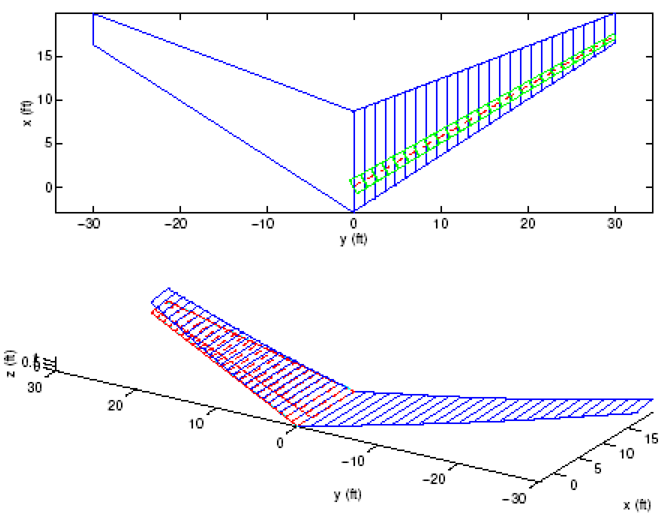
Improving the Performance of Design Decomposition Methods with POD



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Outline

- Motivation
- Proper Orthogonal Decomposition (POD)
- Bi-Level Integrated System Synthesis (BLISS)
- BLISS and POD
- Results
- Conclusions and Future Work

Motivation

- Design decomposition methods for MDO are appealing because they:
  - Are relatively easy to implement.
  - Allow for more autonomy of disciplines.
  - Are more scalable to large numbers of disciplines.
- The computational cost of decomposition methods is typically higher than tightly coupled methods such as Multidisciplinary Feasible (MDF).
- Cost of decomposition methods can be improved with approximation models, response surfaces, curve fits, etc.
- Our past work with POD has shown it may be used as a bandwidth or dimensionality reduction technique.

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).

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

- We have used it for solution approximation and design for 2-D inviscid aerodynamics, including the transonic regime.

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

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

- 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

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

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 $\|\varphi\|^2 = 1$ which may be shown to yield

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

where POD basis is composed of the eigenfunctions of the integral Eq. 3.

- For discrete datasets we will be dealing with a group of N-dimensional vectors in which case we compute an autocorrelation tensor

$$\mathbf{R} = \langle \mathbf{u} \otimes \mathbf{u} \rangle,$$

and the integral eigenvalue problem becomes

$$\mathbf{R}\varphi = \lambda\varphi.$$

POD Theory (cont.)

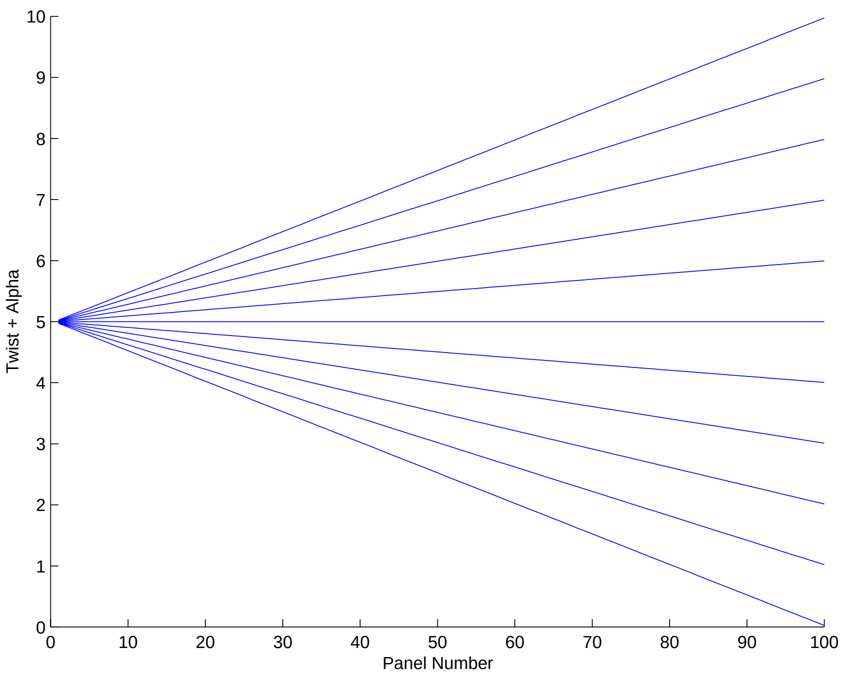
- The member functions of the ensemble can now be decomposed as follows

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

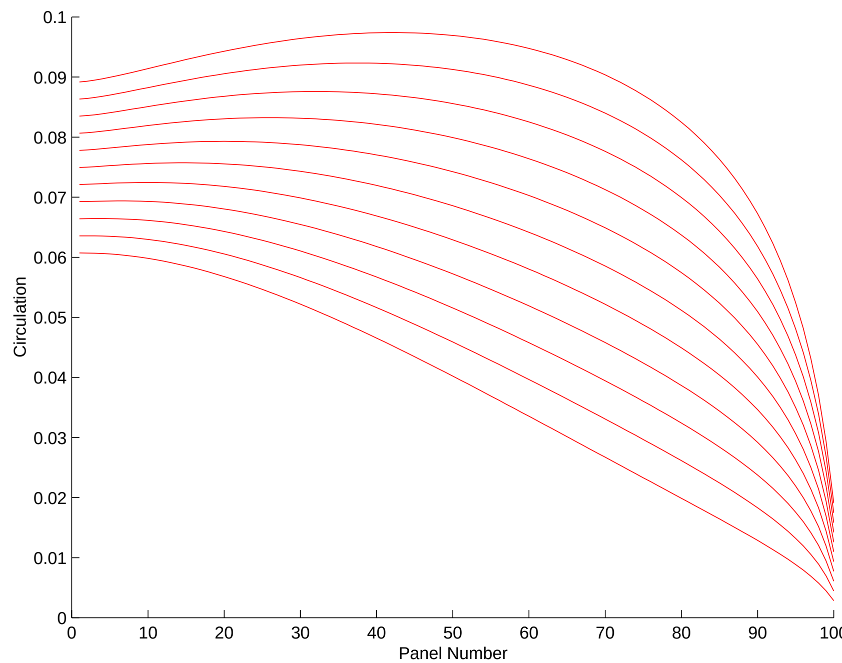
- The main advantage of POD is that it produces the *best* linear representation for an ensemble of functions or flowfields (*snapshots*).

- 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.

POD Example

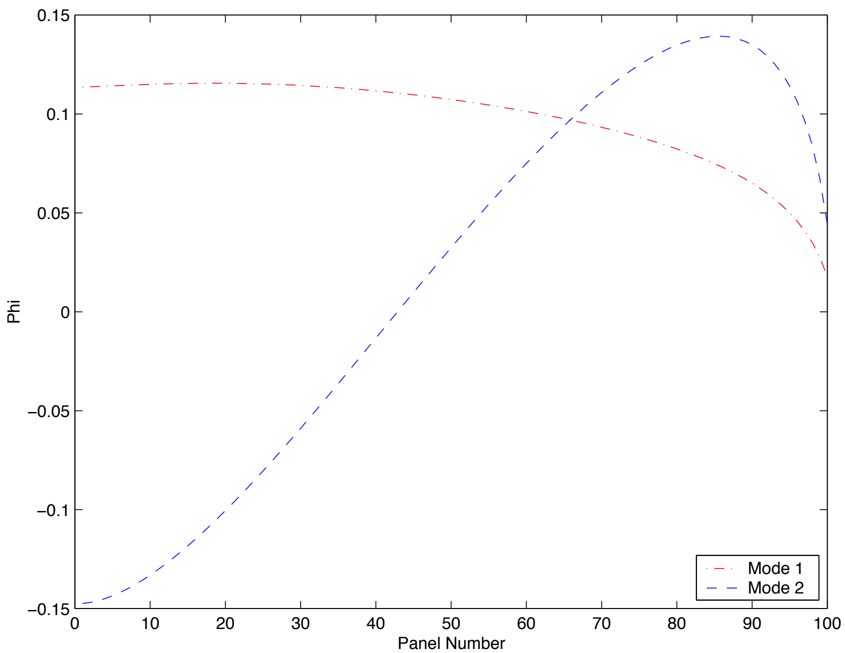


(a) Varying Twist Distributions for Computing Snapshots

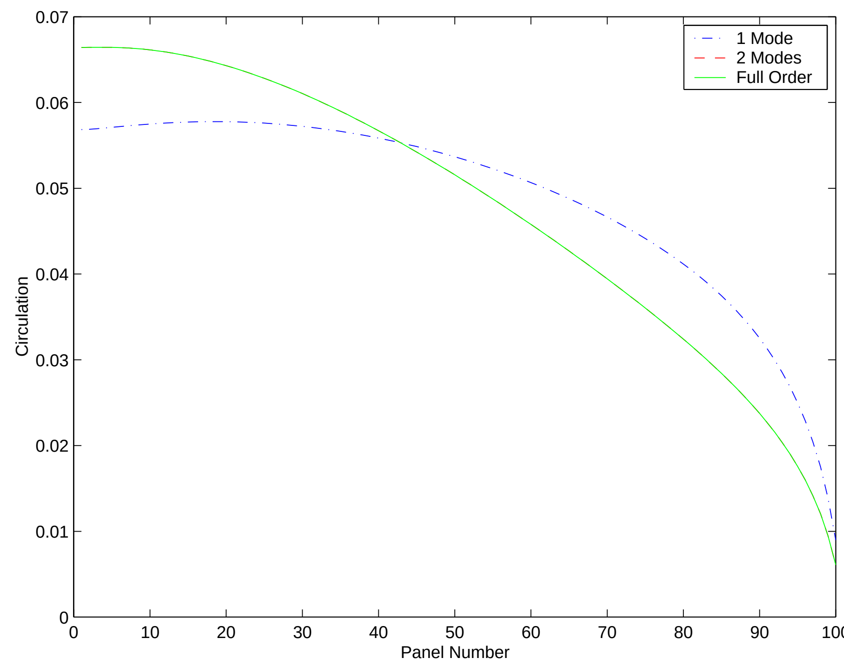


(b) Snapshots: Circulation Distribution for Each Twist Distribution

POD Example (cont.)



(a) Basis (Modes) Computed Using POD



(b) Approximate Solution Using the POD Modes

Method of Snapshots

- 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.

- 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

$$\mathcal{R}_{ij} = \frac{1}{M} \int_{\Omega} u_i \, u_j \, d\Omega \quad i, j = 1, 2, \ldots, M \tag{5}$$

and M is the total number of snapshots.

Method of Snapshots (cont.)

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

$$\mathcal{R}a = \lambda a \tag{6}$$

- The POD basis functions can now be calculated as

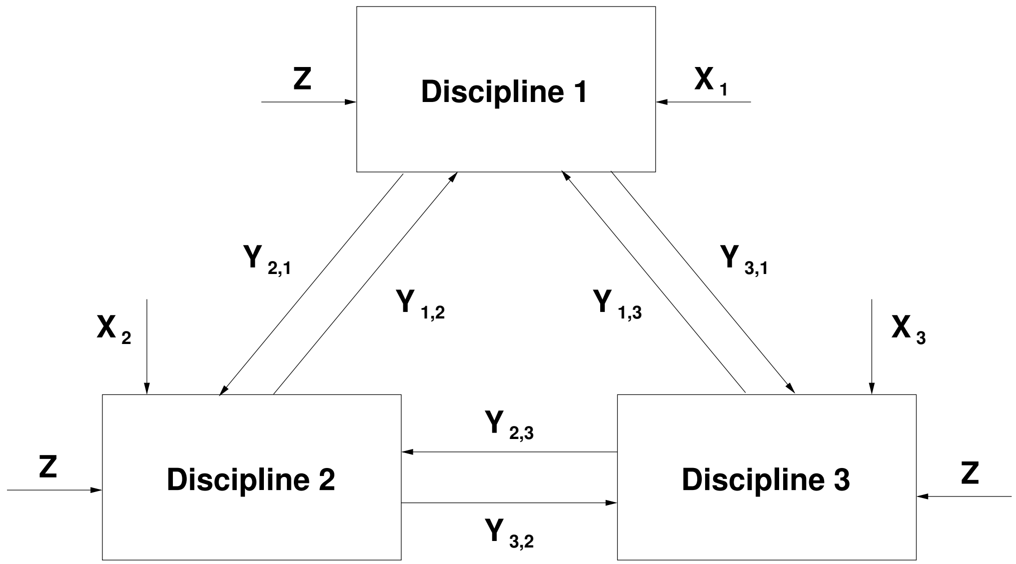
$$\varphi^K = \sum_{i=1}^{M} a_i^K u_i(\mathbf{x}) \quad K = 1, 2, \ldots, M \tag{7}$$

where a_i^K is the i-th element of eigenvector a corresponding to the eigenvalue λ_K.

Bi-Level Integrated System Synthesis (BLISS)

- Decomposes the problem, typically along disciplinary boundaries.
- Sub-problems (with large numbers of design variables) separated from system level optimization (with small number of design variables).
- Each sub-problem concurrently performs an optimization formulated to improve the overall system.
- Sub-problem optimizations alternate with system level optimizations.
- Overall objective is improved, or at least constraint violations are eliminated, during each design cycle.

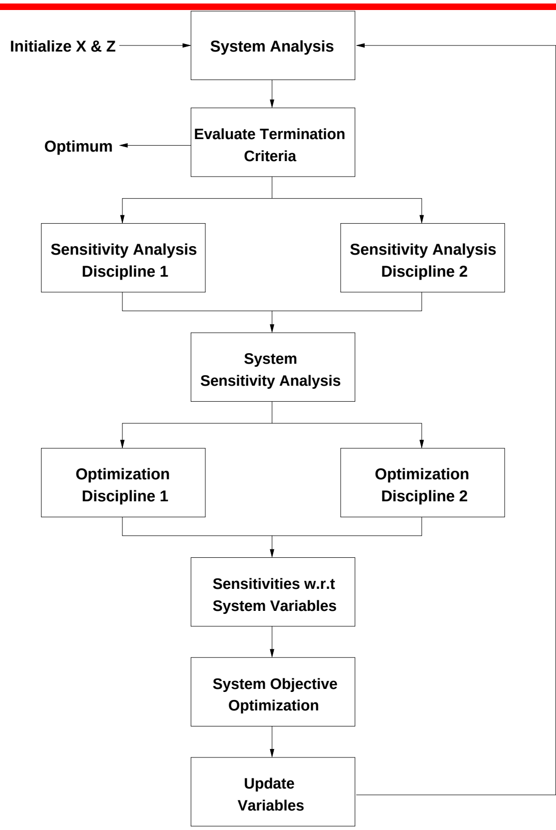
BLISS Discipline Interaction



(a) Interaction of Disciplines in BLISS

- Y are the interaction variables.
  - Y_i is the vector of interaction variables of computed by discipline i.
  - $Y_{i,j}$ is the vector of interaction variables output by discipline j that are inputs to discipline i.

BLISS Procedure



(a) Flowchart for BLISS Procedure

- System analysis is problem dependent and usually iterative.
- After evaluating the termination criteria, we can choose to exit or enter another design cycle.
- First we formulate objective functions for each discipline that will result in minimization of the overall system objective function, Φ, assumed to be one of the elements of Y.

BLISS - System Sensitivity Analysis

- Total derivatives of Y with respect to $x_{r,j}$ (the j^{th} design variable in discipline r) are computed by solving the Global Sensitivity Equations (GSE) for a given $x_{r,j}$

$$[A]\left\{\frac{dY}{dx_{r,j}}\right\} = \left\{\frac{\partial Y}{\partial x_{r,j}}\right\}, \tag{8}$$

where A is a matrix made up of sub-matrices as follows

$$A = \begin{bmatrix} I & A_{1,2} & A_{1,3} \\ A_{2,1} & I & A_{2,3} \\ A_{3,1} & A_{3,2} & I \end{bmatrix}, \tag{9}$$

where I is the identity matrix and $A_{r,s} = -\frac{\partial Y_r}{\partial Y_s}$.

BLISS - Discipline Objective Formulation

- The change in the overall objective function due to a change in the local design variables is

$$\Delta\Phi = \frac{d\Phi}{dX_1}^T \Delta X_1 + \frac{d\Phi}{dX_2}^T \Delta X_2 + \frac{d\Phi}{dX_3}^T \Delta X_3, \qquad (10)$$

and the contribution of the i^{th} discipline is

$$\phi_i = \frac{d\Phi}{dX_i}^T \Delta X_i. \qquad (11)$$

BLISS - Discipline Optimization Problem

- To minimize the overall system objective function each discipline solves an optimization problem such as this for discipline two:

Given:	X_2, Z, and $Y_{2,1}$, $Y_{2,3}$
Find:	ΔX_2
Minimize:	$\phi_2 = \frac{d\Phi}{dX_2}^T \Delta X_2$
Satisfy:	$G_2 \leq 0$

- Constraints are the local constraints, e.g. stress constraints for structures, etc.

- All of the discipline optimization problems can be carried out in parallel.

BLISS - Sensitivities w.r.t System Variables

- After completing the discipline optimizations we can now proceed with the system level optimization using the design variables Z.
- We need the derivatives of Φ with respect to Z.
- BLISS/A computes these derivatives by a modified GSE.
- BLISS/B uses an algorithm that computes them from the Lagrange multipliers of the discipline optimizations.

BLISS - Sensitivities w.r.t System Variables (cont.)

- For $F = F(P)$ and $G_0 = G_0(P)$ (Barthelemy and Sobieski, 1982):

$$\frac{dF}{dP_0} = \frac{\partial F}{\partial P} + L^T \frac{\partial G_0}{\partial P}.$$

which leads to the following for BLISS/B

$$\begin{aligned} \left.\frac{d\Phi^T}{dZ}\right|_0 &= \left(L^T \frac{\partial G_0}{\partial Z}\right)_1 + \left(L^T \frac{\partial G_0}{\partial Z}\right)_2 + \left(L^T \frac{\partial G_0}{\partial Z}\right)_3 \\ &+ \left[\left(L^T \frac{\partial G_0}{\partial Y}\right)_1 + \left(L^T \frac{\partial G_0}{\partial Y}\right)_2 \right. \\ &+ \left.\left(L^T \frac{\partial G_0}{\partial Y}\right)_3\right] \frac{dY}{dZ} + \frac{d\Phi^T}{dZ}. \end{aligned}$$

BLISS - System Level Optimization

- With the sensitivities computed using BLISS/A or BLISS/B the system level optimization can be performed:

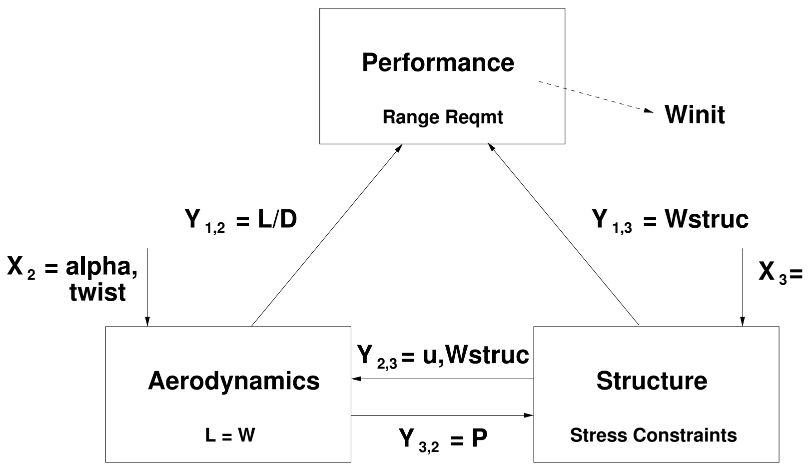
Given: Z and Φ_0
Find: ΔZ
Minimize: $\Phi = \Phi_0 + \frac{dy_{1,i}}{dZ}^T \Delta Z$
Satisfy: $ZL \leq Z + \Delta Z \leq ZU$
$\Delta ZL \leq \Delta Z \leq \Delta ZU$

- ZL and ZU are the bounds on the Z design variables and ΔZL and ΔZU are move limits.

BLISS Example

- We consider a three discipline system with:
  - Aerodynamics consisting of a 1-D panel code.
  - Structures with a single wing spar.
  - Mission performance via the Breguet range equation.

- The objective to minimize is takeoff weight, and the design variables are the twists and thicknesses with lift equal to weight and stress constraints.



(a) Interaction of Disciplines in BLISS for an Aeroelastic Optimization

BLISS and POD

- The need for and benefits of using approximation methodologies in MDO decomposition methods have been demonstrated for BLISS and other algorithms.

- In POD we have an approximation method with similar characteristics to response surfaces, Kriging, etc. but with the ability to incorporate the governing equations of the system and recover the true solution in the limit.

- When making use of approximation methods the difficult question of accuracy and what uncertainty is involved to achieve such computational cost savings arises.

BLISS and POD (cont.)

- In the case of using POD as a bandwidth reduction technique we know the true solution but it is expensive to communicate in the case of high fidelity computational simulations.
- We may want to compress that information, through approximation if necessary, for interaction with others while still using the higher order solution internally.
- If the error is deemed excessive we can request refinement, at some increased cost, through updated models from additional observations or other means such as domain decomposition.

BLISS and POD Procedure

- An initial set of representative data is necessary to compute the POD modes before we can enter the optimization procedure.

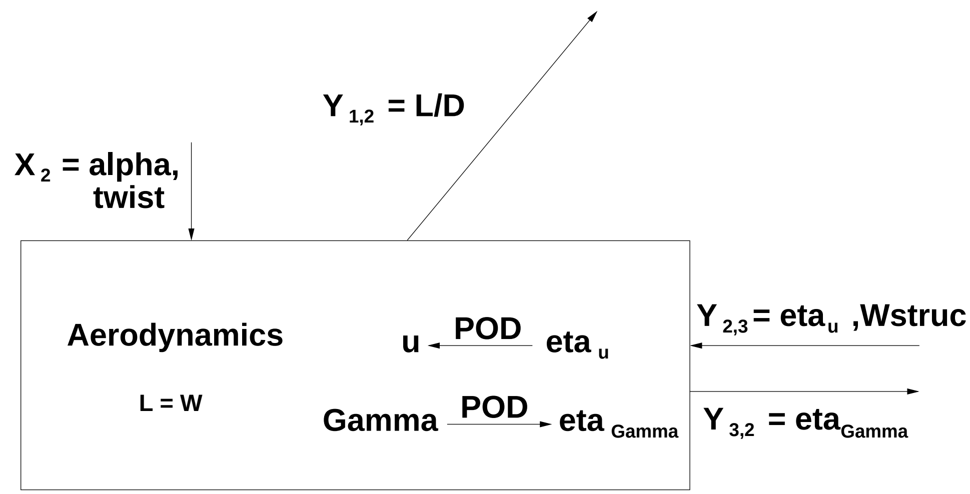
- Snapshots of the interaction variables could come from
  - Running system analyses for a range of design variables.
  - Computations of individual disciplines with anticipated ranges of design variables and interaction variables
  - A database of results from previous optimization runs
  - Any combination thereof.

- It is important that we collect data similar to that we anticipate needing to approximate during the actual optimization to ensure that our approximation model will be as good as possible.

BLISS and POD Procedure (cont.)

- The system analysis is unchanged - no error in overall system objective function.

- Full order, high dimensionality interaction variables computed during the system analysis step are replaced by their low-dimensional, POD coefficient counterparts.



(a) Aerodynamics Discipline in BLISS/POD

- Low-dimensional data such as the structural weight, lift-to-drag ratio, etc. are unaffected by the use of POD.

BLISS and POD Procedure (cont.)

- Computation of the A matrix and right hand side of Eq. 8 is essentially the same but now with many fewer variables.

- The discipline optimizations are unchanged except that the gradients are now an approximation.

- Typically the system variables, Z, tend to be of lower dimensionality compared to the interaction variables, Y, and the application of POD models does not provide compelling advantages.

- As long as the gradient approximations are sufficiently accurate the BLISS algorithm with POD should converge to the correct optimal and feasible solution.

BLISS and POD Procedure (cont.)

- Accuracy of the gradients can be inferred by the measurable accuracy of both the POD approximation and the estimated change in the objective function from the Taylor series expansion.

- There are several options for improving the situation:
  - Save the discipline analyses performed during the course of the optimization procedure to compute updated POD models.
  - Perform domain decomposition and represent a small portion of the domain at full order and the remainder with POD (moving shocks).
  - Go completely full order.

BLISS/POD for Aeroelastic Problem

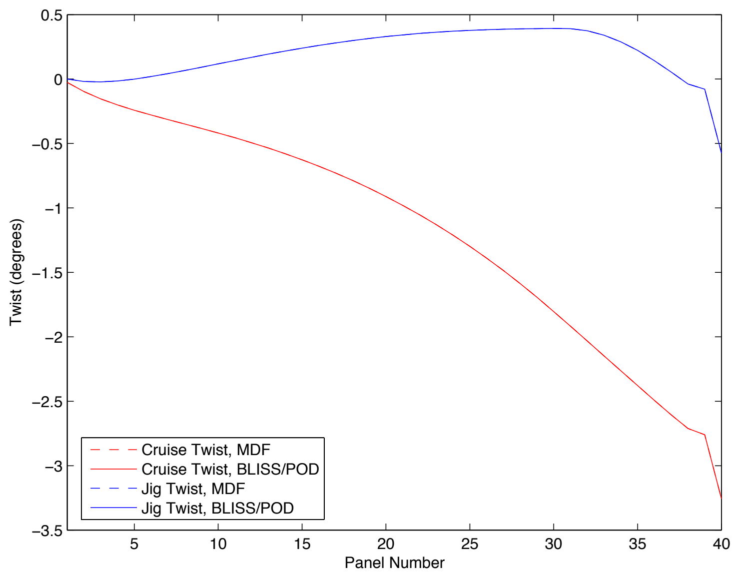
- POD snapshots were obtained by running four aeroelastic solutions and using the corresponding circulations and displacements to compute a set of POD modes for each of these variables.

- For a general problem with more realistic models the number of snapshots necessary will be unknown.

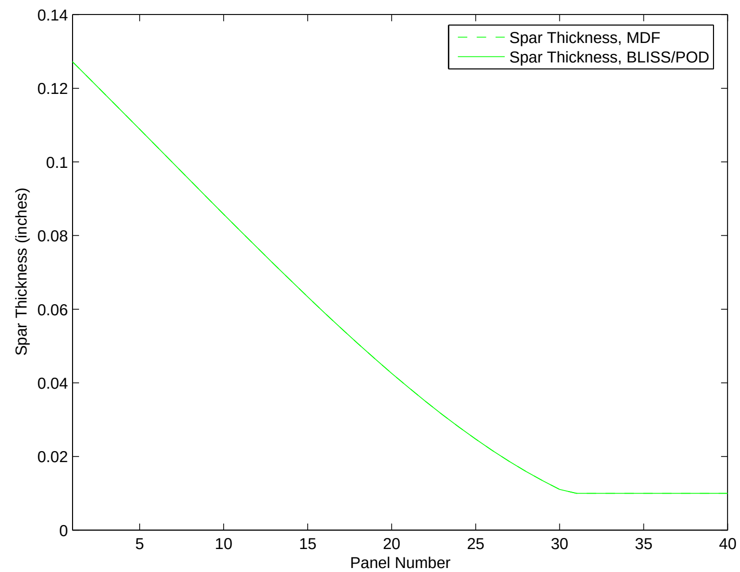
- One option is to compute the eigenvalues as each snapshot becomes available - rapid drops in the eigenvalues indicate that further snapshots will not improve the model.

- Computational effort based on wall clock time.

BLISS/POD for Aeroelastic Problem (cont.)



(a) Twist Distribution



(b) Thickness Distribution

BLISS/POD for Aeroelastic Problem (cont.)

n = 20

	MDF	BLISS	BLISS/POD
Objective	15868.2	15868.3	15868.2
$\|t - t_{MDF}\|$	0.	$9.6e10^{-6}$	$1.5e10^{-5}$
$\|\theta - \theta_{MDF}\|$	0.	$9.6e10^{-6}$	$1.3e10^{-5}$
Time	1.00	8.95	2.63

n = 40

	MDF	BLISS	BLISS/POD
Objective	15845.0	15845.4	15845.3
$\|t - t_{MDF}\|$	0.	$1.8e10^{-5}$	$2.0e10^{-5}$
$\|\theta - \theta_{MDF}\|$	0.	$1.7e10^{-5}$	$1.6e10^{-5}$
Time	1.00	8.77	1.94

BLISS/POD for Aeroelastic Problem (cont.)

- The results of the different optimization methods are essentially the same.

- For BLISS the computational cost was greater by a factor of approximately 8.5, reduced to about a factor of 2 by POD for reasonable size problems.

- Implementation of BLISS is more scalable in terms of numbers of disciplines.

- The lack of need for model refinement to achieve sufficient accuracy *cannot* be expected to hold true for more general problems, particularly high fidelity models.

Conclusions and Future Work

- The use of POD as a bandwidth reduction technique in the BLISS decomposition method for MDO has been demonstrated.
- The use of this technique in a representative aeroelastic design problem achieved computational costs very similar to MDF for moderate size problems.
- Further work will verify the BLISS/POD methodology in high-fidelity multidisciplinary design optimization where the computational cost savings are more compelling and the challenges greater.