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May 11, 2008

Publication Number: CSRCR2008-17

Computational Science & Engineering Faculty and Students Research Articles

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1 Introduction

There are many applications that require the transient simulation of acoustic, elastic or electromagnetic wave propagation. To name a few: structural analysis, blast on structures, vibrations of Navy vessels, sonar, design of piezoelectric transducers for medical ultrasound, medical imaging and therapeutics uses of ultrasound, earth seismic imaging for the Oil Industry and Earthquake Seismology, Optimization driven by Simulation for material identification and optimal design. As such, any significant improvement in the performance of numerical simulators would be very important.

Model Order Reduction (MOR) refers to a collection of techniques to reduce the number of degrees of freedom of the very large scale dynamical systems that result after space discretization of time-dependent partial differential equations in three space dimensions. Some of these techniques have been successfully employed in the simulation of VLSI circuits, computational fluid mechanics, real-time control, heat conduction and other problems [1, 3, 5, 7]. Not much has been done for wave propagation, although it does not seem that there are fundamental difficulties for its application [2].

However, since none of these techniques are trivial to interface with existing large scale high fidelity codes, it is important to be able to select wisely the correct approach, in order to minimize development costs. At this time we have centered our attention into the class of methods that go by the name of **Proper Orthogonal Decomposition (POD)**. We start from the premise that it is possible to run a few full simulations. POD uses snapshots from these simulations to form an orthogonal basis for the solution space. This is a problem-dependent modal decomposition, as opposite to the use of artificial basis functions (Fourier expansions, wavelets). By using truncated Singular Value Decompositions it is possible to reduce even further the size of this basis without sacrificing accuracy. The dynamic of a new problem is obtained by solving projected collocation equations for the time dependent coefficients of a linear combination of the natural basis functions.

A different class of methods, tailored to problems where even a few high fidelity simulations are not an option, is based on Krylov subspace machinery for large-scale matrix computations [5]. These methods generate reduced-order models that are in a certain sense optimal, directly from the large-scale data matrices describing the given linear system. Interfacing these techniques with high-fidelity codes is less trivial, and would require major modifications. Therefore, we will focus first on POD-type methods. In a later stage we will explore hybrid approaches that combine the easy use of POD methods with the powerful approximation properties of Krylov subspace-based order reduction.

2 Model Order Reduction

The purpose of Model Order Reduction (MOR) is to replace a large dynamical system by a smaller one that still captures the dynamics of interest with sufficient accuracy. For wave propagation, when is possible to perform some high-fidelity calculations using existing finite difference or finite element codes, the approach that we will discuss here is called Proper Orthogonal Decomposition (POD), the Karhunen-Loeve Transform, Principal Components Analysis or, in more modern terms, the Singular Value Decomposition. This technique will allow us to analyze a complex spatio-temporal dynamic behavior and extract from it a (small) set of dominant components (data driven modes), separating them from noise and inessential underlying dynamical behavior, while still giving a sufficiently accurate description of the dynamics of interest. It is similar to a mode analysis using Fourier, wavelets or other artificial bases, but in the approach under discussion we will use snapshots extracted from a number of high-fidelity simulations that have appropriate inputs, in order to extract the most important problem specific modes. The ideal application is one in which we have a parametrized model that needs to be calculated many times, such as in optimization, parametric studies, multiple inputs or source wavelets.

The procedure consists of the following steps:

- Some pre-processing in which a few large scale high-fidelity calculations are performed.
- An SVD of the matrix whose columns are spatial snapshots extracted from those simulations is calculated and truncated at the required error level.
- The space-time approximate solution is written as a linear combination of the *m* selected modes (left singular vectors) with (unknown) time dependent coefficients.
- This Ansatz is replaced in the original equations and due to the orthogonality of the modes, a reduced system of ODE's will result. Solving for the coefficients of the linear combination for a problem with new inputs, a very economical procedure results compared to the original high-fidelity calculation.

3 Model Order Reduction by Proper Orthogonal Decomposition

Let us consider a first-order hyperbolic system already discretized in space:

$$\frac{\partial w}{\partial t} = Aw + Bu(t),$$
(1)
$$v = Cw.$$

where $x \in \mathbb{R}^n$, $w(t), B \in \mathbb{R}^M$ and A, C are appropriate matrices. Matrix A is sparse in the finite element or finite differences case, but full if an spectral method is used. The vector u contains the inputs (forcing function, time dependent boundary conditions), while the vector v contains the desired outputs (for instance, seismograms at a few locations). For the state vector w, M is the number of degrees of freedom in space, generally very large.

We assume that we either can observe (measure) the system for various inputs at different times or that we can numerically simulate it. Let $\Phi = \{\phi_i\}$ i = 1, ..., l $(l \ll M)$, be the $M \times l$ matrix whose columns are these spatial snapshots, and let $\Phi = U\Sigma V^T$ be its Singular Value Decomposition, where U, V are orthogonal matrices and Σ contains the singular values σ_i in its diagonal, sorted in descending order of magnitude. Since the vectors in U, V have norm l_2 equal to 1, the singular values measure the 'energy' contained in each one of these modes. The total energy of the system (Frobenius norm) is:

$$E^2 = \sum_{i=1}^{l} \sigma_i^2.$$

If we truncate the SVD at the *mth* term, with $m \leq l \ll M$ then the error (or left-over energy) is:

$$\delta_m^2 = \sum_{i=m+1}^l \sigma_i^2.$$

Thus if we want to preserve a certain fraction of the total energy, say 0 , then m must be chosenso that:

$$\delta_m^2 \cong (1 - p^2) E^2.$$

Let the truncated set of left singular vectors of Φ be called U_m . We now seek solutions of system (1) (with the same spatial discretization), of the form:

$$w(x,t) = U_m a(t),\tag{2}$$

where a(t) is a vector of time dependent coefficients of dimension m to be determined. The coefficients a(t) for a new input are determined via Galerkin collocation. We replace in system (1) the Anzatz (2), obtaining:

$$U_m da/dt = AU_m a(t) + Bu(t),$$

$$v = CU_m a(t).$$

Multiplying by U_m^T the differential equation and since the columns of U_m are orthogonal, we get:

$$da/dt = U_m^T A U_m a(t) + (U_m^T B) u(t),$$

$$v = (C U_m) a(t),$$
(3)

which is the reduced set of ODE's of dimension m, whose solution will produce the time dependent coefficients a(t). The matrix of the reduced system $A_m = U_m^T A U_m$, is not sparse. Combining these coefficients with the spatial modes U_m as in (2) produces the full solution for a new problem.

Summary

The steps to follow then are:

- 1. Run s full simulations with the same spatial mesh (for instance, changing the source location).
- 2. Extract b snapshots from each simulation, for a total of l = b * s columns in Φ .
- 3. Calculate the SVD of Φ (complexity of the SVD for a $M \times l$ matrix is $O(M \times l^2)$).
- 4. Truncate at energy level p < 1.
- 5. With the resulting m modes construct the matrices of the reduced system:

$$A_m = U_m^T A U_m, \quad B_m = U_m^T B(x), \quad C_m = C(x) U_m.$$

- 6. To solve a new problem (say with the source in a different position, or different source input), we solve the reduced systems of ODE's for the coefficients $a_j(t), j = 1, ..., m$, in the representation 2 of the solution.
- 7. Validation: compare reduced results with full high fidelity results (at the sensors!).

Comments

In the previous algorithms there are some undetermined quantities, namely: the number of full simulations s, the number of snapshots b and the energy level p. A possible way of deciding the proper number of simulations and snapshots (besides some experimentation) would be to start with s = 1, and increment it if necessary. A good indicator that we have enough snapshots would be when small singular values start showing. Using an updating algorithm for the successive SVD's would be an efficient way to proceed [6].

Since the real expense is in the simulation, one can take b reasonably large to start with, and let the SVD analysis decide if some snapshots are not contributing energy to the reduced transfer function. In this way there is no *a priori* guess and we would stop as soon as there is enough information content in our data set of snapshots. With regards to the amount of energy that we want to preserve, that would be determined by experimentation or further analysis and/or physical intuition.

The use of a high-order method, such as the one in the pseudo-spectral code SpectralFlex, provides already a beneficial reduction in the initial number of spatial degrees of fredom (by a factor of up to 10,000 in 3D if compared with a second order finite element method). For realistic problems, the original system will still be too large and too time consuming for wholesale real-time simulation, and thus we need to be able to speedup the calculation further by using these order reduction techniques.

4 Example: Scalar wave equation

We consider as a simple test problem to validate these ideas the 1D scalar wave equation in a semi-infinite homogeneous half space, writen in first order form:

$$v_t = \rho^{-1} p_x,$$

$$p_t = K v_x,$$

where v, p are the velocity and the vertical component of the stress, respectively, while ρ, K are density and the constrained modulus. The initial and boundary conditions are:

$$\begin{array}{rcl} v(0,x) &=& 0, \\ p(0,x) &=& 0, \\ v(t,1) &=& 0, \\ p(t,0) &=& Ricker(t), \end{array}$$

where the forcing function is a 50 Hz Ricker wavelet with amplitude 1. We take for this experiment, $\rho = 2000 \ k/m^3$, $c_p = 3000 \ m/s$, $M = 1.8 \times 10^{10} P$.

Once the problem is discretized in space (on a staggered mesh using centered differences) we obtain the following block structure:

$$\begin{bmatrix} w_{1t} \\ w_{2t} \end{bmatrix} = \begin{bmatrix} 0 & A_{12} \\ A_{21} & 0 \end{bmatrix} \begin{bmatrix} w_2 \\ w_1 \end{bmatrix} + 2/\rho \ B \ R(t),$$

where the vectors w_1, w_2 contain the discretized values of v and p respectively, A_{12} , A_{21} are bi-diagonal and B is a vector with all zeroes except for the first component that is equal to 1. The 2 in the forcing term comes from the top and bottom free surface conditions. This is the full system of ODE's that we want to reduce. Due to the special structure it is convenient to continue the reduction in block form. Thus, let Φ_1, Φ_2 be the matrices of snapshots for v, p respectively, and let

$$\Phi_1 = U_1 \Sigma_1 V_1^T, \ \Phi_2 = U_2 \Sigma_2 V_2^T,$$

be their Singular Value Decompositions. Introducing the Ansatz:

$$w_1 = U_1 a_1(t), \ w_2 = U_2 a_2(t)$$

and replacing in the differential equation, after some additional manipulations we obtain the reduced system:

$$\begin{bmatrix} a_1' \\ a_2' \end{bmatrix} = \begin{bmatrix} 0 & U_1^T A_{12} U_2 \\ U_2^T A_{21} U_1 & 0 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} + 2/\rho \begin{bmatrix} U_1^T B_1 \\ 0 \end{bmatrix} R(t).$$

Observe that we can choose a different number of modes for each of the two sets of variables.

5 Numerical Results

We run our finite elements code FLEX for 5000 time steps, with $\delta t = 0.00033$, corresponding to a CFL condition of 0.99 for the problem above and collect 100 equally spaced time snapshots. FLEX uses leapfrog, a second order explicit integrator in time and essentially symmetric differences (on an staggered mesh) in space. For the reduced system we use as time integrator the code SVODE of Brown, Hirschman and Byrne [4] in its stiff option.

The first experiment simply tries to reproduce the results of FLEX by solving the same problem but within the reduced system. In Figure 1 we cross-plot the results of the 2 codes for a snapshot at the 1250th time step. The results are good to eye-ball accuracy. Observe that the two sets of variables differ in about 7 orders of magnitude.



Figure 1: Comparison of FLEX and MOR results. Ricker source at top (left end), t=0.4125. Top figure: velocity; bottom figure: vertical component of the stress.

In the second experiment (Figure 3) we solve the reduced system with a Ricker source at x = 500, with a frequency of 40 Hz and amplitude equal to 2 and show the snapshot at the 750th time step. We still cross-plot with the results for FLEX with the original source in order to verify visually the change in wave form and amplitude. Now we see wave pulses propagating in both direction from the center for the velocity, some extraneous results for the vertical component of the stress and substantial high frequency noise. Observe that the expected vertical stress amplitude is still 1, because of the way in which we apply this forcing function.

Finally, we repeat the second experiment but taking only 66 left singular vectors (i.e., we drop the 40 vectors associated with the smallest singular values, see Figure 2). Now, as hoped, we get much cleaner results and the system has 132 variables instead of 2000, a factor greater than 15 order reduction! (Figure 4).

These results will not be totally surprising to anyone familiar with least squares fitting. The bad results obtained when using too many basis functions are just another manifestation of the phenomenon of overfitting; i.e., we are approximating very faithfully spurious noise and amplifying it as we integrate along. Thus, it is doubly beneficial to filter out these highly oscillatory modes associated with the small singular values, since we also get an additional reduction in the size of the problem, i.e., enhanced data compression plus high frequency noise filtering.



Singular Values and Cummulative Frobenius Norm for 100 Modes

Figure 2: Singular values and cummulative Frobenius norm



Figure 3: Source for MOR at x=500; Ricker wavelet, frequency = 40 Hz, amplitude = 2.



Figure 4: Same as above, but MOR uses only 66 modes, instead of 100

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