A Comparison of Krylov Subspace Methods and Time-Stepping for TEM Simulation

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TEM

Geophysical exploration via transient electromagnetic fields (TEM) is a technique for inferring properties of the subsurface by observing the response over time to controlled electromagnetic sources. Here we consider the forward problem of computing the electromagnetic field due to a vertical magnetic dipole, a configuration often used in practice.

The governing equations are the quasi-static Maxwell's equations

$$\nabla\times\left(\frac{1}{\mu}\nabla\times\boldsymbol{e}\right)+\partial_t\sigma\boldsymbol{e}=-\partial_t\boldsymbol{j}^e, \tag{1}$$

where

$\boldsymbol{e}=\boldsymbol{e}(\boldsymbol{x},t)$	is the electric field,
$\mu=\mu(\boldsymbol{x})$	is the magnetic permeability,
$\sigma=\sigma(\boldsymbol{x})$	is the electric conductivity and
$\boldsymbol{j}^e=\boldsymbol{j}^e(\boldsymbol{x},t)$	is the impressed source current density.

The spatial domain is typically a parallelepiped $\Omega\subset\mathbb{R}^3$ whose upper boundary is either at ground surface level or above it. In the simplest model, the perfect conductor boundary condition $\boldsymbol{n}\times\boldsymbol{e}=\boldsymbol{0}$ is imposed on all six faces of $\partial\Omega$.

The impressed source current is typically of *shut-off* type, i.e., of the form

$$\boldsymbol{j}^e(\boldsymbol{x},t)=\boldsymbol{q}(\boldsymbol{x})H(-t) \tag{2}$$

where H denotes the Heaviside unit step function and the vector field $\boldsymbol{q}$ describes the spatial current pattern.

Yee Discretization

We subdivide the spatial domain Ω into a graded grid with small spacing near the source and increasing spacing as we move away from it. We use a staggered grid (Yee, 1966) with electric components at the center of the edges and magnetic components at the center of the faces, creating a system of elementary electric and magnetic loops, as shown in Figure 1.

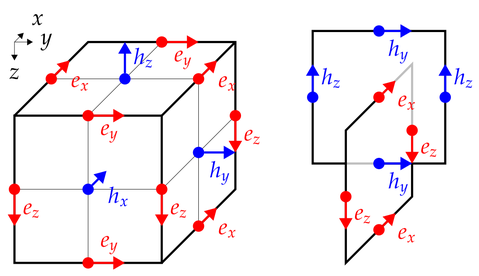

Figure 1: Yee cell and elementary electric/magnetic loops.

Time-Stepping Techniques

The reference of our comparison is the well known Du Fort-Frankel method proposed in (Wang & Hohmann, 1993), which is explicit and solves the coupled first-order Maxwell's equations.

Given an initial electric field $\boldsymbol{e}_0$ at time t_0, and an initial magnetic field $\boldsymbol{h}_0$ at time $t_0+\Delta t_0/2$ we perform a leap-frog iteration. In each step we first compute the electric field $\boldsymbol{e}_j$ from $\boldsymbol{e}_{j-1}$ and $\boldsymbol{h}_{j-1}$ and then the magnetic field $\boldsymbol{h}_j$ from $\boldsymbol{h}_{j-1}$ and $\boldsymbol{e}_j$. With $\delta_{\min}$ denoting the smallest mesh size this method is stable if

$$\Delta t_j=t_{j+1}-t_j<\delta_{\min}\sqrt{\frac{\mu_{\min}\sigma_{\min}t_j}{6}}.$$

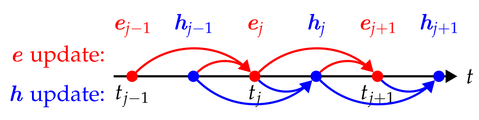

Figure 2: Iteration scheme of the Du Fort-Frankel method.

Apart from Du Fort-Frankel we tested ROCK4, an implementation of fourth order Chebyshev methods. These explicit Runge-Kutta methods are particularly well suited for parabolic initial values problems like those discussed here.

Krylov Subspace Methods

Starting with (1) and omitting the impressed source current the problem is now reduced to the solution of a linear ordinary differential equation of first order

$$\partial_t\boldsymbol{e}=A\boldsymbol{e},\quad \boldsymbol{e}(t_0)=\boldsymbol{e}_0, \tag{3}$$

where the discrete action of $-1/\sigma\,\nabla\times(1/\mu\,\nabla\times\cdot)$ on the spatial discretization of the electric field $\boldsymbol{e}$ is represented by the matrix A. The solution of (3) is given explicitly by

$$\boldsymbol{e}(t)=\mathrm{e}^{(t-t_0)A}\,\boldsymbol{e}_0.$$

Therefore the solution can be obtained by evaluating the exponential function for a large sparse matrix times a vector $\boldsymbol{e}_0$. This is what Krylov subspace methods are well suited for.

Krylov Subspace Methods for Matrix Functions

Given a square matrix $A\in\mathbb{R}^{N\times N}$ (large and sparse), a vector $\boldsymbol{b}\in\mathbb{R}^N$ and a scalar function $f(x)$ which is defined in a neighborhood of the eigenvalues of A, then

$$f(A):=p(A),$$

where $p(\cdot)$ is a polynomial of degree $<N$ that Hermite-interpolates f in the eigenvalues of A. By $\mathcal{K}_m(A,\boldsymbol{b})$ we denote the m-th Krylov space of $\boldsymbol{b}$ and A, that is

$$\mathcal{K}_m(A,\boldsymbol{b})=\mathrm{span}\{\boldsymbol{b},A\boldsymbol{b},A^2\boldsymbol{b},\ldots,A^{m-1}\boldsymbol{b}\}.$$

Since, by definition, $f(A)$ is a polynomial in A of degree $<N$ there holds

$$f(A)\boldsymbol{b}\in\mathcal{K}_N(A,\boldsymbol{b}).$$

The idea of Krylov subspace methods for the approximation of matrix functions can be stated briefly as: Choose Krylov approximations $\boldsymbol{f}^m=p_m(A)\boldsymbol{b}\in\mathcal{K}_m(A,\boldsymbol{b})$ such that $\boldsymbol{f}^m\approx f(A)\boldsymbol{b}$.

There exist very effective methods that achieve good approximates $\boldsymbol{f}^m$ even for fairly small m. Such a method is the *Arnoldi method:*

- Generate an orthonormal basis $V_m=[\boldsymbol{v}_1,\boldsymbol{v}_2,\ldots,\boldsymbol{v}_m]$ of $\mathcal{K}_m(A,\boldsymbol{b})$ using a Gram-Schmidt procedure that satisfies
$$V_m^TAV_m=H_m,$$
where $H_m\in\mathbb{R}^{m\times m}$ is an upper Hessenberg matrix.
- The *Arnoldi approximation of order m* is defined as
$$\boldsymbol{f}^m:=\|\boldsymbol{b}\|V_mf(H_m)[1,0,\ldots,0]^T.$$

If A is Hermitian then H_m is tridiagonal. Instead of orthonormalizing the vector $\boldsymbol{v}_m$ against all preceding $\boldsymbol{v}_1,\ldots,\boldsymbol{v}_{m-1}$, there exists a three-term recurrence involving only $\boldsymbol{v}_{m-2}$, $\boldsymbol{v}_{m-1}$ and $\boldsymbol{v}_m$. This method is called the *Lanczos method* and in comparison to the Arnoldi method

- computation time decreases rapidly (since only 2 orthogonalizations per time step are necessary),
- the memory requirements reduce to storing only 2 vectors of length N for the overall solution process.

Time-Stepped Arnoldi Method

Given $\boldsymbol{e}_0$ at t_0 we are interested in evaluating the electric fields $\boldsymbol{e}_1,\boldsymbol{e}_2,\ldots,\boldsymbol{e}_n$ at times $t_1<t_2<\cdots<t_n$ from a given interval $[t_0,t_n]$.

For each time step j we compute the Arnoldi approximation of order $m=m(j)$

$$\boldsymbol{f}_{j+1}^m\in\mathcal{K}_m(A,\boldsymbol{f}_j^m)\ \text{ for } f(x)=\mathrm{e}^{(t_{j+1}-t_j)x},$$

where $\boldsymbol{f}_0^m=\boldsymbol{e}_0$. From error analysis of Krylov subspace methods it is a well known fact that to guarantee a certain relative error of the Krylov approximation $\boldsymbol{f}_{j+1}^m$ we should choose

$$m=m(j)\sim\|(t_{j+1}-t_j)A\|^{1/2}.$$

The drawback of this method is that we build a new Krylov space for each time step which may be computationally unfeasible.

Arnoldi Method with Recycling

For each time step j we compute the Arnoldi approximation

$$\boldsymbol{f}_j^m\in\mathcal{K}_m(A,\boldsymbol{e}_0)\ \text{ for } f(x)=\mathrm{e}^{(t_j-t_0)x},$$

where we choose $m=m(j)\sim\|(t_j-t_0)A\|^{1/2}$.

Our proposed method reuses the computed basis vectors $\boldsymbol{v}_1,\boldsymbol{v}_2,\ldots,\boldsymbol{v}_{m(j)}$ for the time step $j+1$, just adding the vectors $\boldsymbol{v}_{m(j)+1},\boldsymbol{v}_{m(j)+2},\cdots,\boldsymbol{v}_{m(j+1)}$.

This approach was found to be most efficient, although the number $m(j)$ of required Krylov vectors is slightly larger than that for the *time-stepped Arnoldi method*, since the time-interval is longer.

Restarted Arnoldi Method

If the matrix A cannot be symmetrized, e.g., due to boundary conditions, we may easily run out of memory when using the Arnoldi method, since m vectors of length N need to be stored. To overcome this problem we use a restarted Arnoldi method (Eiermann & Ernst, 2006). The idea of such a method is to compute an Arnoldi approximation $\boldsymbol{f}^m$ for a sufficiently small m and to run a new Arnoldi method using the last computed basis vector as a new starting vector.

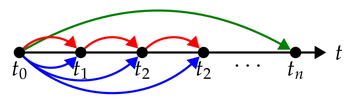

Figure 3: Considered computational strategies.

Numerical Experiments

In our numerical experiments the grid consists of $58\times58\times58$ cells, yielding 565326 degrees of freedom for the electric field.

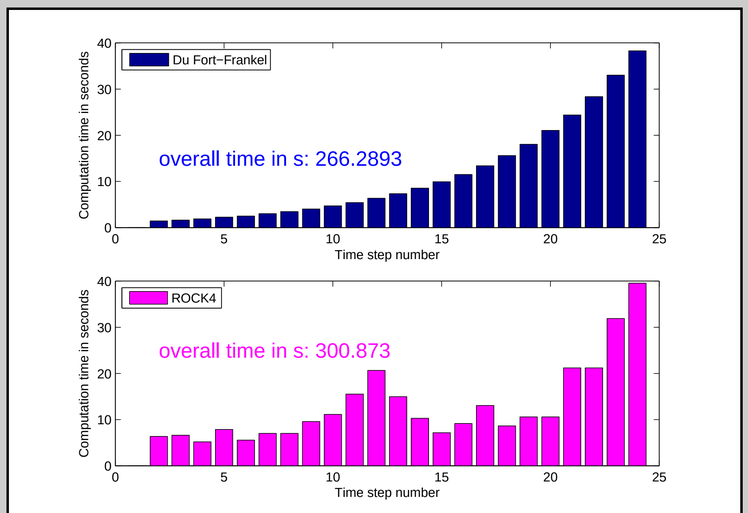

Figure 4: Du Fort-Frankel/ROCK4. Computational effort.

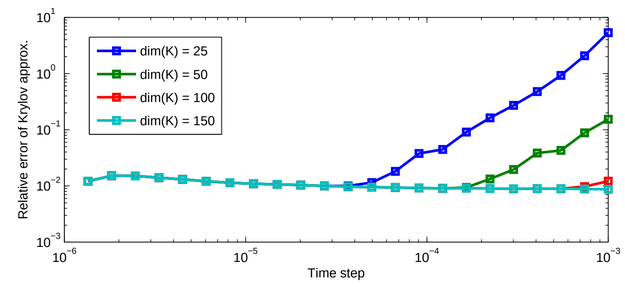

Figure 5: Lanczos time-stepping. Dependence of relative error on time step and fixed Krylov subspace size m. Computational effort is approximately proportional to m.

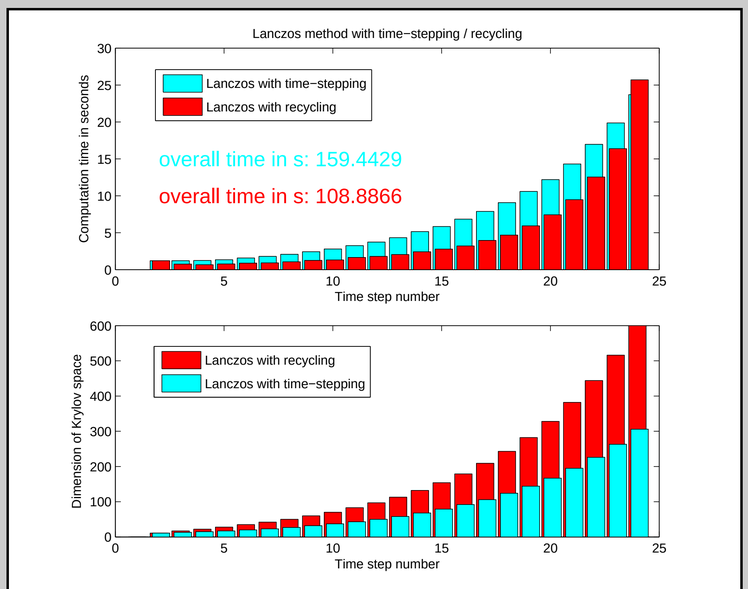

Figure 6: Lanczos time-stepping/recycling. Computational effort and required Krylov subspace size.

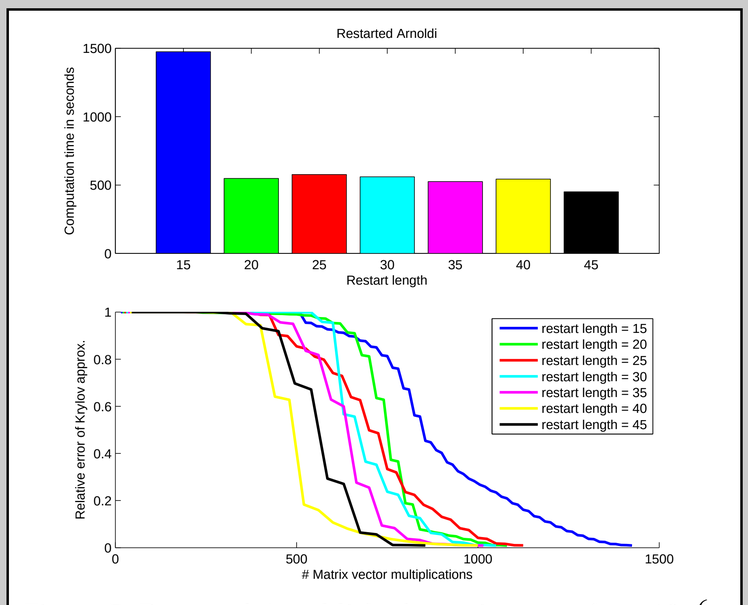

Figure 7: Restarted Arnoldi for large time step from $10^{-6}\,s$ to $10^{-3}\,s$. Computational effort and convergence behavior.

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