Stability-Corrected Wave Functions and Structure-Preserving Rational Krylov Methods for Large-Scale Wavefield Simulations on Open Domains

Vladimir Druskin, Rob Remis, Mikhail Zaslavsky, Jörn Zimmerling

Abstract

In a first-order formulation, simulating wavefield propagation on unbounded domains amounts to solving the large order dynamical system

$$[A(s) + sI]u(s) = b(s) \quad \text{for all } s \in \Omega, \tag{1}$$

where Ω is the frequency interval of interest. In the above equation, $A(s)$ is the spatially discretized first-order hyperbolic wave operator and $u(s)$ and $b(s)$ are the unknown field and known source vectors, respectively. We note that $A(s)$ is frequency dependent in general, due to application of the coordinate stretching or Perfectly Matched Layer (PML) technique. This technique is included to simulate outward wave propagation towards infinity. Taking equation (1) as a starting point, we discuss two Krylov-based solution methods that solve wavefield problems on open domains. Some physical properties of the approximate solutions are discussed as well.

The first method linearizes the discretized wave operator with respect to frequency by setting up a frequency independent PML that constructs a set of *complex* PML spatial step sizes for a given frequency interval Ω [1]. The resulting linearized wave operator A no longer explicitly depends on frequency, but has complex entries and is unstable as well. Fortunately, this matrix can still be used to compute stable time-domain or conjugate-symmetric frequency-domain wave field approximations. Frequency-domain approximations, for example, can be obtained by evaluating the stability-corrected wave function [2]

$$u(s) = [r(A, s) + r(A^*, s)] b(s), \tag{2}$$

where the asterisk denotes complex conjugation and

$$r(z, s) = \frac{\eta(z)}{z + s} \tag{3}$$

is the filtered resolvent with $\eta(z)$ the complex Heaviside function defined as $\eta(z) = 1$ for $\text{Re}(z) > 0$ and $\eta(z) = 0$ for $\text{Re}(z) < 0$. Direct evaluation is not feasible, however, since the order n of matrix A is simply too large. The field vector $u(s)$ is therefore approximated by a polynomial Krylov reduced-order model $u_m(s)$ of order $m \ll n$. Such a model can be computed very efficiently via a three-term Lanczos-type recursion, since there exists a diagonal weighting matrix W such that $A^T W = W A$. Details about the construction of the algorithm, the physical significance of the weighting matrix W, and some of the convergence properties of the above reduction scheme will be discussed.

In the second Krylov reduction method, we do not linearize the wave operator with respect to frequency and we consider equation (1) directly. Specifically, we focus on rational Krylov subspace field approximations to the field vector $u(s)$ satisfying equation (1). Such an approach may be particularly beneficial in case the wavefield response on Ω and at a particular receiver location is dominated by a few modes of the wavefield operator as is the case in many applications in optics, for example [3].

In our rational Krylov reduction method, we construct structure-preserving reduced-order models that belong to the realification of a standard rational Krylov space spanned by the field vectors $u(s_i)$ with $s_i \in \Omega$, $i = 1, 2, ..., m$. Specifically, since there exists a frequency-dependent weighting matrix $W(s)$ such that $A^T(s)W(s) = W(s)A(s)$, we can show that the reduced-order models interpolate the field vector $u(s)$ at the frequencies s_i and s_i^*, for $i = 1, 2, ..., m$, provided the expansion coefficients are determined using a pseudo-Galerkin condition that depends on $W(s)$. Moreover, for monostatic field responses (source and receiver coincide), the derivative of the reduced-order model with respect to s interpolates the derivative of the field at the frequencies s_i and s_i^*, $i = 1, 2, ..., m$. Finally, since space and time are coupled in wavefield problems, we will discuss how the length of the time interval of observation in the time-domain is related to the number of expansion frequencies m and the order n of the total system.

References

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