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Inverse Design of Functional Surfaces through Low Fidelity Modelling

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Abstract :

Functional surfaces are extensively being designed for specific purposes within various industries. The inspiration for many of such surfaces has been derived from biological entities such as shark skin etc. In industry, various surfaces are created by physio-chemical properties of materials with appropriately aligned micro and nanostructures, and sophisticated solutions are found for range of problems. Many drag reducing organisms employ functional surfaces that control near-wall flow characteristics thus affecting their global flow performance. This study focuses on the inverse design of functional surfaces for targeted global flow related effects. At its core, the discussed methodology embeds low fidelity model for surface and corresponding flow events. Desired geometrical parameters are iteratively solved to achieve target flow characteristics.

Mots clefs : Proper Orthogonal Decomposition (POD), Gappy POD, Inverse Design, Functional Surfaces.

1 Introduction

Nature inspired designs potentially offers optimised and innovative solutions for engineering problems. Shark skin, pangolin, lotus leafs, springtails, dessert beetles, moth, butterfly etc. are known to inspire solutions for well-known engineering problems of friction, wettability and reflectively. Riblets discovered on shark skin aided drag reduction [1, 2]. Soil borrowing pangolin has scaled surface to reduce abrasive wear [3]. Lotus leaf employs superhydrophobic surface to keep surface dry and clean. Camouflaged Glasswing butterfly wings embed antireflective functional surface [4]. Moth's eye has antireflective surface with fine array of structures [5].

Extensive literature is available on the application of nature inspired designs. Varanasi et al. [6] employed nanograss and micropillars to enhance critical heat flux of industrial boiler. Study also reported that nanopillars, when applied on top of micropillars, decreased liquid-solid contact angle. Elyyan [7] conducted DNS and LES studies on heat transfer enhancement of dimpled and protruded fins. Larger fin pitch observed higher heat transfer enhancement. In the same study, perforation introduced inside imprint encouraged mixing and enhanced heat transfer.

Numerical simulations have been extensively used to device innovative solution strategies for industrial design. As a result, data driven fluid flow system design has become focal point with increase in computing power. The process to improve on design requirement by optimising given aerodynamic shape within computational manifold is termed as Aerodynamic Shape Optimization (ASO). ASO framework integrates fluid flow model evaluating aerodynamic shape performance subject to flow field or geometric constraints. Additionally, framework embeds mathematical scheme to describe aerodynamic shape with the help of design variables. Numerical optimisation algorithm perturbs design variable resulting in aerodynamic surface change. Fidelity of ASO based results depends on modular components of the framework. For example, high fidelity model capturing true flow physics is important to produce desirable aerodynamic design.

In inverse design methodology, surface characteristics results from specified target flow field. Established iterative process maps changes in flow field to geometry. Under each iteration, developed low fidelity model computes flow characteristics at much lower computational expense. Low fidelity models are types of reduced order models derived by projecting partial differential equation (PDE) solutions on to reduced space spanned by orthogonal basis. This particular method termed as "snapshot method" uses sets of instantaneous flow solutions to compute modes by Proper Orthogonal Decomposition (POD). Derived reduced order model for unsteady aerodynamic application [6-9] have applied this method of snapshot.

POD also sometimes known as principle component analysis, computes empirical orthogonal mode. These modes describe dominant features present within dataset. Variety of applications such as image processing [8], inviscid airfoil design [9] and computation of reduced order dynamic system [10] have previously utilized POD. Everson and Sirovich [11] extended and applied modified POD method to handle incomplete dataset. Termed Gappy POD, the modified version reconstructs incomplete data sets by solving linear system of equations. Wilcox et al. [12] adopted this method to handle incomplete aerodynamic data and inverse design problem. In this manuscript inverse design of functional surface for targeted near wall flow characteristics is described.

2 Proper Orthogonal Decomposition

POD is procedure by which optimal linear basis are obtained to reconstruct original multidimensional data. This reconstruction reduces the order of system from large number to approximate its dynamic behaviour by small number of basis. Basics of POD is briefly summarized. A finite dimensional representation of function u(x) is sought in terms of basis vectors phi(x) as follows:

$$u_M = \sum_{j=1}^{M} a_j \varphi_j(x) \tag{1}$$

Basis are computed from the ensemble of N empirical PDE solutions denoted by $\{u^k\}$. Choice of $\{\varphi_j(x)\}_{j=1}^{\infty}$ is made such that these basis best describes the functions within the ensemble $\{u^k\}$. In other words, the average inner product between the field and the basis is maximised as follows:

$$\max \frac{\langle |u,\varphi|^2\rangle}{\|\varphi\|^2} \tag{2}$$

Here, denotes and denotes the L2 norm. This can be solved by calculus of variations in which $\langle |u,\varphi|^2\rangle$ is maximised subject to constraint $\|\varphi\|^2$=1. Subject to some algebra [10], the basis function that are being sought should satisfy following equation:

$$\int \langle u(x)u(x')\rangle \varphi(x')dx' = \lambda\varphi(x) \tag{3}$$

where λ is a Lagrange multiplier. Hence eigenfunction φ_j of above equation is sought whose kernel is an average autocorerelation function $\langle u(x)u(x')\rangle = R(x,x')$. When ensemble of functions $\{u^k\}$ becomes collection of finite N-dimensional vectors, autocorrelation function becomes autocorrelation tensor. The integral eigen value problem reduces to:

$$R\varphi = \lambda\varphi \tag{4}$$

The basis vectors and corresponding eigen values are hence computes from above problem yielding the expansion of original function:

$$u(x) = \sum_{j=1}^{\infty} a_j\varphi_j(x) \tag{5}$$

For fluid flow problems, eigenvalues represent energy contain within corresponding modes. The ensemble could represent snapshots of various flow variables obtained via experiments or expensive computation. Thus, ordering of eigenvectors as per corresponding eigenvalues computes truncated model of the flow variable.

Gappy POD is an extension of existing POD for missing data reconstruction. The first step is 'data masking' that for a particular flow vector describes where data is available and where it is missing. For a flow snapshot U^k, mask vector is defined as:

$$n_i^k = 0 \quad \text{if } U_i^k \quad \text{is unknown}$$
$$n_i^k = 1 \quad \text{if } U_i^k \quad \text{is known}$$

Here U_i^k denotes the ith element of snapshot vector U^k. To start the process, zero values are assigned to the missing elements in vector U^k. A pointwise multiplication is defined as $(n^k, U^k)_i = n_i^k U_i^k$. A Gappy inner product is hence defined as $(u,v)_n = [(n,u),(n,v)]$, while the induced norm is $(\|v\|_n)^2 = (v,v)_n$.

For a completely known snapshot set $\{U^i\}_{i=1}^m$, let $\{\Phi^i\}_{i=1}^m$ be the POD basis. Consider g to be another solution vector that has some elements missing with corresponding mask vector n. Assuming that behaviour of vector g can be described by existing snapshot set, a complete reconstruction of incomplete g can be represented in terms of p POD basis as:

$$\tilde{g} \approx \sum_{i=1}^{p} b_i\Phi^i \tag{6}$$

Here $\tilde{g}$ is intermediate repaired vector. POD coefficients b_i are computed by minimising error E between original and repaired vectors using gappy norm so that only original existing elements in g are compared :

$$E = \|g - \tilde{g}\|_n^2 \tag{7}$$

By differentiating above equation w.r.t coefficients b_i to minimise error E leads to linear system of equations

$$Mb = f \tag{8}$$

Here $M_{ij} = (\Phi^i, \Phi^j)_n$, and $f_i = (g, \Phi^i)_n$. By solving above equations, coefficients can be obtained to repair intermediate repaired vector $\tilde{g}$. To apply gappy POD for inverse design problem, the snapshots are redefined. Rather than containing only flow characteristics, each snapshot is augmented to contain surface parameter. This methodology is adopted to obtain surface parameters based on the mean velocity profile supplied.

4 Results and Discussions

Application of gappy POD to the inverse design problem is considered. The flow solutions to construct a database is obtained from high fidelity Lattice Boltzmann Method (LBM). A standard grid of 100x100 lattice units has been considered with bounce-back condition for wall. The aim of gappy POD is then to produce functional surface design parameters that dictates target near wall flow characteristics that is not contained within the snapshot collection.

Figure 1 shows mean velocity profile at different design points. Frictional velocity corresponding each design is used to obtain non-dimensional form of mean velocity profiles. Here elemental viscous scaled spacing and height for different functional surface is $s^+ = sU_\tau/\vartheta$ and $h^+ = hU_\tau/\vartheta$ respectively (U_τ = frictional velocity; ϑ = viscocity). Inverse design is based on the ensemble of these velocity profiles.

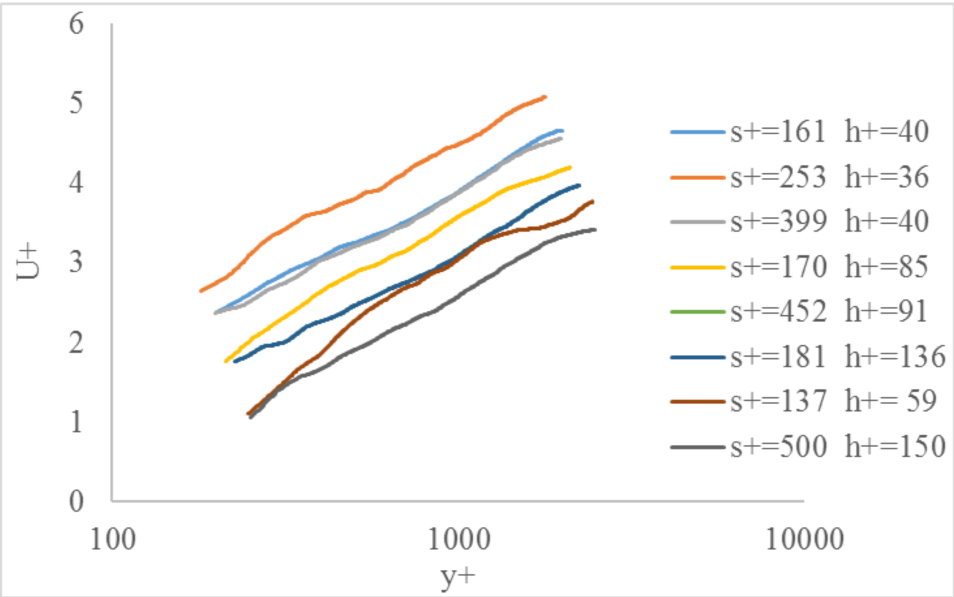

Figure 1. Mean Velocity profiles for different designs.

Figure 2 shows the mean velocity profiles that formed an input to gappy POD inverse design process. These inputs are formed by averaging two distinct velocity profiles from the ensemble. Figure 3 shows the obtained inverse designs for three different mean velocity profile input. It can be seen the Sx+ obtained by inverse design process showed a difference of 5% with that is obtained from high fidelity LBM simulations. About 7% difference is noted between the h+ obtained from inverse design and LBM simulation.

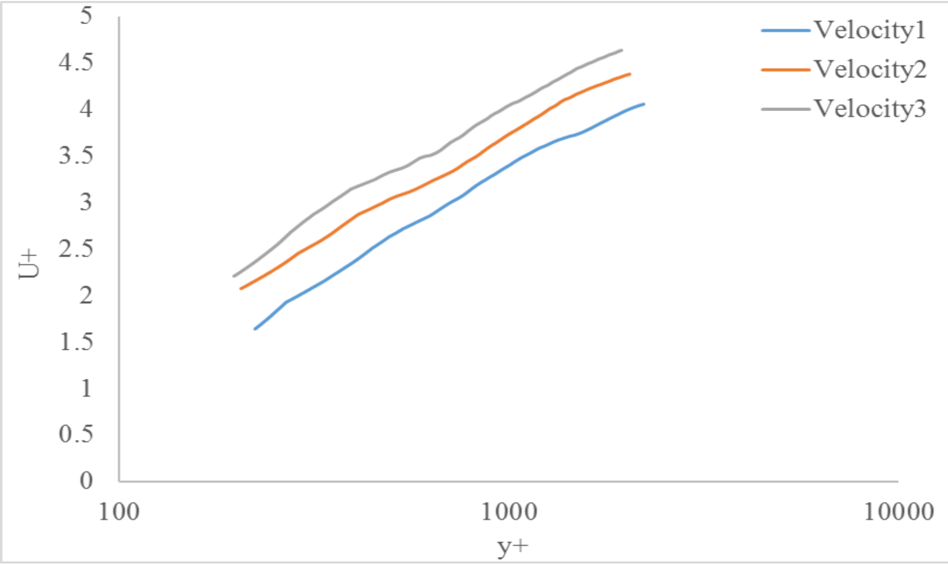

Figure 2. Mean Velocity Profile Input.

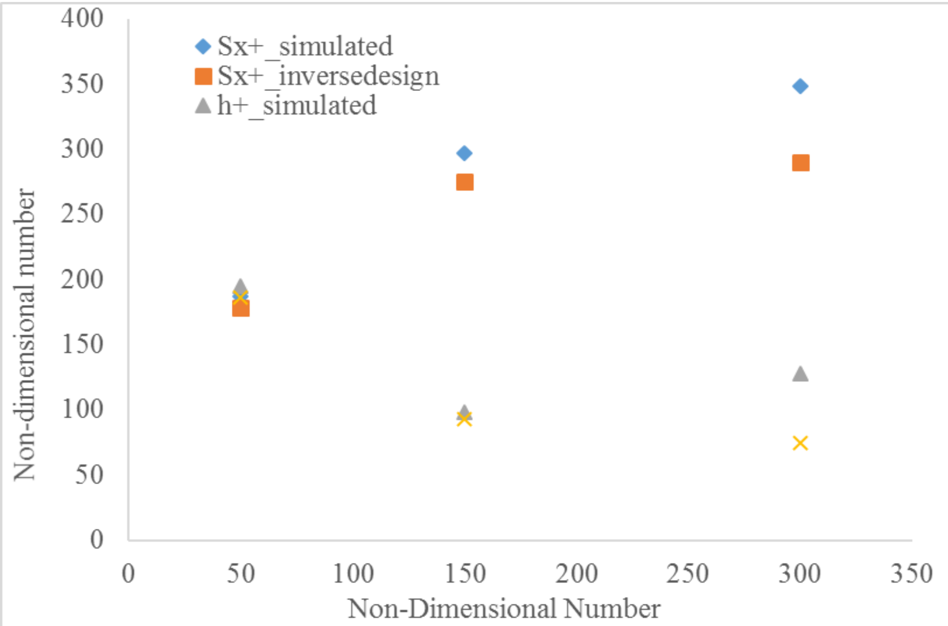

Figure 3. Design Comparision.

Figure 4 shows the mean vecoity profile obtained at the end of inverse design process. As can be seen from the figure, the obtained velocity at the end of inverse design is well correlated with that of target profile. Table 1 shows the corresponding gappy normal error from the inverse design process. It can be seen that Velocity1 has the highest gappy normal error as a target velocity profile.

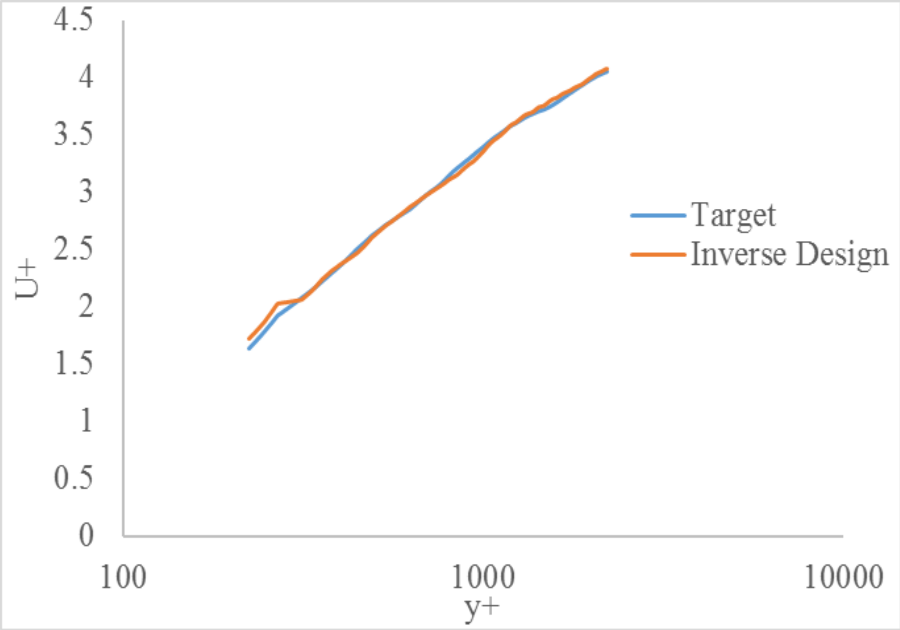

Figure 4. Mean velocity comparision.

Table 1. Gappy nomral error for different mean velocity input.

Velocity	Gappy Error (E)
Velocity1	0.9428
Velocity2	0.3167
Velocity3	0.4764

5 Conclusions

Low fidelity based inverse design process is introduced for functional surface. The process of inverse design is converted into a problem 'missing data' within an ensemble. Ensemble is further expressed in terms of orthogonal basis. The 'missing data' is reconstructed by combining linear basis with appropriately computed coefficients. The propsed method shows a good accuracy of inverse design process for functional surface. The proposed method obtained design parameters within 6% for most of flow range.

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