

# Surrogate Based Optimization Techniques for Aerodynamic Design of Turbomachinery

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## Abstract

Recent development of high speed computers and use of optimization techniques have given a big momentum of turbomachinery design replacing expensive experimental cost as well as trial and error approaches. The surrogate based optimization techniques being used for aerodynamic turbomachinery designs coupled with Reynolds-averaged Navier-Stokes equations analysis involve single- and multi-objective optimization methods. The objectives commonly tried to improve were adiabatic efficiency, pressure ratio, weight etc. Presently coupling the fluid flow and structural analysis is being tried to find better design in terms of weight, flutter and vibration, and turbine life. The present article reviews the surrogate based optimization techniques used recently in turbomachinery shape optimizations.

**Keywords:** Turbomachinery, surrogate modeling, optimization, Pareto optimal front, CFD.

## 1. Introduction

Highly complex flow patterns in turbomachinery are being predicted by solving mass, momentum and energy equations and near accurate solutions at an acceptable level are achieved with the aid of modern development of high speed computers and computational methods. On the other hand, implementation of optimization techniques to design of turbomachinery systems has reduced the computational and experimental expenses. The performance of turbomachinery is directly related to reduction of consumption of fuel, mass, vibration, etc. Hence, this article describes shape optimization of turbomachinery blades targeting to enhance the aerodynamic performance and surrogate based approximation models for the optimization.

The turbomachinery designs require enhancement of performance in terms of thermodynamics parameters; efficiency, pressure ratio and structural parameters; noise, vibration, weight, etc. These parameters are considered to be objectives of designs and the geometric parameters as design variables. If the blade geometry is deduced from the objectives, the design is called inverse design. If the geometrical change is used to predict the objectives, the design called direct design. The present article introduces the direct design procedure.

Reynolds-averaged Navier-Stokes (RANS) equations have been effectively used in turbomachinery applications. These equations require turbulence modeling which is used to predict turbulence structures. Different applications of computational codes are being reported considering different grid resolution, numerical algorithm, and turbulence models, etc. Despite the differences which still exist between numerical simulations and reality, it is possible to predict many of the flow characteristics and the losses due to the non-isentropic features of the flow, for example shocks, viscous layers, tip clearance effects, passage vortices, etc. The accurate flow prediction inside a transonic axial compressor rotor using computational fluid dynamics (CFD) is difficult due to its extremely complex features: three-dimensional, unsteady and vortical nature in the blade passage. However, CFD has obvious advantages over the traditional experimental analysis. CFD helps us to analyze the effects of individual feature more easily as compared to the experimental method [1-7]. Review of preliminary design methods has been reported by Casey [4]. Japikse [1] has reported on the developments of 2D and 3D analysis methods in 1976. Different computational methods for viscous and inviscid flow have been reported by McNally and Sockol [3]. CFD methods for turbomachinery design with their advantages and disadvantages have been discussed by Danton and Dawes [5].

The Mathematical and statistical tools for optimization are being used in optimization area in single as well as multi-disciplinary design and optimization area. These tools combined with numerical analysis methods for flow field have reduced the experimental expenses to design turbomachinery blades in recent years. With the development of CFD analysis methods, accuracy

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of prediction for the flow becomes acceptable for the purpose of blade design [8]. The surrogate based approaches are extensively used in the design of structural and multi-disciplinary optimizations. The surrogate models include polynomial response surface approximation (RSA) [9], Kriging [10], and radial basis neural network (RBNN) [11] and, in addition, weighted average models based on global error measures are also implemented in shape optimization and design. Weighted average modeling is an effective approach to employ multiple surrogates, based on the same training data, to offer approximations from alternative modeling viewpoints [12]. Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) [13, 14] developed by Sandia National Laboratory is used for surrogate analysis. The paper [13] presented and compared a number of algorithmic variations for surrogate-based optimization, including approximate subproblem formulations, merit function selections, iterate acceptance logic options, constraint relaxation approaches and convergence assessment techniques. Li and Padula [15] and Quipo et al. [16] analyzed surrogate based optimization methods.

The present article reviews the optimization techniques, especially the surrogate model based techniques for aerodynamic design of turbomachinery. The previous works related to the applications of these techniques are also introduced.

## 2. Numerical Modeling

For steady incompressible turbulent flows, the continuity and Reynolds-Averaged Navier-Stokes equations are represented as follows:

$$\frac{\partial}{\partial x_i}(\rho x_i) = 0 \quad (1)$$

$$\frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \overline{\rho u_i u_j} \right] + \overline{s_i''} \quad (2)$$

where  $u_i$  and  $u_i''$  are mean and fluctuating velocities, respectively. Source term is represented by  $\overline{s_i''}$ . To solve these equations, turbulence closure model for Reynolds stresses is necessary. A variety of turbulence models have been developed so far, and they are classified as lower-order closure models based on eddy-viscosity hypothesis and second-order closure models. The lower-order closure models include zero-equation, 1-equation, and 2-equation models. And, the typical second-order closure model is Reynolds stress model which solves the transport differential equations for Reynolds stress components.

## 3. Optimization Procedure

Optimization is central of any problem involving decision making which entails choosing among alternatives whether in engineering or economics. The measure of goodness of the alternatives is explained by objective functions or performance indexes. Optimization methodology deals with the selection of the best alternative in the sense of the given designs. In general, optimization problem is defined as:

$$\begin{aligned} &\text{Minimize or maximize } f(x) \\ &\text{Subject to } x \in \Omega \quad (\Omega \text{ is subset of } R^n \text{ and is called the constraint set or feasible set.}) \end{aligned} \quad (3)$$

The function  $f: R^n \rightarrow R$  is objective or cost function to be minimized or maximized. The vector  $x$  is an  $n$ -vector of independent variables; i.e.,  $x = [x_1, x_2, \dots, x_n]^T \in R^n$ . The variables  $x_1, x_2, \dots, x_n$  are called decision variables.

The procedure for surrogate based optimizations is presented in Fig. 1. Initially design space is decided and sampling designs in design space are selected by Design of Experiments (DOE) [9]. At next step, the designs are evaluated by RANS solver and single or multi-objective optimizations are performed.

Design space is defined by the lower and the upper bounds of the variables:

$$x_i^l \leq x_i \leq x_i^u \quad (4)$$

The DOE is the sampling plan to select sparsely distributed design points in design space, where the numerical simulations are to be performed to evaluate the objective functions values. These values are then used to construct the surrogate based approximation models. The DOE includes custom design, screening design, response surface design, full factorial design, Taguchi arrays, mixture design, augment design, and sample size and power [17, 18].

### 3.1 Surrogate modeling

In order to evaluate an objective function as a function of design variables, a lot of numerical simulations are required. For most of thermo-fluids problems, however, a single numerical simulation, such as 3D RANS analysis takes long time to complete. Surrogate modeling is introduced to alleviate this burden by constructing approximation models that mimic the behavior of the simulation model as closely as possible while being computationally cheaper to evaluate.

Single as well as multi-objective optimization procedures are implemented in turbomachinery design and optimization. In single objective optimization, surrogate approximation models are used directly while in multi-objective optimization uses genetic algorithm (MOEA) to predict optimum design. The accuracy of the surrogate depends on the number and location of the samples

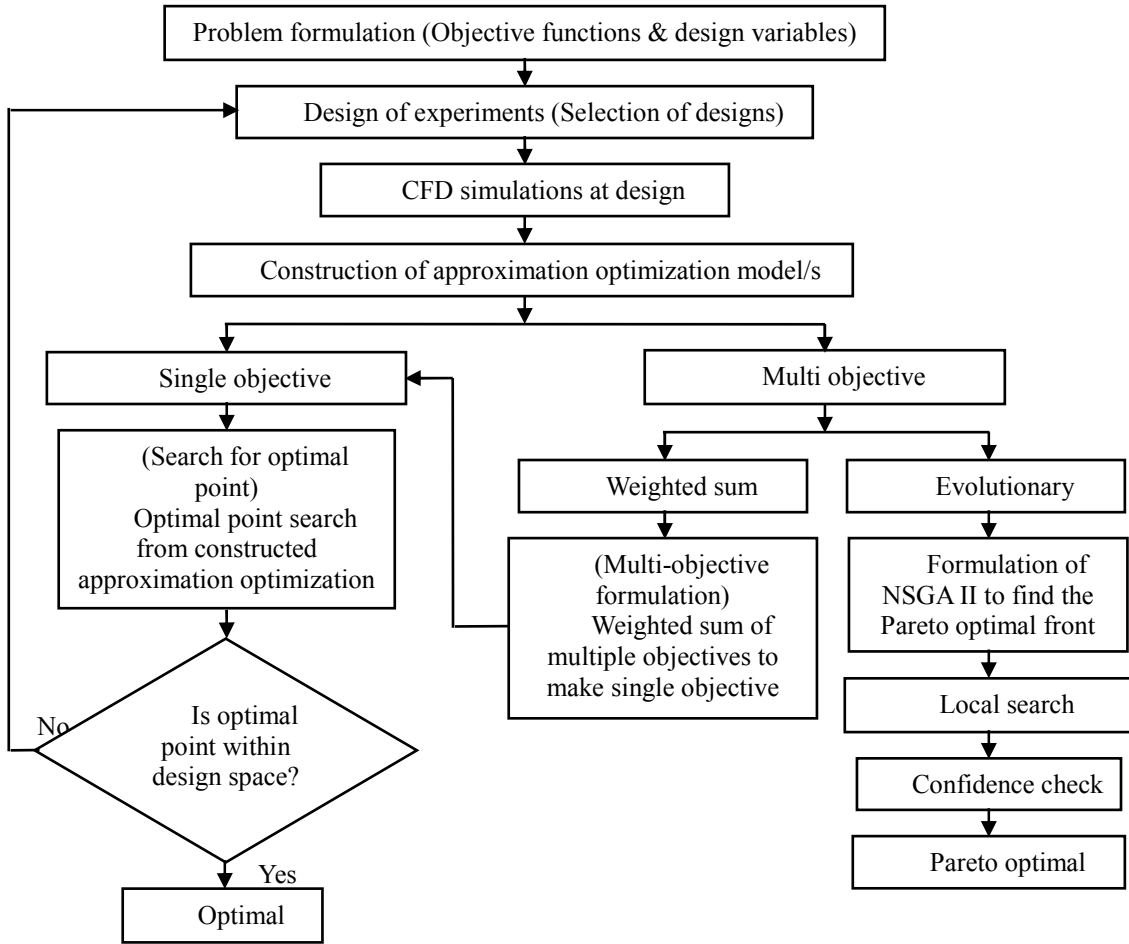


Fig. 1 Optimization procedure

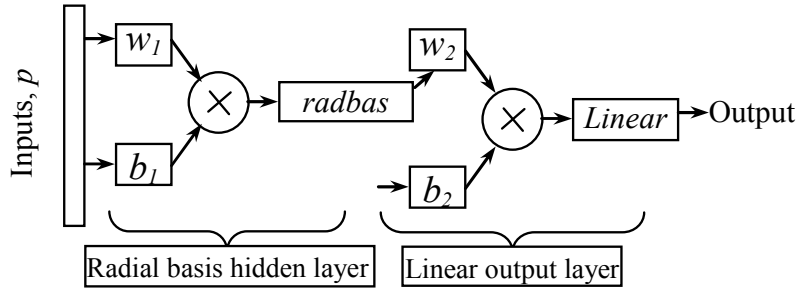


Fig. 2 Radial basis network (single neuron)

in the design space. Various DOE techniques cater to different sources of errors, in particular the errors due to noise in the data or the errors due to an improper surrogate model. Some basic surrogate models are Response Surface Approximation (RSA) [9], Kriging (KRG) [10, 19], Support Vector Machines (SVM) [20] and Radial-Basis Neural Networks (RBNN) [11]. The commonly used basic surrogates are RSA, KRG and RBNN. Recently, Goel et al. [12] proposed some weighted average surrogate models, such as PRESS-Based Averaging (PBA) model. These models are described below.

### 3.1.1 RSA model

RSA is a methodology of fitting a function for discrete responses obtained from numerical calculations. For a second-order polynomial RSA model, the response can be represented by:

$$F(x) = c_0 + \sum_{j=1}^N c_j x_j + \sum_{j=1}^N c_{jj} x_j^2 + \sum_{i \neq j}^N \sum_{j=1}^N c_{ij} x_i x_j \quad (5)$$

where the number of regression coefficients ( $c_i$  and  $c_{ij}$ ) is  $(N+1) \times (N+2)/2$ .

### 3.1.2 RBNN model

The basic concept of RBNN is to simulate human functions of learning from experience, predicting from previous data, etc. The RBNN are two-layered networks with a hidden layer of radial basis transfer function having linear output (Fig. 2). The main advantage of using the radial basis approach is the ability to reduce the computational cost due to the linear nature of the radial

basis functions.

### 3.1.3 KRG model

The KRG method in its basic formulation estimates the value of a function (response) at some unsampled location as a combination of two components, the global model and a systematic departure. Mathematically,

$$\hat{F}(x) = F(x) + Z(x) \quad (6)$$

where,  $\hat{F}(x)$  is the unknown function to be estimated and  $F(x)$  is a known function (usually polynomial) representing the trend over the design space, also referred to as the ‘global’ model. The second part,  $Z(x)$ , creates a localized deviation to interpolate the sampled data points by quantifying the correlation of points with a Gaussian correlation having zero mean and nonzero covariance.

### 3.1.4 PBA model

The predicted response is defined as follows for the PBA model:

$$\hat{F}_{wt.avg}(x) = \sum_i^{N_{SM}} w_i(x) \hat{F}_i(x) \quad (7)$$

where,  $N_{SM}$  is the number of basic surrogate models used to construct weighted average model.  $i^{th}$  surrogate model at design point  $x$  produces weight  $w_i(x)$ , and  $\hat{F}_i(x)$  is the predicted response by  $i^{th}$  surrogate model.

Weights are decided using the guideline that the weights should reflect our confidence in the surrogate model such that the surrogate which produces high error has low weight, and thus low contribution to the final weighted average surrogate, and vice-versa. In this work, global weights are selection using generalized mean square cross-validation error (GMSE) or PRESS (in RSA terminology) that is a global data-based measure of goodness. Generalized mean square cross-validation error calculation procedure is given in the appendix.

The weighting scheme used in PRESS-based averaging surrogate is given as follows:

$$w_i^* = \left( \frac{E_i}{E_{avg}} + \zeta \right)^\kappa, w_i = \frac{w_i^*}{\sum_i w_i^*} \quad (8)$$

$$E_{avg} = \sum_{i=1}^{N_{SM}} \frac{E_i}{N_{SM}}; \kappa < 0, \zeta < 1$$

$$E_i = \sqrt{GMSE_i}, i = 1, 2, \dots, N_{SM} \quad (9)$$

$$GMSE = \frac{1}{k} \sum_{i=1}^k (F_i - \hat{F}_i^{(-i)})^2$$

where,  $\hat{F}_i^{(-i)}$  represents the prediction at  $\mathbf{x}^{(i)}$  using the surrogate constructed with all sample points except  $(\mathbf{x}^{(i)}, F_i)$ . Two constants  $\zeta$  and  $\kappa$  are chosen as  $\zeta = 0.05$  and  $\kappa = -1$  (Goel et al. [12]).

## 3.2 Multi-objective optimization

In multi-objective optimization procedure, two approaches are reported here: (a) weighted-sum-of-objective-functions approach and (b) MOEA approach. Among these weighted sum approach is simplest to use whereas MOEA is based on genetic algorithm.

### 3.2.1 Weighted sum approach

Weighted-sum-of-objective-functions approach [21] which is also known as ‘naïve approach’ is generally used to convert a multi-objective optimization problem to a mono-objective optimization problem. For example, objectives,  $F_1$  and  $F_2$  are linearly combined with a weighting factor;  $w_f$  to constitute a mono-objective,  $F_w$  by naïve approach and the final objective ( $F_w$ ) is defined by

$$F_w = F_1 + w_f F_2 \quad (10)$$

The weighting factor,  $w_f$  is selected as per design requirement. In general, it is the ‘designer’s choice’.

### 3.2.2 Hybrid MOEA approach

Multi-objective approach gives a set of optimal solutions instead of single optimal solution. None of the solutions in this set of optimal solutions can be considered to be better than any other solution with respect to all objectives considered in the problem. These optimal solutions are called Pareto-optimal solutions and their functional space representation is termed as Pareto optimal

front [21]. There are numbers of methods available [21, 22] for solving multi-objective optimization problems but the classical way of tackling multi-objective problems is to convert multi-objective problem into single objective problem. RSA method is applied to get the polynomial equations for each computed objective separately, and these equations are used for multi-objective Pareto optimal front generation. Hybrid MOEA which is used to find Pareto-optimal solutions uses real coded Non-dominated sorting of genetic algorithm (NSGA-II) with local search weighted sum method [22].

#### 4. Objective functions and design variables

Several objectives are being used by the researches such as efficiency, pressure ratio, maximum stress, surge margin, vibration weight, etc. There are hundreds of variables to design turbomachinery blades. Parameterization of blade profile reduces the number of variables and hence reduces the computational costs.

The use of sweep, lean (dihedral), and skew (stacking line in rotational direction) in axial flow compressor rotor has become a matter of interest in the design of turbomachinery blades [23-29]. The blade shape parameters which are used to construct a three-dimensional stacking line is generally introduced to reduce shock losses, corner separation in the blade hub, and tip clearance losses in transonic compressor rotor. For example, Gallimore et al. [23] introduced three-dimensional blade designs using a sweep and a lean in an axial flow compressor rotor for engine. They showed that the positive lean reduced a hub corner and tip clearance losses excepting near the mid-span region. The improvement in the compressor performance as well as the large reduction in the cost and time associated with a rig test was also obtained together with CFD calculations.

The pioneer study on blade sweep in compressors has been done by Bliss [24]. The main objective in this study was to reduce the noise level induced by shock waves. Hah, et al. [25] studied both forward- and backward-swept compressor blades, and showed that a backward-swept blade could suppress the intensity of the shock loss and a forward-swept blade can suppress secondary flow and tip entropy generation. Watanabe and Zangeneh [26] reported that the blade sweep in the design of a transonic turbomachinery blade was an effective parameter to control the strength and position of the shock wave at the tip of the transonic rotors. Denton and Xu [27] investigated the effects of sweep and lean on the performance of a transonic fan, and showed that the stall margin was significantly improved with the forward swept blade although a very little change in the peak efficiency was produced by the blade sweep or lean.

There are a number of studies on the advantages of a skewed rotor. Cai, et al. [28] studied on aerodynamic and aero-acoustic characteristics of an axial flow fan with skewed blade. With the reduction of a secondary flow and the thickness of a rotor wake, they could reduce a broadband noise. Fischer, et al. [29] observed the effect of bowed stators on the performance of a compressor, and showed that the separation was reduced in the bowed stator leading to increase in the stagnation pressure ratio and efficiency.

Cubic spline and Bazier curve based parameterizations have helped to reduce the design variables to modify the camber line and aerofoil profiles [30-39].

#### 5. Applications of surrogate based optimization methods

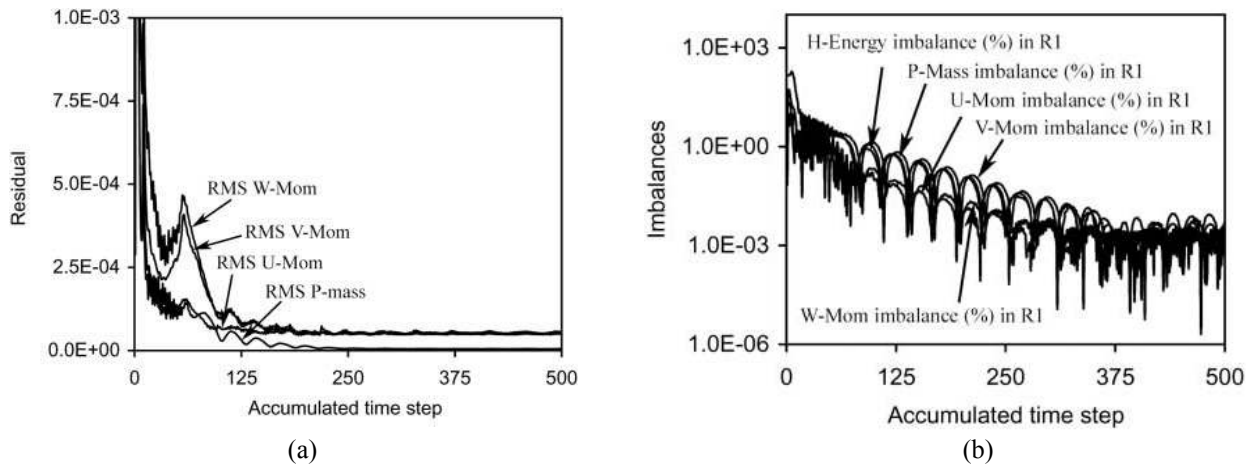
A set of papers [40-81] contributed to single and multi-objective optimizations of turbomachines to enhance their performances. It has been reported that the efficiency is increased due to movement of separation lines towards downstream direction reducing the separation vortex, end-wall losses, etc. These papers describe the blade shape optimization considering stacking line modification in terms of sweeping, leaning or skewing and airfoil shape modification in terms thickness, leading edge, trailing edge modification etc.

RSA model [9] has been widely used as a tool of design optimization for turbomachinery. This is one of the simplest surrogate model, which utilizes information collected from various sources and by different tool. Thus, this method is effective for both of single- and multi-disciplinary optimization problems [40-44].

Multi-disciplinary and multiple operating point optimizations at fixed rotor rotational speed were reported by Pierret et al. [38]. Oyama et al. [63] reported blade profile modification with the help of B-spline curve of NASA rotor 67 to increase adiabatic efficiency by 2%. Chen et al. [69] optimized camber line, thickness distribution and stacking line by polynomial curve to define compressor blade and gained 1.73% improvement of adiabatic efficiency. Maximum camber location effect was studied by Chen et al. [69]. Benini [53] defined blade section profiles by Bezier curve using multi-objective optimization considering total pressure ratio and adiabatic efficiency as objectives for design of a compressor blade. He employed camber line and thickness profile as design parameters. Keskin and Bestle [39] reported Bezier curve parameterization of blade shape to optimize with Pareto optimal design. Optimization of controlled diffusion compressor blade has been reported by Sanger [82].

Queipo et al. [16] and Li and Padula [15] reviewed various surrogate based models used in aerospace applications. Shyy et al. [83] presented global optimization model applying in rocket propulsion design. Zerna et al. [84] developed weighted average surrogate model for alkaline-surfactant-polymer flooding processes design using different surrogates through pointwise error estimation. Goel et al. [12] developed weighted average surrogate models using global data based error and concluded that the weighted average surrogate models provide more reliable prediction method than individual basic surrogates, such as RSA, KRG, and RBNN. Goel et al. [85] and Samad et al. [78, 86] reported on the performances of several surrogate models in several applications, and presented that weighted average surrogate models developed by Goel et al. [12] are reliable in prediction.

Engineering design generally involves multiple disciplines and simultaneous optimization of multiple objectives related to each discipline. These design problems usually known as multi-objective problems require simultaneous consideration of all objective functions to optimize the system. There are numbers of solution methods and algorithms available for solving multi-objective optimization problems [21, 87-91]. In multi-objective optimizations of turbomachinery blade, efficiency, total pressure, static pressure, pressure loss, weight, stress, etc. are used as objectives, and variables related to camber profile and/or stacking line of blade are employed as design variables [35, 39, 42, 51, 57, 70-72, 76, 79]. A multi-objective optimization problem consists of many optimal solutions called Pareto-optimal solutions; therefore a designer's aim is to find as many optimal solutions within the design range as possible. This helps designer to find a global Pareto-optimal front. Each design set corresponding to optimal solution represents a compromise of design objectives. Elitist Non-dominated Sorting Genetic Algorithm (NSGA-II) given by Deb



**Fig. 3** Convergence plots: (a) residual history; (b) imbalances [77]

[22] generates Pareto optimal solution using evolutionary algorithm.

The turbomachinery design and optimization is based on reliability in flow solver, suitable cost function selection and use of practicable search algorithm. The above discussion shows the recent ample efforts of optimization to optimize blade shape of turbomachines have been made. The optimization was performed on the basis of two ideas: (1) the automated design optimization [33, 34, 50 and 52, 92] and (2) CFD simulation and optimization analysis separately [77-81]. As CFD computation takes heavy computational cost, the effort has been made to reduce number of simulation by reducing number of objectives.

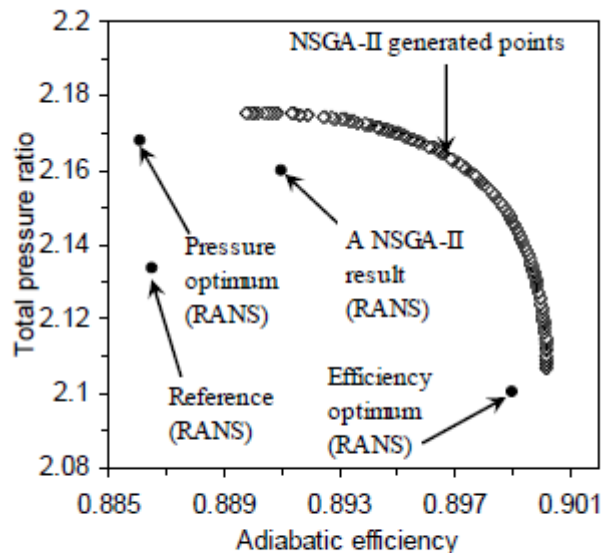
Axial compressor blade shape optimization was performed and reported in literatures [77-81]. The main problem occurs in flow simulation in turbomachinery blade in the proper convergent solution [77]. The Axial transonic blade simulation convergence is shown in Fig. 3 for simulation in Ansys-CFX 11.0 [93] software with 300 000 nodes. Proper grid resolution is also important. This can be performed by grid independency test and comparing with experimental result.

Design space is defined by the lower limit and upper limit of design variable and suitable initial guess of these values helps to reduce the iteration run of optimization [81]. Proper selection of design points in design space is also important. The optimum design should not produce at unsampled location of design space else a higher uncertainty in prediction will be produced [78]. To reduce the uncertainty, multiple surrogate based analysis is suggested because the same set of data can produce different optimum point. PBA surrogate is robust and produce comparative reliable prediction of optimum point [78].

Single objective based optimization gives improvement of one objective and other objective values may reduce. Hence the multi-objective optimization was suggested by Samad and Kim [79]. Multi-objective optimization via Pareto optimal design gives all the objectives considered improved. The axial compressor blade optimization to enhance its efficiency and total pressure ratio was performed by these authors is given in Fig. 4. This figure shows multi-objective optimization produce both the objectives have improved by 0.51 and 1.25%, respectively, while the single objective optimization has failed to improve the both the objectives at the same time.

## 6. Conclusions

The optimization techniques for turbomachinery blades have been reviewed in the present article. Single- as well as multi-objective techniques with three-dimensional Navier-Stokes analysis have been introduced. The RSA, Kriging, RBNN, and weighted average surrogate models are being used for different applications for turbomachinery design optimizations to improve their performances. The genetic-algorithm based optimization methods are widely used for multi-objective as well as multi-



**Fig. 4** Single- and multi-objective optimization [79]

disciplinary optimization methods. The conclusions can be made:

- a) The different blade geometry modification techniques show the reduction of variables to reduce the number of computational runs. Parametric modification of turbomachinery blade gives less number of design variables. A proper convergence of CFD equations is important.
- b) Suitable guess of design space reduces the number of optimization iteration. Proper selection of design points in design is important to reduce uncertainty in prediction.
- c) Multiple surrogates modeling is suggested as this uses same computed results to find different optimum points. Weighted average surrogates have the better prediction capability.
- d) Multi-objective optimization methods can be used if the system contains multiple objectives. This gives simultaneously improvement of all the objectives.

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## Nomenclature

$c$	Regression coefficient	ANN	Artificial neural network
$F$	Objective function	CFD	Computational fluid Dynamics
$F_w$	Combined objective in weighted sum of objectives	DOE	Design of experiments
	model	GMSE	Generalized mean square error
$N_{SM}$	Number of basic surrogate models	KRG	Kriging
$P$	Pressure	LHS	Latin hypercube sampling
$T$	Temperature	MOEA	Multi-objective evolutionary algorithm
$U$	Velocity	NSGA	Non-dominated sorting genetic algorithm
$W$	Weight for PBA model	PBA	PRESS based averaging
$x$	Variables	POF	Pareto optimal front
$w_f$	Weighting factor	PRESS	Predicted error sum of squares
$\xi, \kappa$	Constants of PBA surrogate model	RANS	Reynolds average Navier-Stokes
$\rho$	Fluid density	RBNN	Radial basis neural network
		RSA	Response surface approximation

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