Airfoil Design Optimization Using Reduced Order Models Based on Proper Orthogonal Decomposition

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Motivation

• There is a need for high-fidelity models in the multidisciplinary design and optimization of aerospace systems, but the computational cost is extremely high.

• To be computationally feasible the order of the models may need to be reduced in some situations (e.g. aeroelastcs system with millions of degrees of freedoms) while retaining nice properties - accuracy, equivalence in the limit of large numbers of modes, etc.

• We are investigating POD as an alternate means to form approximate, reduced order models for use in the design environment.
Motivation (cont.)

• Our final goal is to develop a truly multidisciplinary design environment encompassing aerodynamics, structures, propulsion, mission performance, etc., with acceptable computational costs at a higher level of fidelity than is currently possible.

• We are initially investigating POD based models for use in Aerodynamic Shape Optimization (ASO) problems - the parameterization of a surface and the necessary changes to achieve an optimum behavior.

• In theory, within this framework, POD based models can be used both to eliminate system analysis and as a way to compute sensitivities.

• In this work, we have explored both uses of the POD.
Proper Orthogonal Decomposition (POD)

- POD has its roots in statistical analysis and has appeared with various names, including: principal component analysis, empirical eigenfunctions, Karhunen-Loéve decomposition, and empirical orthogonal eigenfunctions.

- POD has been used in a variety of disciplines such as fluid mechanics, image processing, signal analysis, and control in chemical engineering.

- Typically, POD modes have been used to simplify the full Navier-Stokes equations for purposes of turbulence research and modeling, Holmes et. al (1998).

- Rediniotis et. al. (1999) used POD to construct reduced order models of synthetic jet actuators for flow control.
**POD Theory**

- We are seeking representations of a function, $u(x)$, in terms of a basis $\{\varphi_j(x)\}_{j=1}^{\infty}$ which allows an approximation to $u$ to be constructed as

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

- We would like to choose $\{\varphi_j(x)\}_{j=1}^{\infty}$ so that these basis functions describe the functions in the ensemble $\{u^k\}$ better than any other linear basis, which may be expressed mathematically as

$$\max_{\varphi} \frac{\langle |(u, \varphi)|^2 \rangle}{\| \varphi \|^2}$$  \hspace{1cm} (2)
POD Theory (cont.)

• We have a problem of calculus of variations in which we would like to maximize $\langle |(u, \varphi)|^2 \rangle$ subject to the constraint that $\|\varphi\|^2 = 1$. This is a constrained optimization problem where the function to be maximized is given by

$$J[\varphi] = \langle |(u, \varphi)|^2 \rangle - \lambda(\|\varphi\|^2 - 1),$$

where $\lambda$ is a Lagrange multiplier.

• A necessary condition for an extremum of this cost function is that for all variations $\varphi + \delta \psi, \delta \in \mathbb{R}$, the following expression must hold

$$\frac{d}{d\delta} J[\varphi + \delta \psi]|_{\delta=0} = 0$$
• From Eq. 3 and for real functions $u$, $\varphi$, and $\psi$, we have that

$$\frac{d}{d\delta} J[\varphi + \delta \psi]|_{\delta=0} = 2[\langle(u, \psi)(\varphi, u)\rangle - \lambda(\varphi, \psi)] = 0$$

• With some amount of algebra and since the function $\psi$ can be chosen arbitrarily, it can be shown that the basis functions we are seeking must satisfy

$$\int_{\Omega} \langle u(x)u(x')\rangle \varphi(x')dx' = \lambda \varphi(x) \quad (4)$$
POD Theory (cont.)

- The optimal POD basis that we were seeking is composed of the eigenfunctions \( \{ \varphi_j \} \) of the integral equation (4), whose kernel is the averaged autocorrelation function \( \langle u(x)u(x') \rangle = R(x, x') \).

- For the finite dimensional case the ensemble of functions \( u^k \) becomes a group of \( N\)-dimensional vectors and the autocorrelation function transforms into the autocorrelation tensor given by \( R = \langle u \otimes u \rangle \).

- In finite-dimensional spaces, the integral eigenvalue problem becomes

\[
R\varphi = \lambda \varphi.
\]
• The member functions/vectors of the ensemble can now be decomposed as follows

\[ u(x) = \sum_{j=1}^{\infty} a_j \varphi_j(x). \] (5)

• The main advantage of the POD is that it produces the best linear representation for an ensemble of functions or flowfields (snapshots).

• However, when used in the reconstruction of non-linear problems, the level of accuracy is only guaranteed in the limit of large numbers of modes.
• Even in the event that a small number of modes is necessary, we still have to solve an eigenvalue problem of order equal to that of the original problem. This could be mitigated by using iterative techniques to find the eigenvectors corresponding to the largest eigenvalues.

• However, Sirovich (1987) has developed a more elegant procedure called the method of snapshots that reduces the cost of the solution to that of an eigenvalue problem of size equal to the number of modes we intend to use.
Method of Snapshots

- Assume that our ensemble of vectors results from calculations on a grid with a large number \( N \) of points and that the ensemble of functions contains \( M \) snapshots. According to the derivations previously presented, we would have to solve an \( N \times N \) eigenvalue problem.

- Using the method of snapshots, the problem can be easily reduced to an \( M \times M \) eigenvalue/eigenvector problem, which, under the premises of reduced order modeling should be quite a bit more manageable.

- Using the method of snapshots, the resulting elements of the modified autocorrelation matrix are given by

\[
\mathcal{R}_{ij} = \frac{1}{M} \int_{\Omega} u_i(x,y) \ u_j(x,y) \, dx \, dy
\]  

(6)
Method of Snapshots (cont).

• The eigenvectors of $\mathcal{R}$ are computed in an intermediate step

$$\mathcal{R} a = \lambda a$$ (7)

• The POD basis functions can now be calculated as

$$\varphi^K = \sum_{i=1}^{M} a^K_i u_i(x, y) \quad K = 1, 2, \ldots, M$$ (8)

where $a^K_i$ is the $i$th element of eigenvector $a$ corresponding to the eigenvalue $\lambda_K$. 
Method of Snapshots (cont.)

• In the case of the Euler equations, the POD procedure is repeated for each of the primitive variables \((\rho, u, v, p)\) that are needed to compute the conservative state vector \((\rho, \rho u, \rho v, \rho E)\).

• Once these basis modes have been obtained, we can, to a certain degree of accuracy, expand the flow solution about an arbitrary airfoil shape. For example, the density field of these solutions will be expanded in the form:

\[
\rho(x, y) = \sum_{i=1}^{M} \eta_{\rho_i} \varphi_{\rho}^i
\]

where the subscripts indicate the fact that the coefficients of the expansion, \(\eta_{\rho_i}\), are those particular to the expansion of the density field.
Projection

- Traditional uses of POD expansions in fluid dynamics have focused on obtaining modes which are later used to project the time evolution of the full incompressible Navier-Stokes equations.

- This transforms a complicated non-linear partial differential equation (the Navier-Stokes equations) into a number (equal to the number of modes used) of non-linear ordinary differential equations that can be integrated in time to describe the evolution of the fluid system.

- We are not particularly interested in the time evolution of the flow solution at hand. Our flow solutions are *steady* and, for airfoil analysis and design purposes, the design parameters, rather than time, will be identified with the coefficients of a surface parameterization that allows us to change the shape of the geometry of interest.
We are seeking to expand solutions of the flow about arbitrary airfoil shapes using a linear superposition of the POD modes.

We would like the resulting expansion to satisfy, as closely as possible, both the governing equations of the flow, and its wall and far-field boundary conditions.

The approach we have chosen to take is based on the well-known finite-volume procedure which is often used to discretize the governing equations of the flow.
Consider an arbitrary control volume $\Omega$ with boundary $\partial \Omega$. The equations of motion of the fluid can then be written in integral form as

$$
\frac{d}{dt} \int \int_{\Omega} w \, dx \, dy + \oint_{\partial \Omega} (f \, dy - g \, dx) = 0
$$

(10)

where $w$ is the vector of conserved flow variables, and $f$, $g$ are the Euler flux vectors

$$
\begin{align*}
\mathbf{w} &= \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \\
\mathbf{f} &= \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{bmatrix}, \\
\mathbf{g} &= \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho v H \end{bmatrix}
\end{align*}
$$
Projection (cont.)

• Applying Eq. 10 independently to each cell in the mesh we obtain a set of ordinary differential equations

\[ \frac{d}{dt}(w_{ij} V_{ij}) + R(w_{ij}) = 0 \]  \hspace{1cm} (11)

where \( V_{ij} \) is the volume of the \( i,j \) cell and the residual \( R(w_{ij}) \) is obtained by evaluating the flux integral.

• In the steady state, the time derivative term drops out and we are left with

\[ R(w_{ij}) = 0, \]

which already incorporates the wall and far-field boundary conditions in the calculation of the boundary fluxes at the edges of the domain.
Projection (cont.)

- Using a POD expansion we can develop the individual residuals of the
  Euler equations into a local function of the expansion coefficients, \( \eta_l \), for
  each of the primitive fields

\[
\mathbf{R}(\eta_l) = 0, \quad l = 1, \ldots, M. \tag{12}
\]

- This is where the drastic complexity reduction derived from POD can be
  seen. The number of free parameters in the solution of this equation set
  has been reduced considerably.
• Significant reduction in complexity of problem: From a total number of unknowns equal to $4 \times N$, where $N$ is the number of nodes in the grid, to $4 \times M$, where $M$ is the number of modes used for the expansion of each of the solution fields.

• For a typical two-dimensional Euler calculation, $4 \times 161 \times 33 = 21,252$ unknowns are solved for, while for a calculation based on POD using 15 modes, the total number of unknowns is only $4 \times 15 = 60$.

• When this procedure is used in the solution of three-dimensional flows, the reduction in computational cost becomes compelling.
Given that an exact solution to Eq. 12 will typically not be possible since we have drastically decreased the number of free parameters in the problem, we define the following cost function

\[ I_{POD} = \sum_l R^2(\eta_l), \]  

(13)

where the summation, \( l \), is over all the cells in the domain.

This approach renders our problem well-posed and defines the solution that, with a given series of modes, most closely satisfies the equations of motion in a least-squares sense.
The problem of finding the solution to our problem has now been reduced to obtaining the least-squares minimizer, $\eta_l$, of our cost function.

For this work we have chosen to use the method of Levenberg-Marquardt, for which typical solutions for problems involving $15 - 30$ modes can be found in only a few iterations (typically less than $10$).

This projection procedure dramatically reduces the cost of flow calculation from having to solve a complete set of hyperbolic partial differential equations (Euler equations) to the solution of a small set of non-linear equations.

This is reduced order modeling at work!
Results - Flow Computations

• Because any of the snapshots used in constructing a set of modes can be exactly represented by the modes, the projection algorithm should be able to compute the exact solution for any of the geometries represented in the snapshots.

• We parameterize the airfoil surface with a series of Hicks-Henne bump functions, which make smooth changes in the geometry,

\[
b(x) = \{ \sin[\pi x^{\log(1/2)/\log(t_1)}] \}^{t_2} \quad 0 \leq x \leq 1,
\]

where the maximum of the bump is located at \( x = t_1 \) and the parameter \( t_2 \) controls the width of the bump.
Results - Flow Computations (cont.)

Description of snapshots:

- Two baseline airfoils: RAE 2822 and NACA 1413
- Added 14 bump functions, 7 each on the upper and lower surfaces, and distributed evenly along the chord
- Bump amplitude of 0.1% of the chord
- Flow solutions for the baseline airfoils, plus a total 28 of flow solutions for each of the modified airfoils, were computed using FLO82 and used to form the basis modes for $\rho$, $u$, $v$, and $p$, each with a total of 30 modes.
Results - Projection of RAE 2822, $M = 0.50$

(a) Exact Pressure Contours

(b) Projected Pressure Contours
Results - Projection of RAE 2822, $M = 0.50$

(a) Surface Pressure

(b) Error in Lift Coefficient
Results - Projection of RAE 2822, $M = 0.50$

(a) Lift Coefficient Convergence

(b) Drag Coefficient Convergence
Results - Flow Computation (cont.)

- These results validate the projection technique, but not the ability of POD based models to be used for design, since we have only reconstructed information we already knew.

- For design we must be able to compute, to a reasonable degree of accuracy, the flow solutions for new geometries for which we have calculations for similar geometries.

- New set of modes: 30 bump functions used on the NACA 4412 airfoil.

- Attempting to project the NACA 3413 section, using modes based on the NACA 4412 airfoil.

- An exact solution is not guaranteed by the POD procedure.
Results - Projection of NACA 1413, \( M = 0.50 \)

(a) Exact Pressure Contours

(b) Projected Pressure Contours
Results - Projection of NACA 1413, $M = 0.50$

(a) Surface Pressure

(b) Error in Lift Coefficient
Results - Projection of NACA 1413, $M = 0.50$

(a) Lift Coefficient Convergence

(b) Drag Coefficient Convergence
Pressure Modes

(a) Pressure Mode 1

(b) Pressure Mode 2
Pressure Modes

(a) Pressure Mode 3

(b) Pressure Mode 4
Pressure Modes

(a) Pressure Mode 5

(b) Pressure Mode 6
Pressure Modes

(a) Pressure Mode 7

(b) Pressure Mode 8
Results - Projection of RAE 2822, $M = 0.75$

(a) Exact Pressure Contours

(b) Projected Pressure Contours
Results - Projection of RAE 2822, \( M = 0.75 \)

(a) Surface Pressure

(b) Error in Lift Coefficient
Results - Projection of RAE 2822, $M = 0.75$

(a) Lift Coefficient Convergence

(b) Drag Coefficient Convergence
Remarks on Flow Computations

- The lift coefficient convergence is quite rapid, while the drag coefficient takes significantly more modes.

- Nothing about POD implies that using more of the modes that are available will result in a more accurate pressure distribution at the surface of the airfoil.

- Additional modes will add to the overall accuracy when the entire domain is considered, of which the airfoil is only a boundary.

- The sensitivity of the lift and drag coefficients to the number of modes utilized in the projection could be exploited for greater efficiencies - if the cost function is drag coefficient independent, far fewer modes are required.
Results - Inverse Design

• Ability of POD based design models to provide gradients for design optimization was investigated by performing an inverse design in which a target pressure distribution was specified, and the geometry is modified to achieve such a distribution.

• An inverse design cost function is defined as

\[ I_{ID} = \int_{S} (p - p_T)^2 ds, \]  \hspace{1cm} (15)

where \( p_T \) is the target or specified pressured distribution.

• Gradients of the cost function with respect to the design variables were obtained by finite differencing of the POD model.
(a) Geometry for Initial Design  
(b) Pressure Distribution for Initial Design
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 1
(b) Pressure at Design Iteration 1
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 2

(b) Pressure at Design Iteration 2
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 3

(b) Pressure at Design Iteration 3
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 4

(b) Pressure at Design Iteration 4
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 5

(b) Pressure at Design Iteration 5
Results - Inverse Design (cont.)

(a) Geometry after Last Design Iteration

(b) Pressure after Last Design Iteration
Results - Inverse Design (cont.)

(a) Cost Function Convergence
Remarks on Inverse Design

• The use of reduced order models introduces errors into the calculation of the gradients used in the inverse design.

• Despite the errors that will inevitably exist, as long as sensitivities and gradients are generally correct, a significant advantage has been obtained in inexpensively obtaining their values.

• A partial or fully analytical derivative based on the models presented here, or by supplementing the function models with models of the derivatives with respect to design parameters as computed from adjoint methodologies, could significantly increase the usability of these types of reduced order models for design.
• Although this problem was setup so that the exact solution of the inverse design problem could be represented exactly by the modes used, a true design process would not have such \textit{a priori} knowledge of the outcome.

• However, a coupled optimizer could be used to refine the POD based model by adding additional snapshots, which would come from flow solutions that might be computed during the optimization itself, to refine the model as the design evolved. In this case, arbitrary initial conditions and target pressure distributions could be treated.
Conclusions

- The cost of computation of a flow solution is reduced from that of solving a set of partial differential equations to the solution of a coupled set of non-linear equations for steady flows.

- The number of unknowns was reduced by three orders of magnitude for a typical two-dimensional inviscid flow calculation.

- An inverse design problem was performed using information only from a reduced order model.

- Although this reduced order model based design did not attain the exact solution, it moved quite close to the target solution in only a few design steps.
Future Work

• Address means to accelerate the projection solution process, perhaps by multigrid-like / variable fidelity modeling techniques where the POD-based modules are used at the coarser levels of the design procedure.

• Investigate how to select the snapshots to form the best possible set of modes in terms of the accuracy of POD approximations.

• Is there potential to re-use these snapshots within the overall design procedure.
Future Work (cont.)

- Further integration of the design optimization routine with the POD method to allow arbitrary design problems to be posed, with no prior knowledge of the solution.

- Ultimately, we wish to extend this methodology to 3-D aerodynamic flows, both Euler and Navier-Stokes equations.

- By also applying POD to other disciplines, such as structures, mission performance, and ultimately the entire system, we wish to develop a truly multidisciplinary design environment that can exist with an acceptable computational cost and at a higher level of fidelity than is currently possible.