

SURROGATE MODEL WITH CONSERVATIVE ERROR MEASURE FOR THE STAGNATION HEAT FLUX IN ATMOSPHERIC ENTRY FLOWS

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Abstract. *This paper proposes the application of a conservative global error measure estimation to a kriging metamodel of the stagnation pressure and heat flux in the context of the atmospheric reentry of the EXPERT vehicle. In particular, a model based method and a generalized cross validation technique are compared to the actual root mean squared error in order to check whether the estimation is conservative. Furthermore, the quality of kriging metamodeling is compared to the one of classical polynomial chaos response surface by comparing their root mean squared errors.*

1 INTRODUCTION

The control and the post-flight analysis of the reentry trajectory of a space vehicle need an accurate reconstruction of freestream conditions, that is, for example, pressure and Mach number in front of the shock. These quantities can be reconstructed starting from the output of sensors flush-mounted in the vehicle thermal protection system, which are able to measure pressure and heat flux on the spacecraft surface. The problem of rebuilding conditions upstream the shock starting from stagnation measures is an inverse problem that is far from being resolved. Classical freestream reconstruction techniques [16] do not take into account high temperature effects (*e.g.* thermochemical non-equilibrium and surface catalysis), since they usually rely on the calorically perfect gas approximation.

In a recent work, Tryoen et al. in [15] proposed a strategy for rebuilding freestream conditions starting from stagnation pressure and heat flux measures, which they applied to the entry trajectory of the European Experimental Reentry Test-Bed (EXPERT) vehicle. They used generalized polynomial chaos (PC) combined with a non-intrusive spectral projection to propagate the uncertainties through the forward CFD problem. Then, they used the polynomial chaos expansion as a metamodel to compute the solution of the Bayesian inverse problem. In particular, they have shown that the PC response surface for the stagnation heat flux was not sufficiently accurate, featuring also non-physical negative solutions.

The main objective of this work is to propose and assess a kriging-based method in order to build a response surface for the pressure and the heat flux at the stagnation point. Kriging interpolation [3] is based on the idea of approximating the function of interest as a realization of a stationary Gaussian stochastic process. It has been applied widely in geostatistics to interpolate spatially dependent data and is becoming popular also to as a cheap surrogate for expensive predictions in different scientific contexts.

Second objective of this work is to build a kriging metamodel featuring an error measure, that could be considered as *conservative*, *i.e.* the error measure systematically overestimate the real error between the kriging prediction and the exact output value. This property could be of the greatest importance for problems featuring a very large computational cost for a single output evaluation, since a *conservative* error measure permits a robust estimation about the prediction of the kriging surface. In the case under study in this work, this information could be for example used during the trajectory design, relying on robust predictions of pressure and heat flux at the stagnation point. In this work, several error measures are considered, *i.e.* a generalized cross validation (GCV), which is a model independent estimate, and the model based estimate for kriging surfaces. A study in terms of error estimation robustness is presented, by means of a comparison with respect to the actual error measure.

In Section 2, the physical problem and the associated numerical code are briefly described, as well as the different sources of uncertainty on input data. Section 3 illustrates the surrogate models used in this paper. In Section 4, several techniques for building a conservative error estimation are introduced. Then, some results are presented in Section 5. Finally, some conclusions and perspectives are drawn in Section 6.

2 PHYSICAL PROBLEM AND SOURCES OF UNCERTAINTIES

The forward problem consists in computing the quantities of interest, namely the pressure p_{st} and the heat flux q_{st} at the stagnation point, starting from given freestream

conditions, described in table 1, which represent a particular point in the entry trajectory of the EXPERT vehicle, which exhibits chemical non-equilibrium (see Figure 1). The set of equations used to describe the phenomena is a combined physico-chemical

Altitude, Km	T_∞ , K	p_∞ , Pa	M_∞
60	245.5	20.3	15.5

Table 1: Freestream conditions for one point of the trajectory of the EXPERT vehicle.

model, developed by Barbante in [1], able to simulate high temperature reacting flows. Two-dimensional axisymmetric Navier-Stokes equations, supplied with adequate boundary conditions, are combined with the chemical mechanism introduced by Park et al. [12] applied to a mixture of five species air (N , O , NO , N_2 and O_2). Furthermore, the catalyticity of the vehicle surface is taken into account, and it is modeled as a catalytic wall at radiative equilibrium. Hence the input data for the forward model are freestream pressure and Mach number (p_∞ and M_∞), the catalytic recombination coefficient γ and the reaction rate coefficients k_r of the r chemical reactions.

To simulate the forward problem, we use the in-house code COSMIC developed by Barbante [1]. This solver was designed to approximate hypersonic flow models where chemical nonequilibrium effects need to be accounted for. It includes a hybrid upwind splitting scheme, the hybridization of the van Leer scheme [7] and the Osher scheme [11] and includes a carbuncle fix. An axisymmetric condition is imposed on the y axis, while the wall of the body is modeled by a partially catalytic wall at radiative equilibrium. Figure 2 illustrates the temperature field around the nose of the vehicle.

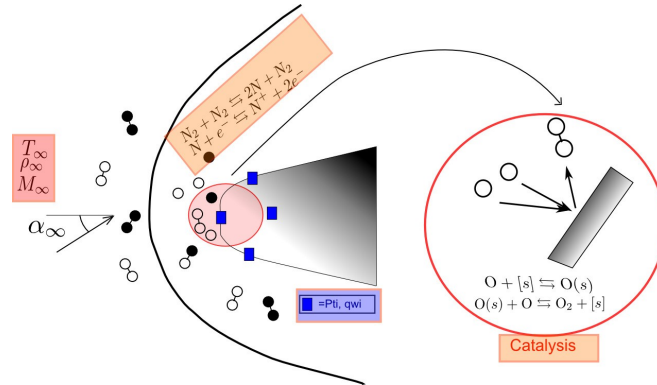


Figure 1: Illustration of the physical problem involved in the atmospheric reentry of the EXPERT capsule

Concerning the uncertainty characterization, the parameters p_∞ , M_∞ and γ are assumed as uniform, and are described in Table 2. Uncertainty is taken into account also on four reactions rates k_r of four chemical dissociation processes (see Table 3).

3 SURROGATE MODELS

In this work, a Generalized Polynomial-Chaos is taken as reference for permitting a deeper analysis about the Kriging performances. In particular, a non-intrusive generalized

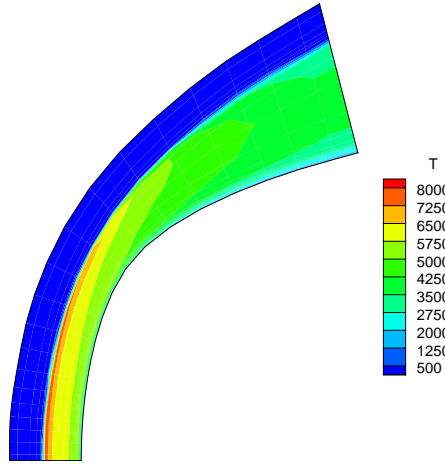


Figure 2: Numerical solution of the temperature field $T[\text{K}]$ around the nose of the capsule at nominal freestream conditions described in Table 1

Variable	Distribution	Minimum	Maximum
p_∞ , Pa	Uniform	16.3	24.3
M_∞	Uniform	13.7	17.3
γ	Uniform	0.001	0.002

Table 2: Uncertainties on freestream conditions and catalytic recombination constant.

Gas reaction	Distribution of $\log_{10} k_r$	σ_r
$\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$	Normal	0.12
$\text{NO} + \text{N} \rightarrow \text{N} + \text{O} + \text{N}$	Normal	0.12
$\text{O}_2 + \text{N}_2 \rightarrow 2\text{O} + \text{N}_2$	Normal	0.10
$\text{O}_2 + \text{O} \rightarrow 2\text{O} + \text{O}$	Normal	0.10

Table 3: Uncertainties on gas reaction rates.

polynomial chaos (PC) as implemented in the NISP (Non-Intrusive Spectral Projection) library has been used. Details about this well-known technique can be found in [6, 4, 2].

3.1 KRIGING SURROGATE

Kriging interpolation([14], [3]), is another suitable technique for building a response surface. Its main idea is to consider the function of interest $f(\mathbf{x})$ as a realization of a stationary Gaussian stochastic process $F(\mathbf{x})$.

$$F(\mathbf{x}) = \mathcal{N}(\mu_k(\mathbf{x}), s_k(\mathbf{x})) \quad (1)$$

In universal kriging, the stochastic process can be written in the form of the sum of a deterministic regression model and a stochastic departure term

$$F(\mathbf{x}) = \sum_{j=1}^n \beta_j y_j(\mathbf{x}) + Z(\mathbf{x}) \quad (2)$$

where $y_j(\mathbf{x})$ are linearly independent known functions, β_j are unknown weights, and $Z(\mathbf{x})$ is a Gaussian process with zero mean and covariance $k(\mathbf{u}, \mathbf{v})$. The departure term is assumed to be correlated as a function of the distance between different points, using usually a Gaussian correlation function [13]

$$k(Z(\mathbf{u}), Z(\mathbf{v})) = \sigma^2 \exp \left\{ - \sum_{j=1}^N \left(\frac{u_j - v_j}{l_j} \right)^2 \right\} \quad (3)$$

The parameters σ and \mathbf{l} , called *hyperparameters*, can be estimated by using the maximum likelihood method, and enter as known parameter in the construction of the kriging surface. Then the aim is to build an interpolation in the form

$$\hat{F}(\mathbf{x}) = \sum_{i=1}^{N_s} f(\mathbf{x}_i) \lambda_i(\mathbf{x}) \quad (4)$$

where $\mathbf{f}_{obs} = (f(\mathbf{x}_1), \dots, f(\mathbf{x}_{N_s}))^T$ are the observation of the function at the N_s training points and $\lambda_i(\mathbf{x})$ are unknown weights. The best unbiased linear predictor can be obtained by minimizing the mean square error between the model and the predictor $MSE = E[F(\mathbf{x}) - \hat{F}(\mathbf{x})]^2$ under the constraint of unbiasedness $E[F(\mathbf{x})] = E[\hat{F}(\mathbf{x})]$. In this way it is possible to obtain the mean of the stochastic process, that can be used as a metamodel for the original function

$$\begin{aligned} f(\mathbf{x}) \sim \mu_k(\mathbf{x}) &= \mathbf{y}^T(\mathbf{x})\boldsymbol{\beta} + \mathbf{c}(\mathbf{x})^T C^{-1}(\mathbf{f}_{obs} - Y^T \boldsymbol{\beta}) \\ \text{with } \boldsymbol{\beta} &= (Y^T C^{-1} Y)^{-1} Y^T C^{-1} \mathbf{f}_{obs} \end{aligned} \quad (5)$$

where $\mathbf{y}(\mathbf{x}) = (y_1(\mathbf{x}), \dots, y_n(\mathbf{x}))^T$ is the vector of basis functions, Y is a matrix whose elements are $Y_{ij} = y_i(\mathbf{x}_j)$, $\mathbf{c}(\mathbf{x})$ is the vector of correlations between the point \mathbf{x} and each training point and C is the matrix of correlations among training points.

It is possible to compute also the process variance [9], which can be used as a local error estimate

$$\begin{aligned} s_k^2(\mathbf{x}) &= k(\mathbf{x}, \mathbf{x}) + \mathbf{a}(\mathbf{x})^T (Y^T C^{-1} Y)^{-1} \mathbf{a}(\mathbf{x}) - \mathbf{c}(\mathbf{x})^T C^{-1} \mathbf{c}(\mathbf{x}) \\ \text{with } \mathbf{a}(\mathbf{x}) &= Y^T C^{-1} \mathbf{c}(\mathbf{x}) - \mathbf{y}(\mathbf{x}) \end{aligned} \quad (6)$$

In our application we limit to use the simpler model called *ordinary kriging*, in which $y_1(\mathbf{x}) = 1$ and $y_j(\mathbf{x}) = 0$ for $j \neq 1$, hence only β_1 needs to be determined.

Also this kind of response surface enables the computation of the values of mean and variance of the function of interest, even if it is not as straightforward and cheap as with PC expansion. For example sampling methods can be applied to the response surface, and statistical moments can be computed via sample expectations.

In this paper, the kriging surrogate model has been constructed using as training points the same set of solutions computed to build the PC expansion, thus not requiring further evaluations of the expensive forward problem. However, there exist in literature more refined techniques to choose training points that allow to obtain a more accurate kriging surface, but this goes beyond the purpose of this work. Furthermore, kriging interpolation is an interesting choice because the variance computed in eq. 6 offers a cheap model based estimation of the error of the response surface (see Section 4).

Note that the kriging process implemented in the ForK library [8], used in this work, includes also the nugget effect variance in the covariance model

$$C_{ij} = k(\mathbf{x}_i, \mathbf{x}_j) + \sigma_n \delta_{ij} \quad (7)$$

This in general is not necessary if the purpose is to interpolate a set of noiseless data, since the interpolation should pass exactly through the training points, but it is however done in order to improve the conditioning of the numerical problem.

4 CONSERVATIVE ERROR ESTIMATION

Let us now explore different techniques for building a kriging metamodel with a *conservative* error estimation, thus computing a robust estimation of the prediction. In particular, a generalized cross validation (GCV), which is a model independent estimate, and the model based estimate for kriging surfaces are here detailed.

As already mentioned in the previous section, for kriging metamodels the local variance of the process (eq. 6) can be used as an estimate of the actual pointwise mean squared error.

$$e(\mathbf{x}) = \sqrt{s_k^2(\mathbf{x})} \quad (8)$$

It is possible to integrate this local error to obtain an estimate of the global root mean squared error (RMSE). In practice the integration is done by a numerical integration technique [5]

$$\text{RMSE} = \sqrt{\frac{\sum_{j=1}^{N_t} e_j^2 \xi_j}{\sum_{j=1}^{N_t} \xi_j}} \quad (9)$$

where $e_j = e(\mathbf{x}_j)$ is the error evaluation at the N_t integration points and ξ_j are the integration weights. It is possible to use the collocation points of a quadrature method as test points to compute the local variance of the kriging surface. Hence a quadrature formula can be exploited to compute the integral in eq. 9. It has to be noticed that this error measure is a model based estimate, because it is based on some assumptions on which the metamodeling technique relies. For example the computations of s_k^2 depends on the assumption on the covariance $k(\mathbf{u}, \mathbf{v})$ to be of Gaussian form.

In literature there can be found many model independent error measures, that are able to deal with many kinds of surrogate models. One of the most popular among these methods is *k-fold cross validation* [10], also called *leave-k-out cross-validation*. In particular, as suggested in [5], one recommended choice is to use *leave-one-out GCV* to estimate the kriging metamodel error. This method consists in fitting a surrogate model on $N_s - 1$ points, by leaving out one design point at a time, then the response is predicted at this point with the metamodel. Then the GCV error can be defined as following, in analogy with the RMSE error

$$\text{GCV} = \sqrt{\frac{\sum_{i=1}^{N_s} \left(f_i - \hat{F}_i^{(-i)} \right)^2 \xi_i}{\sum_{i=1}^{N_s} \xi_i}} \quad (10)$$

where f_i is the design point observed response, while $\hat{F}_i^{(-i)}$ is the prediction at the left-out point using the surrogate built from all the other points. The GCV can be used to estimate the actual root mean squared error of the approximation (RMSE). Although being

relatively expensive for kriging, since the optimization of the kriging parameters must be repeated at each left out point, this error estimate is supposed to perform quite well and most of all to be conservative, *i.e.* not to underestimate the actual error. Moreover, being a model independent error measure, it does not depend on the structure and the parameters of the metamodeling technique, since it only needs the output of the prediction, hence it can be used for black-box metamodeling codes.

In both [5] and [10] it is possible to observe that the quality of the GCV error estimate is truly problem-dependent and it is strongly influenced by different factors, such as the choice of the initial experimental design, although this last aspect could be somehow cured when using adaptivity. Generally, conservativeness is assessed by computing the actual error of the kriging metamodel, by exploiting the knowledge on the real output values on higher level grids.

$$e_a^2(\mathbf{x}_i) = \left(f(\mathbf{x}_i) - F(\mathbf{x}_i)\right)^2 \quad (11)$$

The actual local error can be integrated by using eq. 9 in order to obtain the actual RMSE. It is important to notice that in practical applications the actual RMSE is usually not available, if an excessive computational cost is associated to the forward problem. In this case it is more reasonable to use the whole set of forward evaluations as training points for improving the accuracy of the metamodel.

5 RESULTS

This section illustrates some results about the kriging surfaces obtained on the pressure and heat flux at the stagnation point. First, *exact* evaluations of the fitness functions are performed by running several CFD computations on a Smolyak-Gauss sparse grid in the stochastic space. Three different levels are considered: a second order grid constituted by 120 points, a third order grid of 680 points and a fourth order one of 3060 points (see Tab. 4). These output evaluations are used to compute the projection integrals in order

Order	Number of training points N_s	Number of test points N_t
2	120	2187
3	680	2187
4	3060	2187

Table 4: Number of points for Smolyak-Gauss grids of different order

to get the PC expansion coefficients for the pressure and the heat flux. The actual RMSE error is computed for the PC response surface: the values of the quantities of interest are predicted at the points of the test grid (a second order fully-tensorized grid of 2187 points) and are compared with the actual function values in order to compute the local error (Eq. 11), which can be integrated within Eq. 9 to produce the global error estimate. Results are shown in Tables 5 and 6.

Then, the three different experimental databases are used as training points to build three different kriging surfaces, both for the stagnation pressure and the heat flux. Also for each kriging surface the actual RMSE is computed by predicting the values of the function in the test points and comparing them to the actual function value, already computed with the CFD tool. The kriging variance (Eq. 8) is estimated as well at each

Grid order	RMSE, No=2	RMSE, No=3	RMSE, No=4
2	51.84	-	-
3	162.42	214.94	-
4	384.67	552.23	939.45

Table 5: Actual error measures for the PC interpolation of stagnation pressure p_{st} , Pa

Grid order	RMSE, No=2	RMSE, No=3	RMSE, No=4
2	5.688e4	-	-
3	2.204e5	3.065e5	-
4	5.493e5	7.493e5	1.324e6

Table 6: Actual error measures for the PC interpolation of stagnation heat flux q_{st} , W/m²

point of the test grid and is used to compute the model based estimation of the RMSE. Results are reported in Table 7 for the pressure and in Table 8 for the heat flux.

Order	Actual RMSE	Estimated RMSE	GCV
2	259.77	29.31	696.60
3	74.80	18.56	284.17
4	18.10	8.59	133.67

Table 7: Error measures for the kriging interpolation of stagnation pressure p_{st} , Pa

GCV error estimates for the kriging metamodels are also computed for each of the three sets of design points. These values are compared in Tables 7 and 8 with the actual and the estimated RMSE. It is important to note that for each set of training points the GCV error estimate is conservative, *i.e.* it is always higher than the actual RMSE, while the model based estimate always underestimates the actual error.

Furthermore, in Table 9 and 10 the maximum and the minimum values of the actual local error are shown respectively. Note that the maximum error value is much higher than the mean value computed with the RMSE, but it can be seen that only relatively few points exceed the threshold of 10% of the maximum error, which means that many test points present an error that is at least one order of magnitude less than the maximum error value.

Note also that, from a comparison between values in Tables 5, 6, 7 and 8, in this particular case, the kriging metamodel performs better than the PC expansion in terms of actual RMSE, especially for the stagnation heat flux. This was expected, since the PC metamodel for the heat flux is known to produce points with non-physical negative values.

Finally, the statistics of the quantities of interest are computed by sampling the kriging metamodels. Mean and variance of p_{st} and q_{st} are reported in Table 11, while the whole probability density functions (PDF) is reported in Figure 3.

Order	Actual RMSE	Estimated RMSE	GCV
2	21409	2925	50638
3	15627	5469	65813
4	15367	6510	69759

Table 8: Error measures for the kriging interpolation of stagnation heat flux q_{st} , W/m²

Order	$\max(e_a)$ %	$\min(e_a)$ %	Points above threshold
2	13.77	4.44e-4	859 on 2187
3	4.67	1.38e-4	963 on 2187
4	1.99	1.48e-4	1058 on 2187

Table 9: Relative error bounds for the kriging interpolation of p_{st} and number of test points above the threshold of $0.1\max(e_a)$

Order	$\max(e_a)$ %	$\min(e_a)$ %	Points above threshold
2	47.01	1.38e-3	1149 on 2187
3	22.85	7.44e-5	1507 on 2187
4	58.61	6.03e-4	763 on 2187

Table 10: Relative error bounds for the kriging interpolation of q_{st} and number of points above the threshold of $0.1\max(e_a)$

6 CONCLUSIONS

This paper deals with the computation of a conservative error measure estimation for a kriging metamodel of the stagnation pressure and heat flux in a hypersonic high-temperature reentry flow. The uncertainties in the freestream values and chemical reaction rates are firstly propagated into the forward CFD problem, then CFD solutions on the collocation points of sparse grids of different order are computed. These solutions are used to compute via deterministic numerical integration the coefficients of polynomial chaos expansions of the quantities of interest. Then the same points are used as training points for a kriging interpolation technique. For both surrogate techniques the actual root mean squared error is computed. Results show that in this particular application an with this sets of training and test points the kriging surface performs better as surrogate model than the polynomial chaos expansion, which instead presents also points with non-physical solutions (negative heat flux values). Moreover, two different global error measure estimations are applied to the kriging interpolation: a root mean squared error estimation computed with the model based local variance measure and a leave-one-out generalized cross validation technique. While the first is computationally cheap , the second shows to be always conservative, which means that it never underestimates the actual root mean squared error. Its drawback is the quite elevate computational cost, since for each left-out point (*i.e.* for each training point) the optimization of kriging parameters and hyperparameters should be repeated.

		$No = 2$	$No = 3$	$No = 4$
p_{st} [Pa]	μ	$6.498 \cdot 10^3$	$6.492 \cdot 10^3$	$6.497 \cdot 10^3$
	σ^2	$7.505 \cdot 10^5$	$1.031 \cdot 10^6$	$1.169 \cdot 10^6$
q_{st} [W/m ²]	μ	$2.886 \cdot 10^5$	$2.770 \cdot 10^5$	$2.890 \cdot 10^5$
	σ^2	$1.003 \cdot 10^9$	$2.347 \cdot 10^9$	$1.304 \cdot 10^9$

Table 11: Mean value and variance of the quantities of interest computed with the kriging surrogates built on different order grids

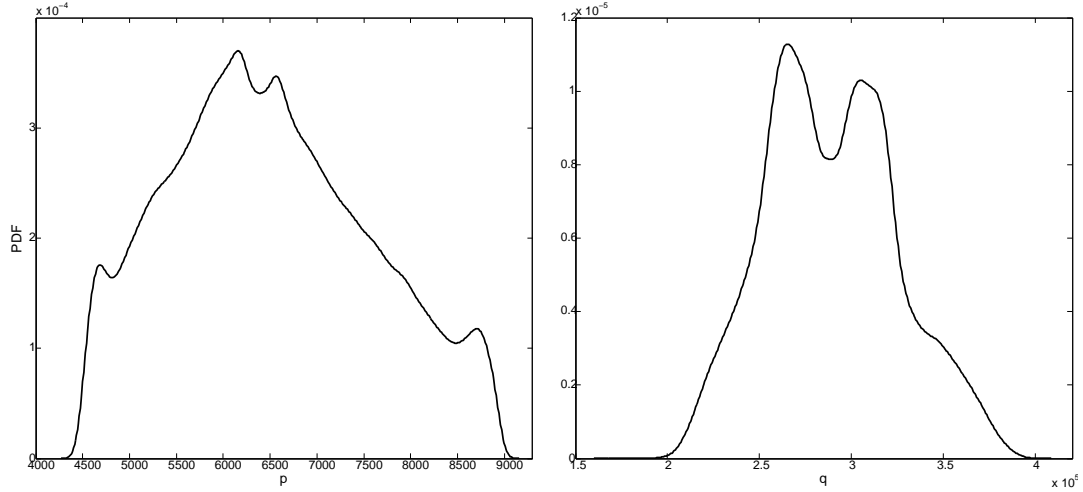


Figure 3: Probability distribution functions of the stagnation pressure and heat flux built with Monte Carlo sampling propagated through the kriging metamodells trained on the fourth order grid

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