Exponential Krylov subspace time integration for nanophotonics applications

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Behavior of light in nanophotonics structures such as photonic crystals or layers of strongly scattering materials is often described by the time dependent Maxwell equations. The equations are usually supplied with the nonreflecting boundary conditions, e.g., the so-called perfectly matched layers (PML). The method of choice for solving these problems by physicists and engineers is the finite difference time domain method. This method is based on the staggered finite differences in space and staggered leap-frog in time.
In this talk we demonstrate that exponential time integration with Krylov subspace evaluations of the matrix exponential actions can be efficient in these applications. We discuss how the following techniques can be employed to achieve this efficiency [2].

1. To keep the Krylov subspace dimension moderate, the rational shift-and-invert (SAI) Krylov subspaces are used [4, 5]. This means that instead of the regular Krylov subspace $\mathcal{K}_m(A, v) = \{v, Av, \ldots, A^{m-1}v\}$, we work with $\mathcal{K}_m((I + \gamma A)^{-1}, v)$ for some $\gamma > 0$.

2. In three space dimensions, the actions of $(I+\gamma A)^{-1}$ should be carried out by iterative linear solvers and we briefly discuss some preconditioning strategies to do this.

3. In our (limited) experience, it is crucial to employ the Krylov subspace in such a way that one (or just several) Krylov subspace(s) suffice for the whole time interval. For non-autonomous problems this leads to block Krylov subspaces [1].

In some cases these techniques result in a method exhibiting an optimal performance in the sense that the number of Krylov subspace outer (for the matrix exponential actions) and inner (for $(I + \gamma A)^{-1}$ actions) iterations do not grow as the spatial mesh gets finer. Finally, we comment on how this approach is related to a general across-time waveform relaxation framework [3]. This facilitates an across-time parallelization of the method, which is a topic of our current research.

References

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