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Abstract. *In this paper, we propose a simultaneous meta-modeling protocol for both input and output spaces. We perform a reparametrization of the input space using constrained shape interpolation by introducing the concept of an α-manifold of admissible meshed shapes. The output space is reduced using constrained Proper Orthogonal Decomposition. By simultaneously using meta-modeling for both spaces, we facilitate interactive design space exploration for the purpose of design. The proposed approach is applied to several industrial problems.*

Keywords: manifold learning; design; reduced order model; optimization; high performance computing

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1 INTRODUCTION

When "high fidelity" computer simulations (finite elements, finite volumes, etc.) are used for calculating the objective functions and nonlinear constraints in the process of optimizing mechanical systems, the CPU time frequently becomes disproportionately large. This brought about a need for efficient surrogate-based methods in design optimization. A popular physics-based meta-modeling technique consists of carrying out the approximation on the full vector fields using Proper Orthogonal Decomposition (POD) and Galerkin projection.
However, this still requires manipulation of the input variables $\bar{V}$. Now for complex shapes the dimensionality d can be very high and can greatly exceed the *intrinsic dimensionality* of the design problem. Another far more serious implication is the generation of inadmissible/infeasible structural shapes, which could eventually lead to crashes of either the mesh generator or the solver. This is due to the difficulties in expressing all the technological and common sense constraints needed to convert a set of geometric parameters to an admissible shape. A final inconvenience is that gradients/sensitivities need to be calculated using either finite differences or the Adjoint method. All these are impediments to truly non-intrusive optimization using a clearly separated *offline/online* approach that would allow for interactive design using, for example, a tablet PC.
A good input-space meta-model needs to be capable of interpolating between admissible instances of the shape representation used to detect the problem dimensionality and generate feasible solutions by design.
In this paper, we develop an approach that builds up a design space by *learning* using *shape interpolation* between shape/mesh instances given by a sequence of parameter values. For this we introduce the concept of the α-manifold. The output space (physics) is modeled using constrained Proper Orthogonal Decomposition giving the smallest set of coefficients $\beta_1 ... \beta_m$ needed to conserve *linear* objective and constraint functions. The POD coefficients for the shape *and* physics are then analyzed *together* to get the local parametric expression for both α's as well as β's in the neighborhood of the evaluation point.
In addition, our approach gives an elegant, practical and straightforward method to compute the so-called "shape derivatives" of the performance objective(s), which are increasingly popular as used in "shape calculus".

2 META-MODELING FOR BOTH SPACES

2.1 Output Space ROM

The POD Reduced Order Model (ROM) strategy for the output space approximates a physical field $\bar{v} \in \mathcal{R}^n$ in the vicinity of the current iteration point $\bar{V} \in \mathcal{R}^d$, where n is typically the size of a FE/CFD mesh/grid, and d is the design space dimensionality. The field vector $\bar{v}(\bar{V})$ may then be approximated around the nominal value $\bar{v}_0$ using a basis $\Psi = [\bar{\psi}_1 ... \bar{\psi}_M]$, typically obtained using a set of *a priori* computer experiments $\bar{V}^{(1)} ... \bar{V}^{(M)}$ using Design of Experiments techniques, or others. This is followed by calculating the projection coefficients i.e. β's.
The reduced-order model is then built either by interpolation of Ψ or by interpolation of the projection coefficients β's using kriging/Radial Basis Functions. Assuming that only the β's depend on the $\bar{V}$ and that Ψ is constant for the design problem, followed by truncating the basis Ψ to a small number ($m << M$) of highly energetic modes, we get

$$\bar{v}(\bar{V}) \approx \tilde{v}(\bar{V}) = \bar{v}_0 + \sum_{1}^{m} \beta_i(\bar{V}) \bar{\psi}_i. \tag{1}$$

Since $\bar{\beta} = \bar{\beta}(\bar{V})$ we need to manipulate the vector of design variables $\bar{V}$ either *after* optimization to verify the design or during the optimization/design to verify intermediate solutions. But as mentioned in the introduction working with $\bar{V}$ can lead to issues like inadmissible geometries (infeasible $\bar{V}$) and thus CAD failures and frequently an elevated problem dimensionality, all of which are even more troublesome when using the meta-model in a non-intrusive procedure.

2.2 Input space ROM

We therefore seek to meta-model the *input space*, in other words the *structural shape* Ω itself in a POD-like manner in order to *implicitly* guarantee admissibility in β-space AND limit the dimensionality *while performing the design*. An ideal representation of Ω for this purpose is by using the shape indicator function χ (written in discrete form as a vector). Let $\chi \in \mathcal{S}$ where $\mathcal{S}$ represent the subspace of admissible shapes for a given design problem. We will represent $\mathcal{S}$ by a smooth manifold in the shape space of the design problem.
To get this shape space, we first perform POD on a sample set of M neighboring admissible shapes ($\chi^1..\chi^M$), giving us a set of projection coefficients allowing us to express any χ^i in terms of the eigenvectors $\bar{\phi}_j$ of C_v where $M << N_c$ = number of snapshots, χ^i = i^{th} individual snapshot and χ_0 is the mean snapshot.

$$\chi^i = \chi_0 + \sum_{j=1}^{M} \alpha_j^i \bar{\phi}_j \tag{2}$$

and obtain a set of M projection coefficients α_j^i for the i^{th} snapshot.
Instead of truncating the vector basis in the usual manner, we then analyze the relationship between these projection coefficients giving us a manifold of admissible shapes (in point-set form). We then detect the dimensionality of this manifold by calculating the covariance matrix of the neighborhood, and perform interpolation on this local manifold using the Diffuse Approximation.
The α-manifold (figure 1) then represents the *inter-relationship* between the α-coefficients by a p-dimensional manifold in $\mathcal{R}^M$ space where $p < M$ [1].

$$\mu(\alpha_1 .... \alpha_M) = 0 \tag{3}$$

and *implicitly* represents all the technological/shape admissibility constraints on the structural shape χ. It thus approaches the true shape space for a given design problem and captures its intrinsic dimensionality ($p \leq d$) [2].
The shape manifold has two important properties:

1. All points on the manifold correspond to admissible shapes (i.e. level set functions)
2. Any point that lies outside the manifold corresponds to a NON admissible shape for the given problem.

The dimensionality $p \leq M$ can easily be estimated using the Fukunaga-Olsen algorithm [5].
Finally we move along the manifold by interpolating between snapshots in a local neighborhood using a local coordinate system $t_1...t_p, h$ where the manifold is given locally by $h = h(t_1...t_p)$. These local co-ordinates $t_1...t_p$ are found by calculating the eigenvectors of the covariance matrix for the local neighborhood

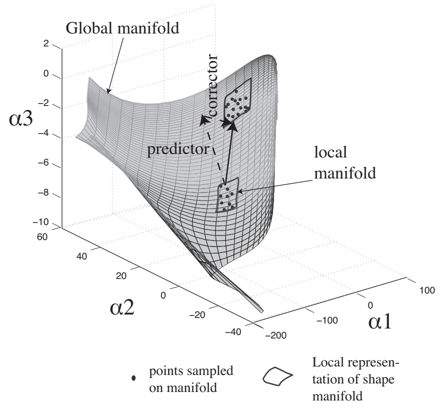

Figure 1: Shape manifold and local diffuse approximation

2.3 Combined input/output meta-modeling

The general approach to simultaneous reduction of both spaces of the design problem is shown in figure 2 with the input space meta-model on the left hand side, and the output space meta-model on the right.

The final step for the simultaneous meta-modeling is to obtain the relationship between the POD coefficients for

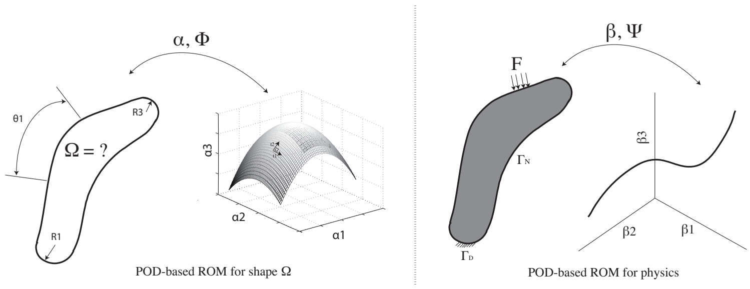

Figure 2: Basic idea of interactive design/optimization

shape (α's) and those for the physical fields (β's). This can be easily obtained using:

$$\bar{\beta} = \bar{\beta}(\bar{\alpha}) = \bar{p}(\bar{\alpha})^T \bar{a} \tag{4}$$

and a polynomial Response Surface.

3 APPLICATION TO PROBLEMS IN MECHANICS

The approach has been successfully been applied to three different problems in computational mechanics:

1. Reduction of dimensionality in design optimization [1, 2, 6]
2. Numerical springback assessment for metal forming [3]
3. Reduced order modeling of material microstructures [4]

Here we show only the first application using an engine intake pipe as a test-case (figure 3 and figure 4). The structural shape is very complex parameterized by using 93 bounded geometric design variables in CATIA, involving an exorbitantly high CAD failure rate of over **60%**:

4 CONCLUSIONS

We introduce a unified meta-modeling scheme intended for use in interactive design or design space exploration in shape optimization. The key contribution is a meta-model for the input space based on constrained shape interpolation using the manifold of admissible shapes in the shape space for a given design problem. This is combined with a

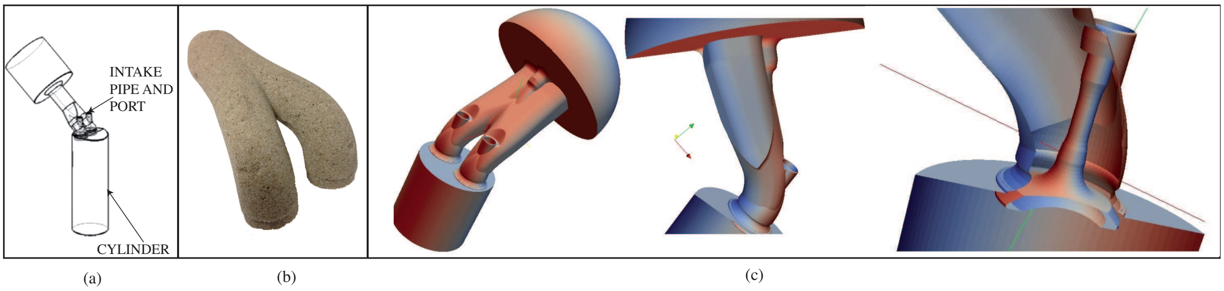

Figure 3: (a) Full system (b) Sand model of intake pipe (c) External & internal details of engine intake

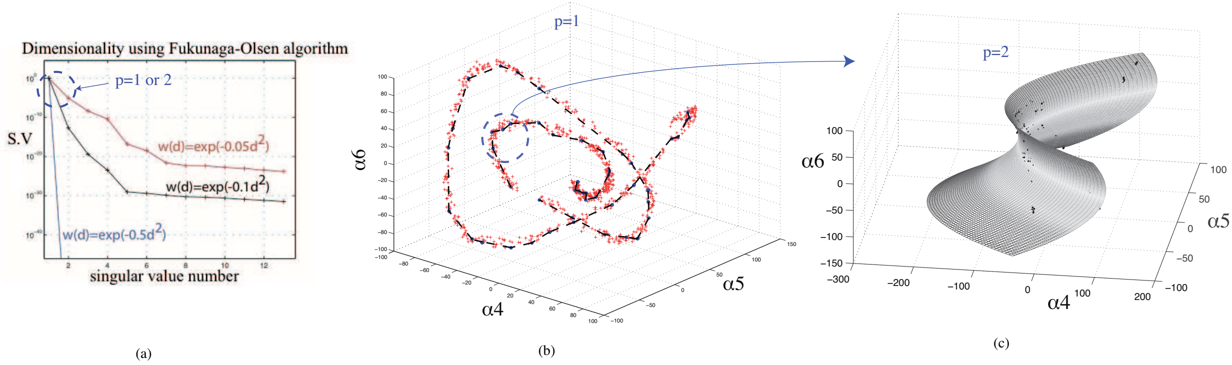

Figure 4: (a) Dimensionality p calculation, (b) Constrained shape interpolation using $p = 1$, (c) α-manifold approximation using $p = 2$ (normalized)

constrained POD meta-model for the output space (physics) using a predictor-corrector algorithm. Interpolation in shape-space (instead of geometric) yields the minimum possible system dimensionality while guaranteeing that we remain in the feasible region (the α-manifold).

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