Robust optimization of supersonic ORC nozzle guide vanes

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Abstract. An efficient Robust Optimization (RO) strategy is developed for the design of 2D supersonic Organic Rankine Cycle turbine expanders. The dense gas effects are not-negligible for this application and they are taken into account describing the thermodynamics by means of the Peng-Robinson-Stryjek-Vera equation of state. The design methodology combines an Uncertainty Quantification (UQ) loop based on a Bayesian kriging model of the system response to the uncertain parameters, used to approximate statistics (mean and variance) of the uncertain system output, a CFD solver, and a multi-objective non-dominated sorting algorithm (NSGA), also based on a Kriging surrogate of the multi-objective fitness function, along with an adaptive infill strategy for surrogate enrichment at each generation of the NSGA. The objective functions are the average and variance of the isentropic efficiency. The blade shape is parametrized by means of a Free Form Deformation (FFD) approach. The robust optimal blades are compared to the baseline design (based on the Method of Characteristics) and to a blade obtained by means of a deterministic CFD-based optimization.

1. Introduction

The use of dense gases as working media in turbomachinery, referred to as Organic Rankine Cycle (ORC) turbines, is proposed as a method of recovery of variable energy sources such as waste heat from industrial processes. Proposed heat sources for ORC turbines typically include variable energy sources such as solar thermal collectors or waste heat from industrial processes. In such conditions, traditional design at nominal operating conditions may lead to poor performance in practice. Optimization under uncertainties is called Robust Optimization (RO). The robustness is determined by a measure of insensitivity of the design with respect to variations of the design parameters, like geometrical tolerances or fluctuations of the operating conditions. To measure the robustness of a new design, statistics such as mean and variance (or standard deviation) of a response are calculated in the RO process. In this work a RO of a supersonic ORC nozzle guide vane is performed with the aim to minimize the variance and maximize the mean value of the isentropic efficiency. An original global optimization methodology has been developed in order to overcome the numerical issues typical of CFD dense gas calculations, which affect convergence and time calculation. A Non-dominated Sorted Genetic Algorithm (NSGA) is coupled with a non-intrusive Uncertainty Quantification (UQ) model which provides the statistics (mean and variance). The UQ subloop is based on a Bayesian-Kriging surrogate trained with the system response to the uncertain variables. For ORC applications, three main sources of uncertainty need to be considered: thermodynamic model, geometry and operational conditions [1].
number of parameters in each category has a strong influence on the feasibility of the UQ analysis and, then, of the RO process. One way to reduce the space parameters dimension is to carry out a sensitivity analysis and show that it is possible to consider only operational (total pressure and temperature) and geometrical (blade thickness) parameters as the main contributors to the total variance of the system output. The nozzle guide vane baseline is designed by means of a Method Of Characteristics (MOC) generalized to accurate Equations Of State (EOS) [2, 3]. A Free Form Deformation (FFD) approach, which allows to easily handle any kind of shape independently from the geometrical complexity, is applied to generate a variety of nozzle designs. The resulting parametrization of the nozzle guide vane shape depends on a relatively low number of parameters. The evaluation of the isentropic efficiency is carried out by means of 2D Reynolds Average Navier-Stokes (RANS) simulations. Given the computational cost of viscous CFD simulations, we propose to speed-up the RO by training a second surrogate Kriging model for the multi-objective fitness function. An adaptive sample infill strategy based on the Multi Objective Expected Improvement (MOEI) is implemented in order to improve the surrogate accuracy during the genetic optimization, with a minimal additional cost.

2. Governing equations and CFD solver
The compressible Reynolds-Averaged Navier-Stokes (RANS) equations are solved, supplemented by a dense-gas EOS, and specifically the Peng-Robinson-Stryjek-Vera (PRSV) cubic equation [4], which has been proven to represent a good compromise between accuracy and computational cost. The caloric behaviour is modelled by assuming that the isocoric specific heat in the dense gas limit follows a simple power law. The governing equations are discretized by using a cell-centered finite volume scheme for structured multi-block meshes of third-order accuracy [5]. To preserve the high accuracy on non-Cartesian grids, the numerical fluxes are constructed by using weighted discretization formulas, which take into account the mesh deformations [6]. The equations are then integrated in time using a four-stage Runge-Kutta scheme. Local time stepping, implicit residual smoothing and multi-grid acceleration are used in order to drive the solution to the steady state. The turbulence is taken into account by means of the Spalart-Allmaras transport equation. The accuracy of the numerical solver has been already demonstrated in previous works [5, 7].

3. Uncertainty Quantification
The evaluation of mean and variance of a Quantity of Interest (QoI), in our case the isentropic efficiency of the ORC expander, is carried out by means of a surrogate model of the output response and a Bayesian-Kriging approach is used. In the Bayesian framework, the Kriging surrogate predicts a set of M values \( y \), conditional on N data \( y^* \), where the data \( y^* \) are a subset of \( y \) selected by the observation matrix \( H \). Assuming that \( y \) and \( y^* \) are normalized such that \( y^* \) has zero mean and unit variance, the covariance matrix \( P \) of the prior distribution \( p(y) \) is defined such that its elements are generated by the Gaussian function:

\[
P = [P_{ij}(\theta)] = \left[ \exp \left( -\frac{h_{ij}^2}{2\theta^2} \right) \right]. \tag{1}\]

where \( h_{ij} = \xi_i - \xi_j \) is the correlation range, \( \xi_i \) the generic coordinate of the prediction \( y \) and \( \theta \) an hyperparameter which need to be estimated. By considering a uniform and uncorrelated observation error \( \epsilon \), the covariance matrix of the likelihood can be also defined as:

\[
R = \epsilon^2 I \tag{2}\]

where \( I \) is the identity matrix. By means of the Bayes theorem it is possible to evaluate the posterior distribution of prediction conditioned on the observation:

\[
p(y|y^*) = \frac{p(y^*|y)p(y)}{p(y^*)} \tag{3}\]
Then, by following Wikle and Berliner [8], the Kriging predictor mean and variance are:

\[ E(y|y^*) = PH^T(R + HPH^T)^{-1}y^* \]  (4)

\[ \text{var}(y|y^*) = [I - PH^T(R + HPH^T)^{-1}]P \]  (5)

The advantage of this methodology is to obtain directly an estimation of the surrogate model accuracy by means of the Kriging variance. Because we deal with an ordinary Kriging model where the hyperparameters need to be estimated, the Maximum Likelihood Estimation (MLE) approach is implemented in order to evaluate the vector \( \theta \) as the solution of the optimization problem:

\[ \max_{\theta} \left\{ - \left( \ln |A| + y^*^T A^{-1} y^* \right) \right\} \]  (6)

where \( A = (R + HPH^T) \). Since the problem (6) is performed over a multidimensional space whose cardinality is given by the number of uncertain variables and the cost varies as \( O(n_sN^3) \), where \( n_s \) is the number of optimization steps and \( N \) is the number of observed samples, it represents a bottleneck for the above methodology. Here the MLE problem is solved by means of the Nelder-Mead downhill simplex method and the inversion of the matrix \( A \) is improved with a Cholesky decomposition. Finally, once the Kriging surrogate has been trained and the hyperparameters estimated, the statistics are calculated by means of a Montecarlo simulation of the model by randomly sampling the uncertain variable distributions.

4. Shape parametrization: FFD method

The FFD methods are widely used in computer graphics to model 3D objects. The term ”free-form” designates: ”whatever the object is, whatever its description and topology, we are able to deform it” [9]. In this sense, these methods are useful when the geometrical complexity is high and a low number of control parameters are required to deform the object. Besides, the use of a combination of Bernstein polynomials allows to take easily into account geometrical singularities, control smoothness and represent the baseline exactly. This approach has been successfully applied in the past to airfoil optimization in external Aerodynamics [10].

The FFD is performed by parametrizing the space surrounding the object of interest (the blade, in our case). A lattice is created, whose node coordinates represent the control points and a deformation space is defined by means of a trivariate (bivariate for 2D case) tensor product Bernstein polynomial. For the 2D case, a baseline point \( X \) can be described in the lattice reference system as [11]:

\[ X = X_0 + sS + tT \]  (7)

where the \((s,t)\) lattice coordinates are limited in the \([0,1]\) interval and can be related to the baseline reference system as \( s = \frac{T \times U (X - X_0)}{T \times U S} \), \( t = \frac{S \times U (X - X_0)}{S \times U T} \), where \( U \) is the direction normal to the object plane. Given a \((l \times m)\) lattice (where \(l\) and \(m\) are the number of interval along the horizontal and vertical direction, respectively) the node locations (i.e. the control points) are calculated as \( P_{ij} = X_0 + \frac{l}{2} S + \frac{m}{2} T \). Then, once the \((s,t)\) coordinates are calculated and the deformation specified by the new \( P_{ij} \) position, the deformed location of a point \( X \) will be given by:

\[ X_{\text{FFD}} = \sum_{i=0}^{l} \binom{l}{i} (1-s)^{l-i} s^i \sum_{j=0}^{m} \binom{m}{j} (1-t)^{m-j} t^j P_{ij} \]  (8)

An application of the above method to the parametrization of an ORC nozzle guide vane is shown in Fig. 1 for a lattice with 12 nodes. The four corners are fixed and only vertical shifts are allowed, leading 8 control parameters, which are the design variables of the subsequent optimization step.
Figure 1. Application of FFD to a supersonic nozzle blade for a $l \times m$ lattice ($l = 6, m = 1$) with 8 control parameters.

5. Robust Optimization strategy

The RO is carried out by coupling a NSGA with the Kriging-based UQ method. The objective functions are the statistical expectaney and variance of a QoI, here the isentropic efficiency. The NSGA is then used to construct a Pareto front of optimal solutions to the problem "find a shape for which the expectation of the QoI is maximal and its variance is minimal". A straightforward coupling of the NSGA with UQ solver is overly costly for the present application, due to the high number of function evaluations, each one involving a CFD simulation. If we consider a Kriging surrogate trained with $10n_{\text{dim}}$ samples, where $n_{\text{dim}}$ is the number of uncertain variables, and a population of 30 individuals in each genetic generation, it results that $300n_{\text{dim}}$ CFD calculations have to be performed for a single genetic step. To reduce the computational cost, a second Kriging surrogate has been developed to predict the response of the multi-objective fitness function, i.e. the mean and variance of the QoI, to the design variables. Since a single output Kriging model is used, the multi-output response is obtained by training two independent surrogates, one for each fitness component. Fig. 2 presents a flow chart of the RO algorithm. The first step consists of a Design Of Experiments (DOE) plan based on Latin Hypercube Sampling (LHS) of the design space. A large training set is sampled with $N > 10n_{\text{dim}}$ samples and, after the evaluation of mean and variance through the UQ, the multi-output Kriging surrogate is trained. This is then used in the genetic algorithm to evaluate the bi-objective fitness function. The cost of the surrogate RO is reduced to $10n_{\text{par}}10n_{\text{dim}}$ CFD calculations, with respect to
the \((n_{\text{gen}} n_{\text{individuals}} 10n_{\text{dim}})\) required by the straightforward RO, where \(n_{\text{gen}}\), \(n_{\text{individuals}}\), and \(n_{\text{par}}\) are the number of genetic generations, individuals and design parameters, respectively. Since the Kriging surrogate automatically provides a surrogate accuracy criterion through the Kriging error estimate, a sample infill strategy can be used to improve the model during the NSGA loop. However, an approach based only on the mean value of the Kriging error can mislead the improvement procedure. This is avoided through a more sophisticated method, described in the next Section.

5.1. Adaptive sample infill strategy
The adaptive infill sampling consists of adding to the initial DOE new samples selected during the NSGA iteration, and to retrain the Kriging model in order to improve its accuracy (see Fig. 2). A possible approach consists in selecting some individuals from the Pareto front according to performances criteria. Unfortunately, this method does not ensure to explore the design parameter space in such a way that the direction of the optimization process is preserved. Besides, the number of samples chosen among the individuals of the Pareto front influences the Kriging accuracy. To overcome these issues, a more efficient approach is to exploit the probabilistic nature of the surrogate error estimate to adapt it in regions where the expected improvement (EI) of the global minimum is maximised [12, 13]. The EI quantifies the probability to improve the surrogate on the design space parameters and, then, a global optimization process of the EI function provides the most suitable location for the new surrogate training. Since we deal with a multi-objective optimization, the EI function will be a surface on a hyper-dimensional parameter space, then a Multi Objective Expected Improvement (MOEI) approach is carried out [13]. The global optimization is performed by means of a differential evolution algorithm. Once the best MOEI is found in the design space, its fitness is calculated using the UQ solver and added to the training set. The accuracy of the surrogate is rapidly improved with a few MOEI evaluations, then it is possible to have accurate predictions of the Pareto fronts by using a number of MOEI (i.e. UQ) evaluations \(n_{\text{MOEI}} \ll n_{\text{gen}}\), as shown in the next Section. The cost of the RO based on the adaptive infill strategy is of \((10n_{\text{par}} + n_{\text{MOEI}}) 10n_{\text{dim}}\) CFD calculations.

6. Numerical results
In this Section the MOEI procedure is first tested on the analytic multidimensional Kursawe function in order to show the feasibility and accuracy of the adaptive infill strategy. Then, the surrogate-based RO algorithm is applied to a supersonic 1D inviscid nozzle with real gas flow, for which it is possible to carry out a reference CFD-based RO. Finally, the RO methodology is applied to a supersonic ORC nozzle guide vane.

6.1. Surrogate-based optimization of the 2D Kursawe function
The adaptive sampling strategy through MOEI is validated against the analytic Kursawe function. This is a multidimensional function with two outputs, widely used for global optimization tests in the form of multi-objective minimization problem. Here the two-dimensional form is used to perform the cycle shown in Fig. 2, without the UQ loop. The Kriging surrogate is trained on an initial LHS training set of 20 samples and used to perform the NSGA. Two calculations, with and without the activation of the MOEI, are carried-out and compared with the exact Pareto front. The maximum number of individuals and generations are set to 50 and 60, respectively, and the MOEI is activated every 20 generations. As a consequence, the Kriging surrogate is updated with only 3 new samples during the genetic loop. Figure 3 compares the exact Pareto front with those provided by the Kriging surrogates with and without MOEI. In the first case the discrepancy is high, whereas the MOEI front is well predicted. To verify the exact position of the two Kriging surrogates respect to the exact Pareto front, the fitness of individuals laying on the approximate Pareto fronts is recalculated with the Kursawe
function. Fig. 4 shows that the MOEI strategy greatly improves accuracy compared to Kriging without adaptive sampling. Other tests have been performed by increasing the space parameter up to 8 dimensions, showing that the MOEI suffers of a curse of dimensionality problem. Indeed the higher is the cardinality, the higher are the number of MOEI calculations required to reach good results by providing more samples to the updated training set. However, the total cost of the algorithm in terms of function evaluations remains much lower than a high-fidelity RO. 

\begin{figure}
\centering
\includegraphics[width=0.4\textwidth]{figure3}
\caption{Pareto fronts comparison among exact Kursawe function and Kriging surrogates with and without MOEI.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.4\textwidth]{figure4}
\caption{Exact Pareto front and comparison with the Kriging surrogate best individuals recalculated with the exact Kursawe function.}
\end{figure}

6.2. RO of a quasi-1D supersonic nozzle

The RO methodology described in the previous section is first applied to a supersonic quasi-1D inviscid nozzle. The flow is modelled by the Euler equations supplemented by the PRSV EOS. More details about the solver can be found in [14]. The working fluid is MDM and the uncertain parameters in terms of mean, percent coefficient of variation (CoV) and probability density function (pdf) are shown in Tab. 1. Three uncertainties are taken into account: two operational (total pressure and temperature \( p_0, T_0 \)) and one geometrical (wall nozzle displacement \( \varepsilon \)) parameters. The nominal operating conditions are normalized with the critical values and are chosen such that a normal shock is set in the nozzle divergent. The chosen CoV ensures that a shock is always present in the convergent, while allowing a significant variation of the shock position. The latter is treated a random QoI, whose mean and variance are estimated through UQ.

\begin{table}
\centering
\caption{Uncertain variables for the 1D supersonic nozzle. Total pressure and temperature are normalised respect to the critical values, \( \varepsilon \) is the wall nozzle displacement.}
\begin{tabular}{lcc}
\hline
Parameter & Mean & CoV\% & pdf \\
\hline
\( p_0 \) & 0.212 & 15\% & UNIFORM \\
\( T_0 \) & 0.0709 & 15\% & UNIFORM \\
\( \varepsilon \) & 1 & 1\% & UNIFORM \\
\hline
\end{tabular}
\end{table}

The RO problem is defined as follows:

\[ \min \alpha |\mu(x_s) - \mu(x_s)_{\text{target}}|, \min \alpha |\sigma(x_s)^2 - \sigma(x_s)_{\text{target}}^2| \] (9)
where \( \alpha \) is the vector of design parameters, \( x_s \) the shock position normalised with the nozzle length, \( \mu_{\text{target}} = 0.7 \) and \( \sigma_{\text{target}}^2 = 1.0 \times 10^{-4} \) two target values to which to converge during the optimization. The nozzle geometry is deformed by means of the FFD and \( n_{\text{par}} = 8 \) control parameters are defined by a \( 6 \times 1 \) lattice around the nozzle with the four corners blocked and only vertical shifts are allowed. The accuracy of the Kriging-based UQ solver is first assessed by means of a convergence study. The QoI is the shock location and the maximum Kriging error estimate \( \varepsilon_{K,\text{max}} \) is computed as a function of the number of samples \( N \). The results, displayed in Figs. 5, 6, show that after 30 samples the Kriging error is below \( 6 \times 10^{-5} \) and small variations of mean and and variance are observed. Then, the UQ-Kriging with \( N = 30 \) is coupled to the NSGA. The results are compared with those of a surrogate-based optimization, with and without MOEI. The initial surrogate is based on a LHS training set of \( 10n_{\text{par}} = 80 \) samples. The results of the RO are shown in Figs. 7, 8, where \( f_1 = |\sigma(x_s)^2 - \sigma(x_s)^2_{\text{target}}| \) and \( f_2 = |\mu(x_s) - \mu(x_s)_{\text{target}}| \). The first figure compares CFD-based and surrogate-based Pareto fronts. The ordinary Kriging surrogate, without MOEI, fails to predicts adequately the high-fidelity Pareto front. On the other hand, by adaptively adding only 3 samples with MOEI

![Figure 5. Maximum Kriging error estimate convergence plot as function of the number of samples.](image)

![Figure 6. Variance and mean convergence plot as function of the number of samples.](image)

![Figure 7. Pareto fronts comparison between high-fidelity CFD RO and Kriging surrogate (with and without MOEI) RO.](image)

![Figure 8. Pareto individuals recalculation for the Kriging surrogate with MOEI and comparison with CFD.](image)
(i.e. one every 5 generations of the NSGA), the prediction is more accurate. To verify if the individuals of the surrogate-based Pareto front with MOEI lie on the high-fidelity one, the fitness function of the non-dominated individuals is recalculated with the CFD solver. Fig. 8 shows an even better agreement between the two fronts, which proves the accuracy and efficiency of the MOEI strategy for the present test case.

6.3. RO of ORC nozzle guide vanes

A deterministic optimization is first performed for the baseline geometry of Fig. 1, obtained by applying an accurate MOC based on a complex EOS for R245FA working fluid (Bufi et al. 2015). The viscous CFD calculations are carried out on a structured $384 \times 128$ mesh, for which $y^+ < 1$. Grid convergence is checked for the wall pressure distribution and isentropic efficiency, showing a maximum difference below 2% and 8% respectively, by referring to a $768 \times 192$ mesh. These convergence levels are acceptable for RO applications. The maximum deformations allowed with the FFD are set to 20% in the lattice reference system, and 8 control points are taken into account, as shown in Fig. 1. In this way the axial chord is kept constant whereas the shape can change freely. In Tab. 2 the nominal design parameters are shown. In Figs. 9,10 the

| Fluid   | $p_0$ | $T_0$ | $\beta$ |
|---------|-------|-------|---------|
| R245FA  | 1.1   | 0.98  | 5       |

Table 2. Nominal nozzle parameters. Total pressure and temperature are normalised with respect to the critical values whereas $\beta$ is the throat-to-exit static pressure ratio.

Mach contour plots are shown for baseline and optimized geometry, respectively. In the first case, the presence of a weak oblique shock at the trailing edge lead the Mach number from 2.37 to 2.31. The optimized blade is narrower and exhibits significantly different shapes at the leading edge. This shows that the MOC procedure provides already a satisfactory design for the divergent part, whereas the convergent benefits from CFD optimization. The throat area per unit depth is 9% higher, leading to a slightly higher massflow rate. The expansion pressure ratio through the nozzle is unchanged, and the exit Mach number is 2.1 for both cases. The optimized shape still exhibits oblique shocks on the trailing edge, but with lower upstream Mach number, so that shocks are weaker. The stagger angle is slightly changed from $72^\circ$ to $71.4^\circ$ and the viscous wake and the separation zone on the suction side, are reduced. These improves the
isentropic efficiency from 0.879 to 0.962 (8%). Afterwards, a RO of the baseline blade is also carried out by maximizing mean $\mu_s$ and minimizing variance $\sigma^2_s$ of the isentropic efficiency and using the multi-objective Kriging surrogate with MOEI adaptive sampling. To evaluate the objective function, the UQ Kriging with 24 samples is used. Total inlet conditions $(p_0, T_0)$ and blade thickness $\varepsilon$ are set as uncertain variables, with the distribution shown in Tab. 4. The choice of beta pdfs, with a proper calculation of the shape parameters based on the known mean and standard deviation, allows to avoid expansions in the liquid-vapor region. The optimization converges after 60 generations with 3 samples adaptively added each 20 generations. The Fig. 11 shows the Pareto front. The recalculated samples show the goodness of the NSGA-Kriging with MOEI surface method. The stochastic performance of deterministically-optimized blade is also represented for comparison. For this blade the average value of the isentropic efficiency is $\mu_{s,\text{det}} = 0.946$, i.e. slightly lower than the deterministic value $\mu_{s,\text{det}} = 0.962$ with a variation of 1.5%. The higher variance compared to the robust individuals shows that the deterministic optimization provides a less robust blade, in spite of the high performances. The stochastic performance of the baseline blade shows that the RO provides a 6% average increase of the isentropic efficiency and a 1% decrease of the standard deviation. In Fig. 12 the robustly optimized shape, selected on the Pareto front (black arrow in Fig. 11), is compared with the baseline and deterministic optimized ones. Once again, the more significant geometrical variations are observed in the subsonic zone.

**Table 3.** Uncertain variables for the ORC supersonic nozzle. Total pressure and temperature are normalised respect to the critical values, $\varepsilon$ is the blade thickness.

| Parameter | Mean | CoV% | pdf   |
|-----------|------|------|-------|
| $p_0$     | 0.98 | 8%   | BETA  |
| $T_0$     | 1.13 | 8%   | BETA  |
| $\varepsilon$ | 1    | 1%   | UNIFORM |

**Figure 11.** Pareto front of the ORC nozzle RO. Horizontal arrow: design compared with the deterministic optimization; vertical arrows: recalculated samples.

**Figure 12.** Comparison among baseline and deterministically and robustly optimized shapes. The robust shape is selected from the center zone of the pareto front.

7. Conclusions
A RO has been carried out for an ORC supersonic nozzle with isentropic efficiency as QoI. The efficiency of the optimization procedure with the NSGA has been improved by means of a Kriging
Table 4. Uncertain variables for the ORC supersonic nozzle. Total pressure and temperature are normalised respect to the critical values, $\varepsilon$ is the blade thickness.

| Parameter | Mean | CoV% | pdf   |
|-----------|------|------|-------|
| $p_0$     | 0.98 | 8%   | BETA  |
| $T_0$     | 1.13 | 8%   | BETA  |
| $\varepsilon$ | 1    | 1%   | UNIFORM |

surrogate model coupled with the MOEI technique for an adaptive sampling strategy. The results have been compared with those obtained from a deterministic optimization, showing that the deterministic shape provides a less robust shape. Indeed, the deterministic design exhibits a not negligible sensitivity to the operational and geometrical uncertain variable variations. The RO provides a good compromise between average performance and stability. Besides, the calculation performances of the RO methodology are promising and able to handle the intrinsic high computational cost of dense gas calculations by reducing the number of CFD simulations. Finally, results show that the initial design of the nozzle divergent, based on MOC along with boundary layer corrections, is little modified by both the robust and deterministic optimization, which affect essentially the design of subsonic part.

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