes.

- **Stagnation pressure loss ratio** ($P_{stagloss}$) is defined as

$$P_{stagloss} = 1 - \frac{P_{s,e}}{P_{s,i}}$$

where $P_{s,e}$ and $P_{s,i}$ are the wall-normal-averaged stagnation pressure quantities at the exit and inlet planes, respectively. Higher values of $P_{stagloss}$ illustrate pressure loss across the combustor and are associated with a decrease in efficiency.

- **Maximum and average root-mean-square (RMS) pressures** ($\text{max } P_{rms}$ and $\text{ave } P_{rms}$) are, respectively, the maximum RMS pressure across the entire spatial domain, and the RMS pressure averaged across the spatial domain between two injectors:

$$\text{max } P_{rms} = \max_{x,y} \sqrt{P(x,y)^2 - [\bar{P}(x,y)]^2}$$

$$\text{ave } P_{rms} = \frac{1}{V} \int_{x,y} \sqrt{P(x,y)^2 - [\bar{P}(x,y)]^2} \ dx \ dy$$

with $V$ indicating the spatial volume of consideration, and $\bar{P}$ denoting time-averaged quantity. We approximate the maximum and integration using the grid at hand. These QoIs reflect the maximum and average pressure oscillation amplitude, which are useful for engine structural considerations.

- **Initial shock location** ($x_{shock}$) is the most upstream shock location, which we currently compute by detecting a rapid pressure change. More upstream locations of the initial shock train are linked with higher chances of unstart and vibration, and degraded safety of the scramjet engine.

Additional information regarding the computational setup, as well as discussions on limitations of the currently available simulations results, can be found in a companion paper submission [31].

### III. Optimization Under Uncertainty

In this section we describe the components of our OUU approach, which encompasses SNOWPAC for the derivative-free optimization solver and DAKOTA for the overall workflow management and multilevel UQ. Recently the two softwares have been fully integrated and are distributed together starting from the version 6.7 of DAKOTA.
Fig. 2 Solution fields of Mach number $M$ (top three) and carbon monoxide mass fraction $Y_{CO}$ (bottom three) simulated at a randomly sampled input settings using the three different grids.

A. Derivative free optimization in (S)NOWPAC

NOWPAC is a derivative-free optimization methods based on a trust region approach using fully linear models for the objective function and the constraint. It was developed for continuous optimization problems of the form

$$\min_{x} f(x),$$
$$\text{s.t. } c_i(x) \leq 0, i = 1, ..., r,$$

with design parameter $x \in \mathbb{R}^d$, objective function $f : \mathbb{R}^d \to \mathbb{R}$ and inequality constraints $c_i : \mathbb{R}^d \to \mathbb{R}$. Likewise to common trust region approaches (see [32] for an introduction), NOWPAC builds local surrogate models $m_k^b$ around...
the current design \( x_k \) within a neighborhood, the trust region, of size \( \rho_k \). Here, \( k = 0 \) represents the initial design. A distinguishing feature that we proposed in [12] is a new way of handling the constraints based on an inner boundary path to ensure feasible trial points. This ensures global convergence to a first-order local optimal design.

With the addition of uncertain parameters \( \theta \in \Theta \) NOWPAC has been successfully extended for stochastic optimization, namely SNOWPAC [13], to find a robust solution to the resulting OUU problem

\[
\begin{align*}
\min_{x} \mathcal{R}^f(x, \theta), \\
\text{s.t.} \quad \mathcal{R}^c_i(x, \theta) \leq 0, i = 1, \ldots, r.
\end{align*}
\]

Here, \( \mathcal{R}^b : \mathbb{R}^d \times \Theta \rightarrow \mathbb{R} \) is a measure for robustness or risk. Common examples for \( \mathcal{R}^b(x, \theta) \) are

- expected value: \( \mathbb{E}[b(x, \theta)] \),
- linear combination of expected value and standard deviation: \( \mathbb{E}[b(x, \theta)] + \alpha \sqrt{\mathbb{V}[b(x, \theta)]]} \),
- probabilistic constraints: \( \mathbb{P}[b(x, \theta) \geq 0] - (1 - \beta) \).

To evaluate those measures, SNOWPAC employs a sampling approach which, however, introduces an error (or noise) \( \epsilon \) depending, e.g., on the number of samples \( N \) used: \( \mathcal{R}^b(x, \theta) = \mathcal{R}^b(x, \theta) + \epsilon \). Therefore, SNOWPAC introduces regularized trust region subproblems to improve the efficiency of the optimization process in the presence of noise.

Additionally, in order to ensure a good quality of the surrogate based on noisy evaluations, we have to enforce an upper bound on the error term \( \epsilon_{\text{max}}^k \rho_k^{-2} \) where \( \epsilon_{\text{max}}^k \) is the maximum noise estimate at step \( k \). We do this by imposing a lower bound

\[
\epsilon_{\text{max}}^k \rho_k^{-2} \leq \lambda_i^{-2}, \quad \text{resp.} \quad \rho_k \geq \lambda_i \sqrt{\epsilon_{\text{max}}^k} = \max \lambda_i \sqrt{\epsilon_{\text{max}}^k},
\]

on the trust region radii for a \( \lambda_i \in [0, \infty[ \). This, however, restricts our trust region from shrinking and delays (or even stops) the convergence of the algorithm. If the trust region size is in range of the noise the achievable accuracy is, therefore, limited.

Thus, to mitigate the noise SNOWPAC biases the sampling estimates \( R^b \) using additional Gaussian process (GP) surrogates [34]. They are probabilistic regression models that not only approximate the function but also give an estimate of the approximation accuracy by means of a standard deviation. More specifically, given a kernel function \( k(x, y) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \), we build a GP posterior function

\[
\begin{align*}
\mu_{\text{GP}}^b(x) &= k(x, X)(K(X, X) + \sigma^2 I)^{-1} R^b(X) \\
\sigma_{\text{GP}}^b(x) &= \sqrt{k(x, x) - k(x, X)(K(X, X) + \sigma^2 I)^{-1} k(x, X)^T}
\end{align*}
\]

where \( \mu_{\text{GP}}^b \) is the GP mean estimate for \( R^b \) and \( \sigma_{\text{GP}}^b \) is its estimated standard deviation. Here, we use a subset \( X = \{x_1, \ldots, x_k\} \) of evaluated design points in a region around the current best design point \( x^* \) such that \( \|x^* - x_i\|_2 \leq 2 \rho_k \). Thus, \( K(X, X) \) is a short notation for the kernel matrix where each entry of the matrix is computed as \( K_{ij} = k(x_i, x_j) \), \( x_i, x_j \in X \), likewise for the row vector \( k(x, X) \). Using the GP surrogate we smoothen the sampling estimates and sampling noises of our current evaluations \( x \in X \)

\[
\begin{align*}
\tilde{R}^b(x) &= \alpha^b \cdot \mu_{\text{GP}}^b(x) + (1 - \alpha^b) \cdot R^b(x) \\
\tilde{\epsilon}^b(x) &= \alpha^b \cdot \sigma_{\text{GP}}^b(x) + (1 - \alpha^b) \cdot \epsilon^b(x).
\end{align*}
\]

Note that with an increasing number of evaluations the GP surrogate will improve and \( \sigma_{\text{GP}}^b(x) \) will therefore decrease. Thus, the weight \( \alpha^b = \epsilon^b \sigma_{\text{GP}}^b(x) \) is chosen such that the influence of the GP surrogate increases and the noise estimate \( \tilde{\epsilon}^b(x) \) decreases. Based on eq. [7] we can reduce the trust region further and finally proceed in the optimization. To conclude, SNOWPAC balances two sources of approximation error: on the one hand, there is the structural error in the approximation of the local surrogate models which is controlled by the size of the trust region radius; on the other hand, we have the inaccuracy in the Gaussian process surrogate itself which is reflected by its standard deviation. This results in an optimization method which can even progress despite a small sample size.

**B. MLMC error estimators for OUU in DAKOTA**

In this section we briefly present the MLMC sampling approach that we employed for the forward UQ step. As described in the previous section, SNOWPAC is designed to work with any sampling method provided its capability to
evaluate the standard errors for the statistics. In recent years, multifidelity sampling strategies has been introduced to alleviate the limitations of the plain onte Carlo (MC) estimators (see for instance [35] for a unified treatment of several multifidelity approaches), i.e., its slow convergence with the number of realizations. In our application we rely on the spatial and temporal resolution to build low-fidelity approximations, therefore it is legitimate to use a MLMC estimator [17]. The main task to be accomplished by the MLMC here is to efficiently evaluate the statistics of each QoI, namely the expected value \( \mathbb{E}[\cdot] \) and variance \( \text{Var}[\cdot] \). More precisely, for a given QoI \( Q \), we desire to adopt a robustness measure given by the linear combination of its expected value and standard deviation, i.e. \( \mathbb{E}[Q] + \alpha \sqrt{\text{Var}[Q]} \) (see Sec. III.A). Moreover, the noise introduced by the sampling method is quantified by an approximation based on the combination of the standard error for the (multilevel) sample mean and standard deviation. The MLMC method in its classical form [17] has been introduced to evaluate the expected value, and it is also common to evaluate its performance by estimating the standard deviation of the estimator distribution. Let \( \ell = 0, \ldots, L \) denote a sequence of resolution levels with \( L \) being the finest resolution level. The MLMC estimator for the expected value of \( Q_L \) (the QoI evaluated at the finest resolution level) and its variance are defined as

\[
\mathbb{E}[Q_L] \approx \hat{Q}_L^{ML} = \sum_{\ell=0}^{L} \frac{1}{N_{\ell}} \sum_{i=1}^{N_{\ell}} (Q_{\ell}^{(i)} - Q_{\ell-1}^{(i)}) = \sum_{\ell=0}^{L} \hat{Y}_{\ell}
\]

where \( \hat{Y}_{\ell} \) is the difference function between two consecutive levels (we assume \( Y_0 = Q_0 \)) and \( \hat{Y}_{\ell} \) is its estimator at the \( \ell \)th level. The MLMC is effective whenever it is reasonable to assume \( \text{Var}[Y_L] \to 0 \) for \( l \to \infty \), and therefore the number of samples \( N_{\ell} \) decreases for an increasing \( \ell \). Once the cost of each sample and the variance of \( Y \) is estimated at each level \( \ell \), the number of samples \( N_{\ell} \) to be evaluated can be obtained in closed form [17] in order to obtain an estimator with a prescribed variance \( \text{Var}[\hat{Q}_{L}^{ML}] \). Alternatively, if the number of evaluations is constrained at the finest resolution level, the optimal samples profile can be obtained (see for instance [27]).

The distribution of the MLMC estimator approaches the normal distribution for a large number of samples, therefore its standard error can be obtained directly as the square root of \( \text{Var}[\hat{Q}_L] \)

\[
\text{SE} [\hat{Q}_L] = \sqrt{\text{Var}[\hat{Q}_L]}.
\]

The derivation of the multilevel estimator for the standard deviation requires the derivation of the multilevel estimator for the variance. Moreover, the standard error for the standard deviation cannot be derived in closed form and it needs to be approximated.

1. Standard error of the sample variance

The multilevel expansion for the variance of \( Q_L \) can be written as

\[
\text{Var}(Q_L) = \sum_{\ell=0}^{L} \mathbb{E} \left[ (Q_\ell - \mathbb{E}[Q_\ell])^2 - (Q_{\ell-1} - \mathbb{E}[Q_{\ell-1}])^2 \right] = \sum_{\ell=0}^{L} \mathbb{E}[P_{\ell}^2] - \mathbb{E}[P_{\ell-1}^2]
\]

where we define a new quantity \( P_{\ell}^2 = (Q_\ell - \mathbb{E}[Q_\ell])^2 \) and, as usual, we assume \( P_{-1}^2 = 0 \). In order to derive the estimator, it is necessary to write an unbiased estimator for each expected value term \( \mathbb{E}[P_{\ell}^2] \), which corresponds to the variance of \( Q_\ell \). Therefore, the unbiased estimator is obtained by employing the Bessel correction

\[
\mathbb{E}[P_{\ell}^2] \approx \hat{P}_{\ell}^2 = \frac{1}{N_{\ell} - 1} \sum_{i=1}^{N_{\ell}} (Q_{\ell}^{(i)} - \hat{Q}_\ell)^2
\]

and the variance for \( Q_L \) is

\[
\text{Var}(Q_L) \approx \hat{s}_{ML}^2 = \sum_{\ell=0}^{L} (\hat{P}_{\ell}^2 - \hat{P}_{\ell-1}^2)
\]

The overall variance estimator \( \hat{s}_{ML}^2 \) is also unbiased since it is derived as a sum of unbiased estimators. Similarly to the MLMC estimator for the expected value, if the estimators are independent level by level, the variance of \( \hat{s}_{ML}^2 \) is equal to
the sum of the variance of the estimators at each level

$$\text{Var}[s_{\text{ML}}^2] = \sum_{\ell=0}^{L} \text{Var}[\hat{P}_\ell^2] + \text{Var}[\hat{P}_{\ell-1}^2] - 2 \text{Cov}(\hat{P}_\ell^2, \hat{P}_{\ell-1}^2).$$  \hspace{1cm} (15)

Two additional terms appear in the previous expression and they need to be evaluated. The variance of the estimator \(\text{Var}[\hat{P}_\ell^2]\) at each level \(\ell\) and the covariance term between \(\hat{P}_\ell^2\) and \(\hat{P}_{\ell-1}^2\). The first term is computed by resorting to the fourth central moment for \(Q_{\ell}\), defined as \(\mu_{4,\ell} = \mathbb{E} \left[ (Q_{\ell} - \mathbb{E} [Q_{\ell}])^4 \right] \)

$$\text{Var}[\hat{P}_\ell^2] = \frac{1}{N_\ell} \left( \mu_{4,\ell} - \text{Var}^2[Q_{\ell}] \right) + \frac{2}{N_\ell(N_\ell - 1)} \text{Var}^2[Q_{\ell}].$$  \hspace{1cm} (16)

A multilevel expansion for this moment leads to an expression similar to the variance Eq. (14), where the sample estimator for the fourth moment \(\hat{P}_\ell^4\) should be derived

$$s_{\text{ML}}^4 = \sum_{\ell=0}^{L} \hat{P}_\ell^4 - \hat{P}_{\ell-1}^4.$$  \hspace{1cm} (17)

However, in this case the estimator \(s_{\text{ML}}^4\) is not unbiased, because it is derived from biased estimators for \(\hat{P}_\ell^4\) if a straightforward sample average is adopted

$$\hat{P}_\ell^4 = \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} Q_{\ell}^{(i)} \left( \sum_{j=1}^{N_\ell} Q_{\ell}^{(j)} \right)^4.$$  \hspace{1cm} (18)

In this case we can still obtain a correction for \(\hat{P}_\ell^4\), however it is much more involved than the Bessel factor introduced for the variance and we only report here the final result

$$\hat{P}_\ell^{4,\text{unbiased}} = \frac{1}{N_\ell^2 - 3 N_\ell + 3} \left[ \frac{N_\ell}{N_\ell - 1} \hat{P}_\ell^4 - (6 N_\ell - 9) \left( \frac{s_{\text{ML}}^4}{N_\ell} \right) \right].$$  \hspace{1cm} (19)

We note here that in the previous equation we approximated the square of the variance with the square of the unbiased estimator \(s_{\text{ML}}^4\), which itself cannot be guaranteed to be unbiased.

Finally, the unbiased multilevel estimator for the fourth moment is

$$s_{\text{ML}}^{4,\text{unbiased}} = \sum_{\ell=0}^{L} \hat{P}_\ell^{4,\text{unbiased}} - \hat{P}_{\ell-1}^4.$$  \hspace{1cm} (20)

The covariance term that appears in Eq. (15) has a more complex expression, however an unbiased estimator for it can be easily obtained by only resorting to unbiased estimators for both mean and variance

$$\text{Cov}(\hat{P}_\ell^2, \hat{P}_{\ell-1}^2) = \frac{1}{N_\ell} \left( \mathbb{E} \left[ P_\ell^2 P_{\ell-1}^2 \right] - \text{Var}[Q_{\ell}] \text{Var}[Q_{\ell-1}] \right)$$

$$+ \frac{1}{N_\ell(N_\ell - 1)} \left( \mathbb{E} [Q_{\ell} Q_{\ell-1}] - \mathbb{E} [Q_{\ell}] \mathbb{E} [Q_{\ell-1}] \right)^2,$$  \hspace{1cm} (21)

where

$$\mathbb{E} [P_\ell^2 P_{\ell-1}^2] = \mathbb{E} [Q_{\ell}^2 Q_{\ell-1}^2] - 2 \mathbb{E} [Q_{\ell-1}] \mathbb{E} [Q_{\ell}^2 Q_{\ell}]$$

$$+ \mathbb{E} [Q_{\ell-1}] \mathbb{E} [Q_{\ell}^2] - 2 \mathbb{E} [Q_{\ell}] \mathbb{E} [Q_{\ell} Q_{\ell-1}]$$

$$+ 4 \mathbb{E} [Q_{\ell}] \mathbb{E} [Q_{\ell-1}] \mathbb{E} [Q_{\ell} Q_{\ell-1}] + \mathbb{E}^2 [Q_{\ell}] \mathbb{E} [Q_{\ell}^2 Q_{\ell-1}] + 3 \mathbb{E}^2 [Q_{\ell}] \mathbb{E}^2 [Q_{\ell-1}].$$  \hspace{1cm} (22)
2. Standard Error for the sample standard deviation

Unfortunately the SE for the multilevel standard deviation cannot be derived in closed form. This limitation is not peculiar to the ML approximation but it also affects the single level approximation of the sample standard deviation \( \hat{s} \). Let consider a single level case where for simplicity we omit the level index. The sample standard deviation can be obtained by the unbiased estimator for the variance \( \hat{s}^2 \) as

\[
\hat{s} = \sqrt{\hat{s}^2} = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (Q^{(i)} - \hat{\theta})^2}.
\] (23)

It is usually possible to resort to two approximations to estimate the standard error. The first is to assume that the distribution of the population is normal. In this case we can write an expression for the standard error \( SE[\hat{s}] \) as

\[
SE[\hat{s}] = \frac{\hat{s}}{\sqrt{2(N-1)}}
\] (24)

following [36]. However, in many practical situations, the distribution of the population is not normal and, therefore the previous expression is only an approximation in this respect.

The second approximation consists in applying the so-called Delta Method [37] which enables us to approximate the probability distribution of a function of an asymptotically normal distributed estimator. In our case, we want to compute the square root of the sample variance for which we know its standard error \( SE[\hat{s}^2] \). The standard error for the variance can be found in [37] without any assumption on the sample size and the population’s distribution

\[
SE[\hat{s}^2] = \sqrt{\frac{1}{N} \left( \mu_4 - \frac{N-3}{N-1} (\text{Var}[Q])^2 \right)}.
\] (25)

By means of the Delta Method we can approximate

\[
SE[f(\hat{\theta})] \approx |f'(\hat{\theta})|SE[\hat{\theta}],
\] (26)

where in our case \( \hat{\theta} = \hat{s}^2 \) and \( f(\hat{\theta}) = \hat{\theta}^{-1/2} \). The final expression for the consistent approximation for the standard error is obtained by resorting to the sample standard error and variance estimators

\[
SE\left[\sqrt{\hat{s}^2}\right] = \frac{1}{2\sqrt{N}} \sqrt{\frac{1}{N} \left( \mu_4 - \frac{N-3}{N-1} (\hat{s}^2)^2 \right)}.
\] (27)

In the previous expression an estimator for the fourth central moment should be used. We can adopt an expression for it similar to Eq. (19).

In order to develop an intuition for the different approximations we perform few numerical tests. We select two analytical functions, one linear and one non-linear, and we compare the results of the different standard error approximations against the values computed with a large number of repetitions. We consider the following functions

\[
f(X) = X
\]

\[
f(X_1, X_2, X_3) = \sin(X_1) + 7 \sin^2(X_2) + \frac{1}{10} X_3^4 \sin(X_1)
\] (28)

with both normal and uniform distributed input, namely \( X \sim \mathcal{U}(-\pi, \pi) \) and \( X \sim \mathcal{N}(0, \frac{\pi}{2}) \).

In Fig. [3] we report the results for the standard error for both uniform and normal input for the linear function. We report the results for both the variance and the standard deviation. In the case of the variance, we compare the standard errors evaluated with and without the unbiased estimator for the fourth central moment. We note only a marginal beneficial effect of including the unbiased estimator for the fourth central moment, however, as expected, the effect of the correction is more significant for a small number of samples, while the two approximations are indistinguishable for a larger number of samples. For the standard error of the standard deviation we note that the approximation for normal populations is exact when the input is normal (as expected given the linearity of the function). However, this approximation performs worse than the Delta Method for uniform input.
Fig. 3  Comparison between several approximations for the Standard Error for the Variance (left column) and the Standard Deviation (right column) for the linear function. Both cases of normal (top row) and uniform (bottom row) input are considered.

Similar qualitative results are obtained for the Ishigami function for both normal and uniform input, see Fig. 4. Even in this case the unbiased estimator for the fourth central moment leads only to marginally improved results for small numbers of samples. However, for the standard deviation the normal population’s distribution approximation exhibits a bias with respect to the reference solution for all the sample sizes. On the contrary, the Delta method approximation leads to a result that converges to the reference solution for sample sizes larger of approximately 100 samples.

From the numerical test cases reported in both Fig. 3 and Fig. 4 we conclude that the most robust estimation for the standard error is given by the Delta Method with unbiased estimation for the fourth central moment. This approximation is used in all the numerical results presented in the following.

IV. Numerical Results

In this section, we describe the OUU problem setup and results for a model test case and two scramjet design problems based on simulations of the HDCR.

A. Model problem

As a first step to verify the optimization pipeline we developed a model problem intended to replicate certain aspects of the scramjet application. It should, however, also be less time consuming with respect to computational effort to give a reasonable time frame for active development and testing. Using the publicly available software Stanford University Unstructured Code (SU2) as CFD solver and gmsh for automatic meshing, we, therefore, defined a 2D inviscid fluid flow problem for a duct geometry inspired by the HDCR setup. We added a wedge right at the beginning of the cavity to create a shockwave in the flow to imitate the behavior of the fuel injection in the scramjet. Using the automatic
meshing capabilities we can easily introduce different meshing resolutions for the MLMC approach introduced in III.B. Though these results were presented in [40] we would like to reiterate them here to show the validity of the approach before moving to the more realistic HDRC application.

**Fig. 5** SU2 channel flow scenario

The full geometry and a flow solution are reported in Fig. 5. We introduce three uncertain parameters \( \{ \xi_i \}_{i=1}^3 \) as inlet conditions for the flow, where \( \xi_1 = p_{0, in} \) is the stagnation pressure, \( \xi_2 = T_{0, in} \) is the temperature and \( \xi_3 = M_{0, in} \) is the Mach number. As design parameters we picked parameters of the wedge. Namely, the position of the rightmost wedge point \( x_b \), the length of its lower side \( l_b \), its height \( h_b \), length of top side \( l_t \) and distance \( ltp \) of the top rightmost point to the wedge rightmost point \( x_b \). Additionally, the different mesh discretizations are visualized around the wedge in Fig. 6 where COARSE, MEDIUM and FINE resolutions are shown for reference. The computational times for the different resolutions are approximately 10s, 30s and 300s, respectively.

Finally, the upper and lower bounds of the different parameters are summarized in Table 1.
With the capabilities of (S)NOWPAC in DAKOTA we can easily compare between different optimization and sampling methods on this application. We decided on comparing the deterministic optimization scenario where we set the uncertain parameters to their nominal values with the optimization problem under uncertainty. We define the OUU problem as

$$P^*_{loss}(x^*) = \min_{x} \mathbb{E}[P_{loss}(x, \xi)]$$

s.t. $0.51 \leq \mathbb{E}[T_c(x, \theta)] - 3\sigma[T_c(x, \xi)]$,

where the objective function $P_{loss}$ and the constraint $T_c$ are defined as follows:

$$P_{loss} = \left( \frac{p_{0,in} - \frac{1}{L_y} \int_{out} p_{0}(y)dy}{p_{0,in}} \right)$$

$$T_c = \frac{1}{L_x} \int_{L_c} T(x)dx,$$

where $L_c$ describes the length of the cavity domain, used for computing the average cavity temperature.

Additionally, for the OUU problem we discuss the results using a standard Monte Carlo estimator on the FINE grid compared to using the newly developed MLMC estimator leveraging the COARSE, MED and FINE grid. The different samples used are given in Table 2. Here, the number of MLMC samples are chosen such that they match the accuracy of the (MC) approach.

| Method  | COARSE | MED | FINE |
|---------|--------|-----|------|
| (DET)   | 0      | 0   | 1    |
| (MC)    | 0      | 0   | 54   |
| (MLMC)  | 179+20 | 20+5| 5    |

Table 2  Number of samples on each resolution used for each approach. (DET) describes using the deterministic optimizer NOWPAC at nominal value of stochastic parameters. (MC) uses SNOWPAC using Monte Carlo sampling estimators. (MLMC) employs SNOWPAC with an MLMC estimator on three different resolutions.

We compare the different results obtained from the three methods of choice quantitatively in Table 3. Overall, we receive slightly different designs for the three strategies, and MC shows the best objective value. Moreover, the lower
constraint is active for the MLMC approach. Regarding the cost, we can see the advantage of using MLMC compared to MC: we reduce the number of FINE grid evaluations from 9396 for MC to 870 for MLMC for the same number of evaluation steps while still being similar in the objective. This results can be seen in Table 3 and also already suggested in benchmark results in [12]. NOWPAC converges and finds a local optimum quickly after 73 steps since there is no noise restriction on the trust region. The constraint is not getting active in this case. An additional result that we observed is that due to high noise in the estimators we only see a slow convergence in the stochastic methods MC and MLMC. Because of that, the trust regions size shrinks slowly and we selected a maximum number of optimization steps as stopping criteria.

The final designs for the duct plus the flow fields of the pressure are shown in Fig. 7. Although we reach different designs for each we see the attenuating effect on the initial shockwave induced by the decreased slope or height of the wedge. Relating these qualitative with the quantitative results from Table 3, we deduce further that the objective functions inhibit multiple local minima found by the different optimization approaches.

| Problem | \( x^\star \) | \( P^\star_{\text{loss}} \) | \( c^\star \) | Cost: (C, M, F) |
|---------|----------------|-----------------|-------------|----------------|
| (DET)   | [1.46, 11.25, 2.51, 17.62, 79.50] | 0.4902          | 0.6732      | (0, 0, 73)    |
| (MC)    | [2.06, 8.63, 3.84, 20.5, 79.5]   | 0.4807          | 0.5355      | (0, 0, 9396)  |
| (MLMC)  | [2.37, 10.63, 3.52, 20.5, 79.75] | 0.4840          | 0.5138      | (34626, 4350, 870) |

Table 3 The table shows the design \( x^\star \), objective \( P^\star_{\text{loss}} \), constraint \( c^\star \) and cost for the different methods on different resolutions COARSE (C), MEDIUM (M) and FINE (F). The red color shows active constraints.

To summarize, this test benchmark and its results give us the following two main contributions: first, we are able to test, verify and validate our method on a benchmark example which is computationally inexpensive and simple to modify, e.g., with respect to different resolutions. This stands in contrast with the scramjet application which, as we will discuss in the next section, takes multiple days to compute. By using the test benchmark we could, thus, set up the coupling of SNOWPAC with DAKOTA as preparation for the scramjet runs. Second, the numerical results also give insight on the different approaches used. By comparing the number of blackbox evaluations on the different resolutions we can clearly see the computational advantage of using a multilevel sampling approach which still resulted in a similar final objective value. Therefore, these results encouraged us to also apply a multiscale approach in the following for the scramjet which we will talk about next.

B. HIFiRE Direct Connect Rig simulations

In this section we document our progress in the design of a scramjet engine by using DAKOTA, SNOWPAC and RAPTOR. We consider two cases: an initial bi-level setup that uses only two resolution levels and the final OUU setup that uses all the resolution levels, namely \( d/8 \), \( d/16 \) and \( d/32 \).

For both OUU problems we identified the following optimization formulation: we want to maximize the performance of the engine in term of combustion efficiency \( \eta_{\text{comb}} \) subject to a robust measure for constraints on the burned equivalence ratio \( \phi_{\text{burn}} \), the maximum or the spatial average (for the bi-level and full setup, respectively) RMS pressure, \( \max P_{\text{rms}} \) or \( \text{ave} P_{\text{rms}} \), which are indicators for the loading on the structure, the stagnation pressure loss \( P_{\text{stagloss}} \) which is a surrogate
for the thrust generated, and the shock train initial location $x_{\text{shock}}$. These constraints are defined by evaluating the (statistical) performance of the nominal configuration. Description for all QoIs can be found in Section II.

We consider five design parameters reported in Table 4 with their allowable ranges. Eleven input parameters are allowed to bear uncertainty, and are listed in Table 5.

| Design Parameters | Range       | Description                                      |
|-------------------|-------------|--------------------------------------------------|
| $\phi_G$          | [0.5, 1.0]  | Global equivalence ratio (total of primary and secondary) |
| $\phi_R$          | [0.25, 0.35]| Ratio of primary to secondary injector equivalence ratios |
| $x_1$             | [0.231, 0.2564] m | Primary injector $x$-location                |
| $x_2$             | [0.40755, 0.43295] m | Secondary injector $x$-location             |
| $a_1$             | [5, 25]$^\circ$ | Primary injector angle                         |

Table 4 Design parameter for the RAPTOR LES optimization scramjet problem.

| Parameter | Range | Description |
|-----------|-------|-------------|
| $p_0$     | [1.406, 1.554] $\times 10^6$ Pa | Stagnation pressure |
| $T_0$     | [1472.5, 1627.5] K | Stagnation temperature |
| $M_0$     | [2.259, 2.761] | Mach number |
| $I_i$     | [0, 0.05] | Turbulence intensity horizontal component |
| $R_i$     | [0.8, 1.2] | Ratio of turbulence intensity vertical to horizontal components |
| $L_i$     | [0.8] $\times 10^{-3}$ m | Turbulence length scale |

| Fuel inflow boundary conditions: | Range | Description |
|---------------------------------|-------|-------------|
| $I_f$                           | [0, 0.05] | Turbulence intensity magnitude |
| $L_f$                           | [0, 1] $\times 10^{-3}$ m | Turbulence length scale |

| Turbulence model parameters: | Range | Description |
|------------------------------|-------|-------------|
| $C_R$                        | [0.01, 0.06] | Modified Smagorinsky constant |
| $Pr_t$                       | [0.5, 1.7] | Turbulent Prandtl number |
| $Sc_t$                       | [0.5, 1.7] | Turbulent Schmidt number |

Table 5 Uncertain model input parameters. The uncertain distributions are assumed uniform across the ranges shown.

1. Initial bi-level results

In this section we report the initial results obtained for a bi-level setup; we only used two resolution levels, namely $d/8$ and $d/16$. For this setup we deployed the following workflow:

- Deterministic surrogate-based optimization in order to compute the initial design point (only $d/8$ realizations);
- OUU optimization by using a fixed samples profile: for a total of 20 $d/8$ and 5 $d/16$ simulations.

The deterministic optimization is performed by constructing a Gaussian process surrogate with the 32 corners and 21 random points for a total of 53 evaluations for the $d/8$ resolution. Moreover for the nominal point, the expected values for all the constraints are evaluated to provide a reference for the optimization. Our goal is to improve the objective function while not degrading the constraints. The allowable values for the nominal design point ($d/8$) are reported in Table 6.
Allowable constraint values for the $d/8$ problem, i.e., mean values for the constraints with respect to the design point.

| QoI      | Allowable                        |
|----------|----------------------------------|
| $\phi_{\text{burn}}$ | $\geq 0.1843$ (nominal $d/8$) |
| $\max P_{\text{rms}}$ | $\leq 0.1677$ (nominal $d/8$) |
| $x_{\text{shock}}$ | $\geq 32d$                     |
| $P_{\text{stagloss}}$ | $\leq 0.3768$ (nominal $d/8$) |

Table 6

After the optimization on the Gaussian process surrogate the initial point is obtained and the values for the design variables are reported in Table 7. We note that for the secondary injector position the initial value is equal to the lowest range value. For this initial design, we also report the correspondent objective function and constraints values in Table 8. For the constraint values we note that all of them are active except the shock location.

| Design parameter | Value |
|------------------|-------|
| $\phi_G$         | 0.5751|
| $\phi_R$         | 0.3227|
| $x_1$            | 0.2540|
| $x_2$            | 0.4076|
| $a_1$            | 15.55 |

Table 7

The deterministic design point is used to initiate the OUU algorithm. We use a fixed samples profile for each UQ evaluation by means of a MLMC estimator with 15 $d/8$ realizations and 5 discrepancy evaluations between $d/16$ and $d/8$. In this formulation we include a robustness measure equal to $\pm 3\sigma$. An initial optimization design is obtained as reported in Table 9. This design point is obtained after the initial surrogate evaluation (which requires 6 evaluations) and one optimization step for a total of 7 MLMC evaluations (each with a total of 20 $d/8$ and 5 $d/16$). The initial deterministic design proved to be an infeasible starting point with respect to the probabilistic constraints and therefore the algorithm is operating in feasibility restoration mode.

The performance of the system for the initial and the nominal design are compared in Table 10. The constraint violation is reduced by 30% at a cost of a reduced $\eta_{\text{comb}}$. A comparison between the nominal and design point is reported in Fig. 8 where the contours for Mach number and carbon monoxide concentration are shown.

2. Preliminary results for the final OUU formulation

For this problem we selected the $d/32$ resolution to be our highest fidelity and $d/16$ and $d/8$ as our mid- and lo-fidelity models, respectively. In order to define the levels we performed a numerical study on the nominal configuration (the one with design parameters chosen to be the center of the ranges reported in Table 4). For this nominal configuration, we performed a forward UQ study with a total of 1053 random realizations for $d/8$, 122 for $d/16$ and 23 for $d/32$. Each

| QoI      | Value |
|----------|-------|
| $\eta_{\text{comb}}$ | 0.3096 |
| $\phi_{\text{burn}}$ | 0.1843 |
| $\max P_{\text{rms}}$ | 0.1677 |
| $x_{\text{shock}}$ | 78.33 $d$ |
| $P_{\text{stagloss}}$ | 0.3768 |

Table 8

Objective and constraints values for the final design point for the deterministic optimization for the bi-level HDCR problem (only $d/8$ simulations).
### Table 9  Initial optimization design obtained after 7 iterations for the bi-level HDCR problem.

| Design parameter | Nominal | Latest Iteration |
|------------------|---------|------------------|
| $\phi_G$         | 0.5751  | 0.5733           |
| $\phi_R$         | 0.3227  | 0.3229           |
| $x_1$            | 0.2540  | 0.2535           |
| $x_2$            | 0.4076  | 0.4078           |
| $a_1$            | 15.55   | 15.74            |

### Table 10  Performance comparison between the initial and the nominal design for the bi-level HDCR problem.

| QoI                          | Nominal | Latest Iteration |
|------------------------------|---------|------------------|
| $\eta_{\text{comb}}$        | 0.3214  | 0.3150           |
| $\mathbb{E}[\phi_{\text{burn}}] - 3\sigma[\phi_{\text{burn}}]$ | 0.1309  | 0.1437           |
| $\mathbb{E}[\max P_{\text{rms}}] + 3\sigma[\max P_{\text{rms}}]$ | 0.4148  | 0.3974           |
| $\mathbb{E}[x_{\text{shock}}] - 3\sigma[x_{\text{shock}}]$ | N/A     | N/A              |
| $\mathbb{E}[P_{\text{stagloss}}] + 3\sigma[P_{\text{stagloss}}]$ | 0.4810  | 0.3917           |

**Fig. 8**  Comparison between the nominal design (top of each pair) and the first design point (bottom of each pair) for variables $M$ (top two) and $Y_{CO}$ (bottom two) from the HDCR OUU problem RAPTOR LES. Solutions plotted are from $d/16$ resolution.
evaluation of the RAPTOR code produces a full time history of the flow quantities that are a posteriori integrated in time in order to obtain the QoIs. We assessed the impact of the error committed during the time integration by letting some of the simulations converge for a long time and evaluating from them the reference values. Afterward, we used the reference solutions for each mesh to compute the $L^2$ error for several choices of initial time coordinates and averaging window lengths. This information enabled us to select the right combination of parameters in order to minimize the cost of each evaluation for the three meshes (by integrating the solution in time long enough to obtain a converged solution without incurring in an unnecessary computational cost). Furthermore, we verified that with the selected choices of these parameters, we obtained converging statistics for the dataset evaluated with respect to the nominal conditions. The choice of these parameters finally give us the relative computational cost of an evaluation on each mesh. We report the computational cost in Table 11.

| Grid Size | Relative Computational Cost |
|-----------|-----------------------------|
| $d/32$    | 1                           |
| $d/16$    | 0.125                       |
| $d/8$     | 0.01575                     |

Table 11 Relative computational cost for a simulation of different mesh. The costs are normalized with respect to the high-fidelity cost.

For this case we use a fixed MLMC sample profile of 20 $d/8$ evaluations, 10 difference values given by $d/16$ and $d/8$ realizations and 5 difference values between $d/32$ and $d/16$. As a reference, we note that this samples profile corresponds to a computational cost of approximately $7 d/32$ evaluations.

This optimization is still ongoing and so far we have evaluated 10 design points
- The design points 1 through 6 are needed to compute the surrogate;
- Evaluation 7 is found after the optimization in feasibility restoration mode. This evaluation is rejected due to a negative acceptance ratio since the surrogate has to be improved first;
- Evaluation 8 is randomly added to enrich the surrogate;
- Evaluation 9 is found after the optimization in feasibility restoration mode. This point is rejected for the same reason of Evaluation 7;
- Evaluation 10 is randomly added to enrich the surrogate.

We note here that each design point evaluation described above requires a MLMC estimator evaluation. The whole set of design point evaluations accounted for a total of 500 combined RAPTOR LES realizations which correspond to a computational cost of approximately $70 d/32$ realizations. At this point of the optimization process we cannot extract any conclusive information regarding the design and we will report the results of this optimization in a future communication.

V. Conclusions

We present an overview and progress update on optimization under uncertainty efforts under the DARPA EQUiPS ScramjetUQ project. In particular, we detail activities in integrating the SNOWPAC and DAKOTA software packages, which require new algorithm advances for coupling the derivative-free optimization in SNOWPAC together with the multilevel uncertainty quantification capabilities in DAKOTA. A scramjet inspired model problem is first used to demonstrate the efficiency of the multilevel approach in contrast to a single fidelity method. For this test case, a comparison between stochastic and deterministic optimization results is also conducted. Next, we present details regarding the setup and preliminary steps needed for the scramjet OUU task using large eddy simulations of supersonic reactive flows inside the HiFiRE Direct Connect Rig. While this campaign is highly computationally intensive and currently on-going, initial results are presented and discussed.

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