#### Dynamic Domain Decomposition and Error Correction for Reduced Order Models



Patrick A. LeGresley and Juan J. Alonso Dept. of Aeronautics & Astronautics Stanford University

41st Aerospace Sciences Meeting Reno, Nevada January 6, 2003

### Outline

- Motivation
- Proper Orthogonal Decomposition (POD) Theory
- Flow Analysis Procedure
- Domain Decomposition
- Error Estimation
- Flow Computation & Drag Minimization Results
- Conclusions & Future Work

#### Motivation

- The application of reduced order models based on Proper Orthogonal Decomposition (POD) to aerodynamics has been restricted to subsonic flows or flows with weak shocks which had little movement.
- The inherent simplicity of the linear basis generated via POD also limits it to representing phenomena which have been observed in the dataset used to construct it.
- A simple example illustrates the problem.

#### Motivation (cont.)



4

### Motivation (cont.)



## Motivation (cont.)

- Lucia (2001) proposed and demonstrated the decomposition of a flow with moving shocks into a subdomain in which the flow is represented with a POD model and a small subdomain in which a full order flow solver is used.
- Extend domain decomposition as a dynamic, *a posteriori* verification and if necessary, correction of the approximate solution.
- The fidelity can be varied from extremely low only a handful of degrees of freedom coming solely from POD to very high as the model recovers the fidelity of a full order solver in the limit. This makes for a good fit for multilevel optimization

### **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

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

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

$$\max_{\varphi} \frac{\langle |(\mathbf{u},\varphi)|^2 \rangle}{\|\varphi\|^2} \tag{2}$$

### **POD Theory (cont.)**

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

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

$$u(x) = \sum_{j=1}^{\infty} \eta_j \varphi_j(x).$$
(4)

### **POD Theory (cont.)**

• In the case of the Euler equations we use a *vector* state variable

$$\mathbf{w} = (\rho, \rho \mathbf{u}, \rho E),$$

where  $\rho$ ,  $\rho u$ , and  $\rho E$  are the density, momentum, and total energy respectively and the variables are assumed to have zero mean.

• The inner product is then computed as

$$(\mathbf{w}^{(l)}, \mathbf{w}^{(m)}) = \int_{\Omega} \sum_{k=1}^{N} \mathbf{w}_{k}^{(l)}(\mathbf{x}) \ \mathbf{w}_{k}^{(m)}(\mathbf{x}) \ d\Omega.$$
(5)

where  $N = dim(\mathbf{w})$ .

#### Flow Analysis Procedure

• Approach is based on a *finite-volume* discretization in which the equations of motion of the fluid can be written in integral form as

$$\frac{d}{dt} \iint_{\Omega} \mathbf{w} \, dx \, dy + \oint_{\partial \Omega} \, (\mathbf{f} \, dy - \mathbf{g} \, dx) = \mathbf{0} \tag{6}$$

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

$$\mathbf{w} = \left\{ \begin{array}{c} \rho \\ \rho u \\ \rho v \\ \rho E \end{array} \right\}, \quad \mathbf{f} = \left\{ \begin{array}{c} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{array} \right\}, \quad \mathbf{g} = \left\{ \begin{array}{c} \rho v \\ \rho uv \\ \rho uv \\ \rho v^2 + p \\ \rho vH \end{array} \right\}$$

## Flow Analysis Procedure (cont.)

• Applying Eq. 6 independently to each cell in the mesh we obtain a set of ordinary differential equations

$$\frac{d}{dt}(\mathbf{w}_{ij}\,V_{ij}) + \mathbf{R}(\mathbf{w}_{ij}) = \mathbf{0},\tag{7}$$

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

$$\mathbf{R}(\mathbf{w}_{ij}) = \mathbf{0}.\tag{8}$$

• An exact solution of Eq. 8 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.)

- One can use any weighted residual method such as collocation, least squares, and the Galerkin method.
- Method used here is to minimize the residuals in a least squares sense.
- Defining the square of the residuals where  ${\bf R}$  can now be expressed as a function of  $\eta$

$$\tilde{R}(\eta) = \sum_{i,j} \mathbf{R}(\eta)^2 \tag{9}$$

• The governing equations for the POD solution are then

$$\hat{R}_k(\eta) = \frac{\partial \tilde{R}}{\partial \eta_k} = 0.$$
(10)

# Flow Analysis Procedure (cont.)

- Cost of the approximate solution is proportional to the number of modes used in the approximation and also has a dependence on the number of degrees of freedom in the original problem.
- Can lessen the impact of dimensionality for the non-linear case by not using every single residual in the least squares fit.
- This approach essentially achieve somes of the low cost of collocation with less dependence on the choice of collocation points and are sometimes referred to as least squares collocation.

#### **Domain Decomposition**

- Coupling is essentially the same as that used in mutliblock solvers where the spatial domain of the problem is broken into blocks and communication between subdomains is accomplished using halo cells surrounding each subdomain.
- However, the coupling does require attention to the interface between the approximate solution generated via POD and the full order solver.
- Sources/sinks of mass, momenta, and energy in the first level of halo cells surrounding the full order domains to leave a conservative interface between the POD and full order solver.

## **Domain Decomposition (cont).**

- Lagged iterations, beginning with a pure POD solution, between the POD and full order solver are used to generate the solution of the coupled system.
- The number of iterations required to solve the full order equations in the coupled system is approximately the same as the number of iterations required to solve the real full order system, but now there are far fewer equations.
- There is additional cost to recompute the solution in the POD subdomain as the solution in the full order subdomain evolves, typically one or two more iterations beyond the three or four required to get the initial POD solution.

#### **Error Estimation**

- The coupling of the POD and full order solver allows one to generate solutions of widely varying computational cost, but as is often the problem in reduced order modeling the degree of accuracy is unknown.
- Ideally we would like to have error bounds, but this may have nearly the same cost as computing the solution of the problem we are trying to approximate in the first place.
- We can however prioritize which portions of the domain to augment with additional basis functions to generate the best solution for a given computational cost.

#### **Error Estimation (cont).**

• Let subscript POD denote the solution as computed using POD

$$\mathbf{w}_{POD} = \sum_{m=1}^{M} \eta_m \varphi_m(\mathbf{x}) \tag{11}$$

and DD the solution using the POD basis functions plus some additional top hat basis functions,  $\hat{\varphi_n}$ ,

$$\mathbf{w}_{DD} = \sum_{m=1}^{M} \eta_m \varphi_m(\mathbf{x}) + \sum_{n=1}^{N} \hat{\eta_n} \hat{\varphi_n}(\mathbf{x}).$$
(12)

• Define  $w_{DD}^{POD}$  as the solution using the expansion in (11) transferred to the basis in (12).

### **Error Estimation (cont).**

• The residual operator representing the governing equations are

$$\left\{ \begin{array}{c} \hat{R}_k(\eta) \\ R_k(\hat{\eta}_n) \end{array} \right\} = R_{DD} = \mathbf{0}.$$
 (13)

• The residual operator can be expanded as

$$\mathbf{R}_{DD}(\mathbf{w}_{DD}) = \mathbf{R}_{DD}(\mathbf{w}_{DD}^{POD}) + \frac{\partial \mathbf{R}_{DD}}{\partial \mathbf{w}_{DD}} \Big|_{w_{DD}^{POD}} (\mathbf{w}_{DD} - \mathbf{w}_{DD}^{POD}) + \cdots$$

• This can be inverted to give the error in the state vector

$$\left(\mathbf{w}_{DD} - \mathbf{w}_{DD}^{POD}\right) \approx - \left[\frac{\partial \mathbf{R}_{DD}}{\partial \mathbf{w}_{DD}}\Big|_{w_{DD}^{POD}}\right]^{-1} \mathbf{R}_{DD}\left(\mathbf{w}_{DD}^{POD}\right).$$
(14)

### **Error Estimation (cont).**

- How useful and costly this estimate is depends on the number of additional basis functions that are introduced.
- For this work we found that introducing new basis functions in blocks of 8 by 8 cells (in a computational domain which was 160 by 32 cells) gave a good compromise between capturing higher order effects and computational cost.
- Each block was assigned a value equal to the norm of the change in pressure for the cells inside that block to give priority to placing basis functions that lead to a local change.

#### **Results - Flow Computation**

• Error Estimation for the RAE 2822 Airfoil



# **Results - Flow Computation (cont).**

• POD with Domain Decomposition for the RAE 2822 Airfoil at M=0.67



(a) Surface  $C_P$  Distribution



(b) Percentage Error in  $C_P$  (Boundary of Domain Decomposition Denoted with Dashed Line)

### **Results - Drag Minimization**

- Geometry of the airfoil is modified to reduce drag at fixed lift.
- To generate the snapshots a baseline NACA 4410 airfoil was perturbed with 4 Hicks-Henne bump functions on both the upper and lower surfaces.
- $\bullet$  Flow solutions for the 9 airfoil geometries were computed at Mach 0.67 and angles of attack of  $1.5\,^\circ$  and  $1.6\,^\circ$
- The drag minimization was carried out using the NACA 4410 airfoil at Mach 0.67 and an angle of attack of 1.5 °.
- Gradients were computed by finite differencing of the approximate POD model to determine the direction of change and a line search was made at each iteration to determine the best step size.

• 75% POD / 25% Full Order



(a) Initial Solution, POD with DD:  $C_l~=~1.017,~C_d~=~0.0115;$  Full Order:  $C_l~=~1.018,~C_d~=~0.0115;~\alpha~=~1.50~^\circ$ 



(b) After 5 Design Iterations, POD with DD:  $C_l = 0.993$ ,  $C_d = -0.0088$ ; Full Order:  $C_l = 1.018$ ,  $C_d = 0.0034$ ;  $\alpha = 1.40^{\circ}$ 



(a) Drag Coefficient Design History

(b) Comparison of Geometry for Approximate and True Solution

• 50% POD / 50% Full Order



(a) Initial Solution, POD with DD:  $C_l = 1.017$ ,  $C_d = 0.0115$ ; Full Order:  $C_l = 1.018$ ,  $C_d = 0.0115$ ;  $\alpha = 1.50^{\circ}$ 



(b) After 5 Design Iterations, POD with DD:  $C_l = 1.027$ ,  $C_d = 0.0003$ ; Full Order:  $C_l = 1.018$ ,  $C_d = 0.0020$ ;  $\alpha = 1.58^{\circ}$ 



(a) Drag Coefficient Design History

(b) Comparison of Geometry for Approximate and True Solution

#### **Conclusions & Future Work**

- A procedure with continuously variable fidelity has been developed to use POD-based reduced order models for aerodynamic problems with moving shocks.
- To investigate the suitability of these types of models for use in design, a drag minimization problem was performed with final results which were very similar to the full order results.
- When fully integrated into a multilevel optimization procedure this method will produce accurate optimization results at significantly reduced computational cost and allow new design problems which are currently infeasible to be considered.