Matrix exponential and Krylov subspaces for fast time domain computations: recent advances

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We show how finite difference (or finite element) time domain computations can be accelerated by employing recent advances in the matrix exponential time integration and Krylov subspace techniques.

Matrix exponential time integration: no time stepping!

The finite difference time domain (FDTD) method is an efficient tool to model photonic nanostructures numerically. The standard FDTD method can be seen an application of the staggered leap frog time integration to the system of ordinary differential equations

$$y'(t) = -Ay(t), \quad y(0) = v, \qquad A \approx \begin{bmatrix} 0 & \mu^{-1}\nabla\times \\ \varepsilon^{-1}\nabla\times & \sigma\cdot \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

Here A is the discrete Maxwell operator discretized in space by the standard staggered Yee method. μ, ε and σ are (relative) permeability, permittivity and conductivity, respectively. The vector function $y(t)$ contains unknown components of the magnetic and electric fields.

By using the matrix exponential operator, solution of the system can be written as $y(t) = \exp(-tA)v$. Numerical algorithms, which are based on this approach, are called exponential time integration methods. The essential point is that not the matrix exponential itself but rather *its action* on the vector v is computed. An attractive feature of the formula $y(t) = \exp(-tA)v$ is that it provides solution for virtually any time moment, without time stepping. Often, this leads to a significantly faster time solution than with the standard time integration, such as the classical FDTD method.

Rational shift-and-invert Krylov subspace techniques

An efficient way to compute the actions of $\exp(-tA)$ is by employing the so-called Krylov subspace methods. In this approach a projection of A onto the Krylov subspace $\text{span}\{v, Av, A^2v, \ldots, A^{k-1}v\}$ is used and the approach is efficient as soon as $k \ll n$. Recently, an improvement has been proposed to the Krylov subspace methods for computing the actions of the matrix exponential, namely, the shift-and-invert Krylov subspace method. This method belongs to the class of the rational Krylov subspace methods. It provides a very fast and often grid independent convergence for the price of solving linear systems. We discuss its implementation issues.

Block Krylov subspaces to accommodate source terms

Source terms are often dealt with incorporating an inhomogeneous term $g(t)$ into the discretized Maxwell equations, e.g.,

$$y'(t) = -Ay(t) + g(t), \quad y(0) = v.$$

The presence of the source term renders the formula $y(t) = \exp(-tA)v$ invalid and usually one applies a time stepping where the matrix exponential approach can used at each time step. We propose another, often more efficient, approach. It is based on a low rank approximation of the source term $g(t)$ and a special block Krylov subspace method.