# Krylov Subspace Approximation for TEM Simulation in the Time Domain

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## Summary

Forward transient electromagnetic modeling requires the numerical solution of a linear constant-coefficient initial-value problem for the quasi-static Maxwell equations. After discretization in space this problem reduces to a large system of ordinary differential equations, which is typically solved using finite-difference time-stepping. We compare standard time-stepping schemes such as the explicit and unconditionally stable Du Fort-Frankel scheme with the more recent Runge-Kutta-Chebyshev methods, which are designed specifically for parabolic initial value problems, with Krylov subspace techniques for the explicit solution of the initial value problem using the matrix exponential. Besides the classic Arnoldi/Lanczos approximation we also consider restarted Arnoldi approximations as were recently proposed in (Eiermann & Ernst, 2006). These restarted schemes have the advantage of requiring only an a priori fixed amount of memory storage, a significant aspect in the context of 3D simulations.

We also present a recent efficient implementation (Afanasjew, Ernst, Güttel, & Eiermann, to appear) of the restarted Arnoldi method for evaluating the matrix exponential.

## 1 TEM – Governing Equations

Geophysical exploration using 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.

## 2 Semidiscretization in Space

Omitting the impressed source current $\boldsymbol{j}^e(\boldsymbol{x},t)$ in (1)—since we are looking at times $t>0$—the PDE becomes

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

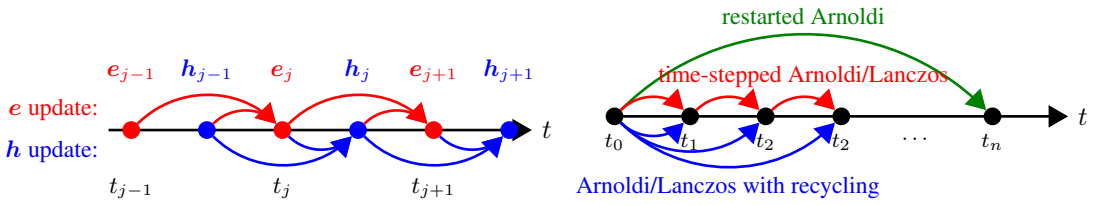


**Figure 1:** Leap-frog iteration of the Du Fort-Frankel method with time-interleaved electric and magnetic fields (left). Considered computational strategies for Krylov subspace methods (right).

To discretize this equation in space, we introduce a graded tensor-product mesh on the spatial domain $\Omega$, which is refined near the source. The curl-curl equation is then discretized using the well-known Yee finite-difference scheme (Yee, 1966), which transforms the PDE to the linear first-order ordinary differential equation

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

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

$$\boldsymbol{e}(t) = \mathrm{e}^{(t-t_0)A}\, \boldsymbol{e}_0. \tag{3}$$

Our objective, given an initial field $\boldsymbol{e}_0$ at $t = t_0$, is to evaluate the solution $\boldsymbol{e}(t)$ at given discrete time values $t_1 < t_2 < \cdots < t_n$ in an integration interval $[t_0, t_n]$.

## 3 Time-Stepping

Semi-discretized initial-value problems like (ODE) are traditionally solved using a time-stepping scheme. The reference scheme for our comparisons is the Du Fort-Frankel scheme, an explicit time-integrator with a weak stability constraint on the time step, which was proposed for TEM forward modelling in (Wang & Hohmann, 1993).

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 (Figure 1, left). 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

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

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.

## 4 Krylov Subspace Methods

As an alternative to time-stepping, one could evaluate (3) directly, which entails multiplying a matrix exponential with the initial vector $\boldsymbol{e}_0$. As the matrix $A$ is large and sparse, this can be achieved efficiently with a Krylov subspace approximation. This gives rise to various implementations depending on time and memory constraints. Some computational strategies based on Krylov subspace methods are illustrated in Figure 1 (right).

### 4.1 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

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

Krylov subspace methods approximate $f(A)\boldsymbol{b}$ by suitable vectors $\boldsymbol{f}^m = p_m(A)\boldsymbol{b} \in \mathcal{K}_m(A, \boldsymbol{b})$ from lower order Krylov spaces, i.e., with $m \ll N$. The basic steps are as follows:

- Generate an orthonormal basis $V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m]$ of $\mathcal{K}_m(A, \boldsymbol{b})$ using the *Arnoldi process*, yielding the projected matrix $H_m := V_m^T A V_m \in \mathbb{R}^{m\times m}$, which is an upper Hessenberg matrix.
- The *Krylov subspace approximation of order* $m$ is defined as

$$\boldsymbol{f}^m := V_m f(H_m) V_m^T \mathbf{b} = \|\mathbf{b}\| V_m f(H_m)[1, 0, \ldots, 0]^T.$$

If $A$ is Hermitian then the *Lanczos process*, in place of the Arnoldi process, may be used to generate the basis. In this case $H_m$ is tridiagonal and, instead of orthonormalizing each vector $\boldsymbol{v}_m$ against all preceding vectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m-1}$, there exists a three-term recurrence involving only $\boldsymbol{v}_{m-2}$, $\boldsymbol{v}_{m-1}$ and $\boldsymbol{v}_m$.

### 4.2 Time-Stepped Arnoldi Method

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 known 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.

### 4.3 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 $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_{m(j)}$ for the time-step $j + 1$, just adding the vectors $\mathbf{v}_{m(j)+1}, \mathbf{v}_{m(j)+2}, \ldots, \mathbf{v}_{m(j+1)}$.

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.

### 4.4 Restarted Arnoldi Method

The restarted Arnoldi method introduced in (Eiermann & Ernst, 2006) generates a succession of Krylov spaces of a fixed maximal size $m$. The approximations are then chosen from the union of all Krylov spaces generated up to that point. The advantage is that one never needs to store more than $m$ basis vectors. Moreover, for the exponential function required in this context, the superlinear convergence of the unrestarted method is retained.

In (Afanasjew et al., to appear), this method was further enhanced by evaluating $f(H_m)$ using a suitable rational approximation of fixed order, which amounts computationally to the solution of a small number of linear systems of equations with coefficient matrix $H_m$, a small, constant amout of work in each restart cycle. Moreover, error estimators giving upper and lower bounds of the approximation error can be generated inexpensively in each step.

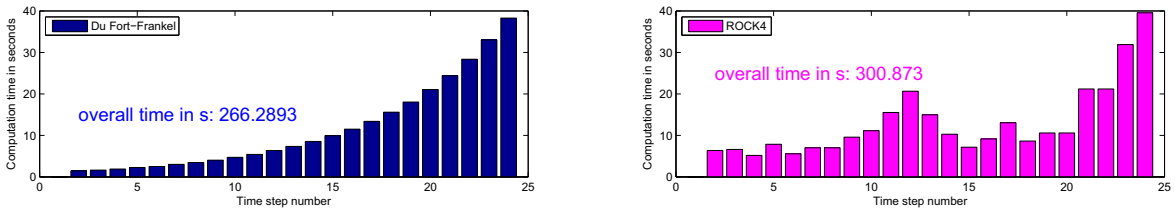


**Figure 2:** Du Fort-Frankel/ROCK4. Computational effort.

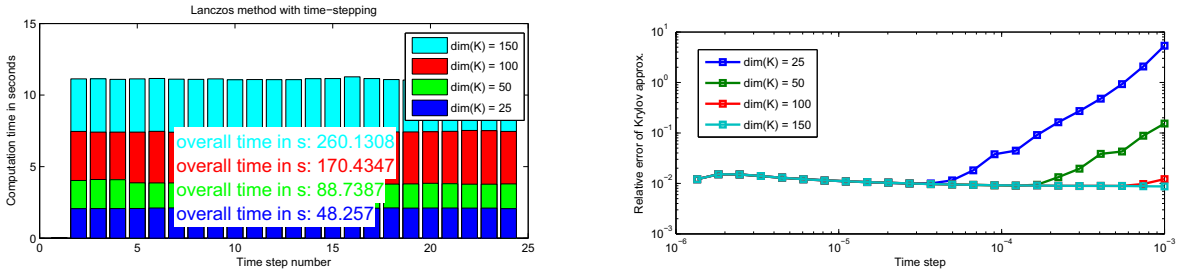


**Figure 3:** Lanczos method with time-stepping. Here $m$ is constant for all time steps $j$.

## 5 Numerical Experiments

We solve (1) on a cube with constant conductivity and permittivity. The finite-difference mesh consists of $58 \times 58 \times 58$ cells, resulting in $565,326$ degrees of freedom for the electric field. We evaluate the solution at $24$ logarithmically equispaced times between $10^{-6}$ s and $10^{-3}$ s. All computations were performed until the relative error was below $10^{-2}$.

In Figure 2 we compare the performance of the Du Fort-Frankel method with the more sophisticated ROCK4 method. As can be seen in the bar graphs, ROCK4 gets outperformed despite perfoming fewer time steps. We believe that this is due to its relatively high per-step overhead compared to the simplistic iteration scheme in Du Fort-Frankel.

Turning to the Krylov subspace methods, Figure 3 shows the computational effort for the time-stepping strategy. The times are merely illustratory since using a constant Krylov subspace size for every (exponentially growing) time step is wasteful. The figure nicely relates the size of the Krylov subspace to the achievable relative error.

The tradeoff between computation time and memory consumption can be seen in Figure 4. We compare the running time—total and per time step—and the size of the required Krylov subspace, that directly corresponds to the required memory. In this example, having enough memory available can save up to a third of the overall computation time.

Table 1 summarizes the performance of the restarted Arnoldi method for a single large time step from $10^{-6}$ s to $10^{-3}$, requiring an error below $10^{-12}$. While the non-restarted Krylov algorithms perform faster they require a—in most cases—prohibitively big amount of memory compared to the constant storage requirements for the restarted variant.

Finally, Figure 5 contains a plot of the transient of the electric field at a distance of $26.2$ m from the source. We see a good agreement between the transients produced by both methods. The faster Krylov method is even somewhat closer to the analytic solution since it—in contrast to the Du Fort-Frankel method—does not require discretization in time.

| $m$ | time[s] | mvp | error |
|---|---|---|---|
| 70 | 112 | 1400 | 9.13e-13 |
| 90 | 118 | 1350 | 2.01e-13 |
| full 2-pass | 144 | 2144 | 9.93e-13 |
| full 1-pass | 86 | 1072 | 9.93e-13 |

**Table 1:** Computing times for the restarted Arnoldi method for various restart lengths.

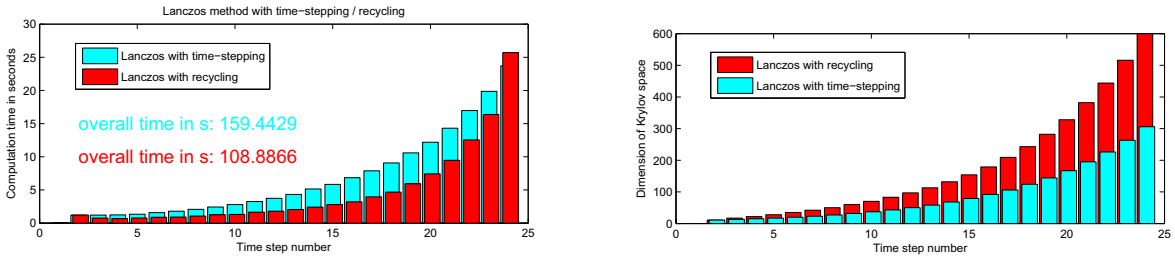


**Figure 4:** Comparing Lanczos time-stepping and recycling.

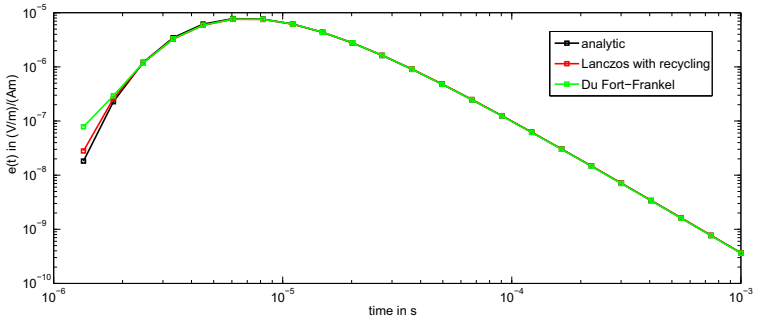


**Figure 5:** Transient electric field at a distance of 26.2 m from the source.

## Conclusions

Krylov subspace approximation is an efficient computational tool for integrating the initial value problem (ODE), arising in TEM forward modelling. The restarted Arnoldi method for the matrix exponential offers the possibility for the user to tradeoff storage requirements against speed, a possibility not offered by competing Krylov subspace methods such as SLDM.

## Acknowledgments

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