Phase-preconditioned Rational Krylov Subspaces for wave simulation in open domains

Vladimir Druskin, Rob Remis, Mikhail Zaslavsky, Jörn Zimmerling

Abstract

Interpolatory Rational Krylov Subspaces (RKS) are a powerful tool for model order-reduction of large dynamic systems, preconditioning of shifted systems and spectral approximation. RKS model-order reduction of diffusive PDEs for instance clearly outperforms time stepping algorithms. However, RKS are barely used for model-reduction of large-scale dynamic systems representing wave propagation on unbounded domains. This, despite the fact that RKS show excellent convergence for resonant structures where the wave field can be expanded in a few eigenmodes of the system.
For non-resonant structures RKS techniques are less attractive as the frequency domain transfer function is highly oscillatory and the RKS approach is fundamentally limited by the Nyquist-Shanon sampling rate. More specifically, at least two interpolation points per period of the cut-off frequency of the transfer function are required, which can lead to thousands of interpolation points for large-scale wave propagation and thus prohibitively large RKS as these interpolation points need to be solved for every right hand side. We suggest to precondition the RKS via the phase term of the WKB approximation, easily obtainable from the eikonal equation.
This preconditioning makes the number of interpolation points dependent on the complexity of the wavespeed model rather than the Nyquist-Shanon sampling rate, which in turn is proportional to the largest arrival time present in the transfer function. Phase-preconditioning not only allows a reduction of interpolation points with respect to the Nyquist-Shanon rate but also allows us to reduce the number of spatial discretization points. After factoring out the main phase dependency of the wavefield it becomes spatially smooth which significantly lowers the number of points per wavelength needed for accurate modeling. Last, the preconditioned RKS basis only weakly depends on the right hand side of the system which allows a third level of model reduction. Specifically, the number of right hand sides for systems with multiples sources and receivers can be reduced with respect to standard techniques.
In summary, phase-preconditioning allows a reduction of all three computational aspects of wave simulation: number of RKS shifts, number of spatial discritization points and number of right hand sides.

1 Problem definition

After spatial discretization of a second-order wave equation on an open domain we obtain the nonlinear shifted-system

$$(\mathsf{A}(s) - s^2\mathsf{I})\mathsf{u}(s) = \mathsf{b} \tag{1}$$

with the wave operator $\mathsf{A}(s)$, wavefield u, right hand side b and Laplace paramter s. To model wave propagation on an unbounded domain we use a near-optimal PML as described in [1], which leads to the dependence of the operator $\mathsf{A}(s)$ on the Laplace parameter. The wave operator inherits the poperties of the underlying physics, such that it is follows the Schwartz reflection principle $\mathsf{A}(\bar{s}) = \bar{\mathsf{A}}(s)$, is symmetric with respect to a diagonal symmetry matrix $\mathsf{WA} = \mathsf{A}^T\mathsf{W}$ and is passive.

The symmetry and Schwarz reflection principle can be used to design a structure preserving rational Krylov subspace method that interpolates the original problem tangentially for coinciding source and receiver locations. Such an approach works well if the Hankel singular values of the system decay rapidly, meaning that only a few modes contribute to the solution as is the case for resonating structures with a few excited and observable modes [2]. Then the frequency domain response is well-described by a low-degree rational function and a rational Krylov technique will therefore quickly capture the desired wave field response. For waves characterized by large travel times, however, this may no longer be the case, since such responses are highly oscillatory in the frequency domain and sampling should at least take place at half the Nyqvist-Shanon sampling rate. As an illustration, consider a coinciding source/receiver pair with a reflector located at a travel time of $T^{\mathrm{arr}}/2$ away from the source. A transmitted pulse will arrive (without distortion) at the receiver after T^{arr}, so that the receiver measures the source wavelet convolved with $\delta(t - T^{\mathrm{arr}})$. In the frequency domain this translates to multiplication with $\exp(-sT^{\mathrm{arr}})$, which means that according to the Nyquits-Shanon sampling theorem the maximum frequency domain sampling distance is $\Delta\omega = \frac{\pi}{T^{\mathrm{arr}}}$. Clearly, the number of required frequency domain samples increases as the travel time increases leading to prohibitory large rational Krylov subspace approximations for these fields.

2 Phase Preconditioning

Intuitively we want the size of the Krylov subspace to depend on the complexity of the wavespeed model rather then the largest arrival time. To achieve this we propose to precondition the rational Krylov subspace method with the phase term obtained from the eikonal equation $|\nabla \mathsf{T}_{\mathrm{eik}}(x)|^2 = \frac{1}{c(x)^2}$, with wave speed $c(x)$. Every vector of the RKS is decomposed into a spatially smooth incoming and outgoing field amplitude by factoring out the WKB-phase term. More specifically, we decompose a single frequency solution $\mathsf{u}(s_j)$ as

$$\mathsf{u}(s_j) = g(s_j \mathsf{T}_{\mathrm{eik}})\mathsf{u}_{\mathrm{out}}(s_j) + g(\bar{s}_j \mathsf{T}_{\mathrm{eik}})\mathsf{u}_{\mathrm{in}}(s_j), \tag{2}$$

where $g(s\mathsf{T}_{\mathrm{eik}})$ is the WKB phase term. At evaluation of the reduced-order model all field amplitudes are then phase-corrected with the phase corresponding to the WKB-phase term of the evaluation frequency. The reduced-order solution can then be represented as

$$\mathsf{u}_m(s) = g(s\mathsf{T}_{\mathrm{eik}}) \sum_{j=1}^{m} a_j(s)\mathsf{c}_{\mathrm{out}}(s_j) + g(\bar{s}\mathsf{T}_{\mathrm{eik}}) \sum_{j=1}^{m} d_j(s)\mathsf{c}_{\mathrm{in}}(s_j), \tag{3}$$

were $g(s\mathsf{T}_{\mathrm{eik}})$ denotes the phase term of the WKB approximation and the coefficients $a_j(s)$ and $d_j(s)$ follow form a Galerkin condition. Clearly this makes the basis of the rational Krylov subspace frequency *dependent*, which is necessary in order to precondition a spectral problem like equation (1) for all shifts s. Doing so can be seen as spectral weighting were the residues associated with poles far away from the evaluation frequency are deweighted by projecting the operator $\mathsf{A}(s)$ onto the frequency dependent subspace. Spectral problems can in principle not be preconditioned by one preconditioner for all shifts s, as one can in practice not achieve perfect pole zero cancellation. Thus, convergence of a RKS method can only be enhanced by increasing the subspace size, which is computaionally advantageous if the computational cost is dominated by solving shifted systems rather then projection of the operator onto the subspace, as is the case in the cosidered example of wave operators. This is the central idea of the presented approach.

The amplitudes $\mathsf{c}_{\mathrm{out/in}}(s_j)$ obtainable via one-way wave equations are spatially smooth compared to the original wavefield $\mathsf{u}(s)$. Therefore, they can be computed on a much coarser grid then necessary to accurately compute the original wavefield, which significantly reduces the cost of subspace construction. Admittedly, coarse spatial discretization increases numerical dispersion, which can be counterbalanced by correcting the wavespeed $c(x)$ for numerical dispersion while constructing the RKS. The basic idea is that numerical differentiation of the WKB phase term should cancel the asymptotically dominant term $-s^2\mathsf{I}$ in the wave equation (1). After subspace construction with a dispersion corrected, coarse operator we project a wave operator of high accuracy onto the phase-preconditioned subspace to obtain the phase-preconditioned reduced-order model.

Since the subspace is phase corrected the reduced-order model can now extrapolate, meaning the reduced-order model can be evaluated for shifts outside the convex hull of interpolation points. Especially if $c(x)$ is a smooth function this allows extrapolation to frequencies which are not resolvable with the grid used to construct the RKS. For smooth configurations taken from geophysics we obtain accurate results for wavelets with a cutoff frequency of roughly 2.7 spatial points per wavelength with a second order operator.

In this contribution we discuss extensions of the outlined method to systems with multiple sources and receivers and discuss how right hand sides can be reduced on top of reduction of the spatial grid and frequency domain interpolation points. We present numerical experiments showing that reduced-order models with phase preconditioning can indeed extrapolate.

References

[1] Vladimir Druskin, Stefan Güttel, Leonid Knizhnerman "Near-Optimal Perfectly Matched Layers for Indefinite Helmholtz Problems", *SIAM Review*, No 1, Volume 58, pp. 90-116, 2016,doi:10.1137/140966927

[2] Peter Benner, Serkan Gugercin, Karen Willcox, "A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems", *SIAM Review*, No 4, Volume 57, pp. 483-531, 2015, doi:10.1137/130932715