Investigation of Non-Linear Projection for POD Based Reduced Order Models for Aerodynamics

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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 unfeasible for realistic problems.

• Application of the adjoint equation has produced remarkable improvements in the ability to design for specific optimal behavior, but is limited in that it cannot be used to treat arbitrary cost functions.

• Response surfaces have disadvantages because the polynomial interpolate has no physical basis and there is no way to tell how well an approximate solution will agree with the exact solution.

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

• In a manner analogous to the multigrid method used to accelerate convergence of a flow solution, design optimization will be performed on a series of low to high order models to accelerate the optimization process.

• 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.
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.

• A typical use of POD in fluid mechanics has been 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.

• Pettit et. al. (2000) constructed reduced order models using POD for supersonic flutter prediction.
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 be constructed as

\[
u_M = \sum_{j=1}^{M} \eta_j \varphi_j(x)
\]  

(1)

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

\[
\max_{\varphi} \frac{\langle |(u, \varphi)|^2 \rangle}{\| \varphi \|^2}
\]

(2)
POD Theory (cont.)

- We have a calculus of variations problem in which we would like to maximize $\langle |(u, \varphi)|^2 \rangle$ subject to the constraint that $\|\varphi\|^2 = 1$ which may be shown to require that the basis functions satisfy

$$\int_\Omega \langle u(x)u(x') \rangle \varphi(x') dx' = \lambda \varphi(x). \quad (3)$$

- The POD basis is composed of the eigenfunctions of the integral Eq. 3.

- The member functions of the ensemble can now be decomposed as follows

$$u(x) = \sum_{j=1}^{\infty} \eta_j \varphi_j(x). \quad (4)$$
• 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.
Method of Snapshots

- Sirovich (1987) has developed a 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.

- Using the method of snapshots the modified autocorrelation matrix is

\[
R_{ij} = \frac{1}{M} \int_{\Omega} u_i u_j \, d\Omega \quad i, j = 1, 2, \ldots, M
\]  

and \(M\) is the total number of snapshots.
Method of Snapshots (cont.)

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

$$\mathcal{R}a = \lambda a$$  \hspace{1cm} (6)

- The POD basis functions can now be calculated as

$$\varphi^K = \sum_{i=1}^{M} a^K_i u_i(x) \quad K = 1, 2, \ldots, M$$  \hspace{1cm} (7)

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 we use a \textit{vector} state variable

\[ \mathbf{v} = (\rho, \mathbf{u}, p), \]

where $\rho$, $\mathbf{u}$, and $p$ are the density, cartesian velocity components, and pressure respectively and the variables are assumed to have zero mean.

- The inner product is then computed as

\[ (\mathbf{v}^{(l)}, \mathbf{v}^{(m)}) = \int_{\Omega} \sum_{k=1}^{N} \mathbf{v}^{(l)}_{k}(\mathbf{x}) \mathbf{v}^{(m)}_{k}(\mathbf{x}) \, d\Omega. \] (8)

where $N = \text{dim}(\mathbf{v})$. 
Flow Analysis Procedure

• Using the basis modes the flow solution can be expanded in the form

\[ \mathbf{v}(\mathbf{x}) = \sum_{i=1}^{M} \eta_i \varphi_i(\mathbf{x}). \]  

(9)

• Traditional uses of POD expansions in fluid dynamics have used this modal expansion to project the time evolution of the full incompressible Navier-Stokes equations.

• 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 geometry.
Flow Analysis Procedure (cont.)

- 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.
Flow Analysis Procedure (cont.)

• 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

\[
w = \begin{Bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho E
\end{Bmatrix}, \quad f = \begin{Bmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho u H
\end{Bmatrix}, \quad g = \begin{Bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
\rho v H
\end{Bmatrix}
\]
Flow Analysis Procedure (cont.)

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

\[ \frac{d}{dt}(w_{ij} V_{ij}) + R(w_{ij}) = 0, \]  

(11)

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

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

(12)

- An exact solution of Eq. 12 using the reduced basis will typically not be possible since we have drastically reduced the number of available degrees of freedom.
Flow Analysis Procedure (cont.)

- The expansion coefficients should therefore be computed in such a way that the governing equations are satisfied as closely as possible.

- We define the POD residual to be

\[
R_{\text{POD}}(w_{ij}) = 2 + \frac{R^{+}(w_{ij})}{R^{-}(w_{ij})} + \frac{R^{-}(w_{ij})}{R^{+}(w_{ij})} = 0, \quad (13)
\]

where the $+$ and $-$ denote the positive and negative contributions to the residual.

- This non-dimensionalizes the residuals of continuity, momenta, and energy so that the residuals are given even weighting.
Flow Analysis Procedure (cont.)

• Using the linear expansion, the flow variables in Eq. 13 can be considered functions of the expansion coefficients and the POD residual can be expressed as

\[ R_{\text{POD}}(\eta_l) = 0, \quad l = 1, \ldots, M. \]  

(14)

• An exact solution of Eq. 14 will usually not be possible so we define a POD cost function

\[ I_{\text{POD}} = \sum_n R_{\text{POD}}^2(\eta_l), \]  

(15)

to render the problem well posed and define the solution that for a given set of modes most closely satisfies the governing equations.

• The flow solution procedure consists of finding the least squares minimizer of Eq. 15, with solutions typically requiring 5 to 10 iterations.
Flow Analysis Procedure (cont.)

• The summation in Eq. 15 should be over every cell in the domain if the governing equations are to be satisfied as closely as possible over the entire domain.

• For the types of problems we are considering in which the airfoil geometry is to be perturbed the effects of these changes will decay as the distance from the airfoil increases.

• The approximate flow solution is unchanged by including cells beyond the 20-30% closest to the body.
Computational Costs

- The FLO82 flow solver, using a 5-stage Runge-Kutta scheme and multigrid, requires the equivalent of approximately 1,000 residual evaluations over the entire domain when artificial dissipation evaluations are also considered.

- The cost of the approximate flow solution from a set of basis modes is equivalent to about 50 evaluations of the residual over the entire domain.

- Over an order of magnitude decrease in computational cost is achieved for two-dimensional flows, and the reduction in three-dimensions is even greater.
Implementation Issues

- We do not wish to duplicate the efforts that produced existing analysis codes for various disciplines, rather, to generate a common interface so that data can be exchanged between programs.

- To implement our design environment, we use the Python language as a top level interface to the various subroutines, codes, and visualization programs.

- Python interfaces allow us to retain all of the speed advantages of compiled C/C++ or Fortran code over interpreted languages such as Java or Python, which are typically substantially slower.

- Interfaces to the engines of Matlab and the Visualization Toolkit (VTK) are available for plotting and data visualization.
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 RAE 2822 airfoil surface with a series of Hicks-Henne bump functions, which make smooth changes in the geometry.

• To define the snapshot geometries 14 bump functions, 7 each on the upper and lower surfaces, were used.

• Bump amplitude was 0.1% of the chord.
Results - Projection of Korn, $M = 0.50$

(a) Snapshots and Korn Airfoil

(b) $C_P$ Comparison for Korn Airfoil
Results - Projection of NACA 4410, $M = 0.50$

(a) Snapshots and NACA 4410 Airfoil

(b) $C_P$ Comparison for NACA 4410 Airfoil
Results - Projection of NACA 1413, $M = 0.50$

(a) Snapshots and NACA 1413 Airfoil

(b) $C_P$ Comparison for NACA 1413 Airfoil
Results - Convergence of $C_l$

(a) Normalized $C_l$ error for NACA 4410 Airfoil  
(b) Normalized $C_l$ error for NACA 1413 Airfoil
The use of POD models for design optimization was investigated by performing an inverse design. Although this problem can be efficiently treated using an adjoint formulation, we use it as a model problem.

An inverse design cost function is defined as

\[ I_{ID} = \int_S (p - p_T)^2 ds, \]  

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

Design variables were the amplitude of 20 bump functions.

Gradients of the cost function were obtained by finite differencing.
Results - Inverse Design (cont.)

(a) Geometry for Initial Design

(b) Pressure Distribution for Initial Design
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 5

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

(a) Geometry at Design Iteration 10

(b) Pressure at Design Iteration 10
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 15

(b) Pressure at Design Iteration 15
Results - Inverse Design (cont.)

(a) Cost Function Convergence
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 20

(b) Pressure at Design Iteration 20
Results - Inverse Design (cont.)

(a) Geometry at Design Iteration 25
(b) Pressure at Design Iteration 25
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.

• Although this reduced order model based design did not attain the exact solution, a significant reduction in computational cost is achieved with a quite small degradation in accuracy.
Conclusions

• A flow solution computation 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 computational cost is reduced by approximately an order of magnitude for two-dimensional flows.

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

• The design results show that a significant computational cost reduction is achieved with minimal degradation in accuracy.
**Future Work**

- Replace finite differencing with complex step to extend the usefulness of a given set of modes and reduce the need to compute additional flow solutions and new modes.

- Investigate use of these models on more complicated transonic flows.

- Ultimately, we wish to extend this methodology to 3-D aerodynamic flows, both the 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.