Krylov Subspace Methods for an Initial Value Problem Arising in TEM

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Problem Description

Our Aim

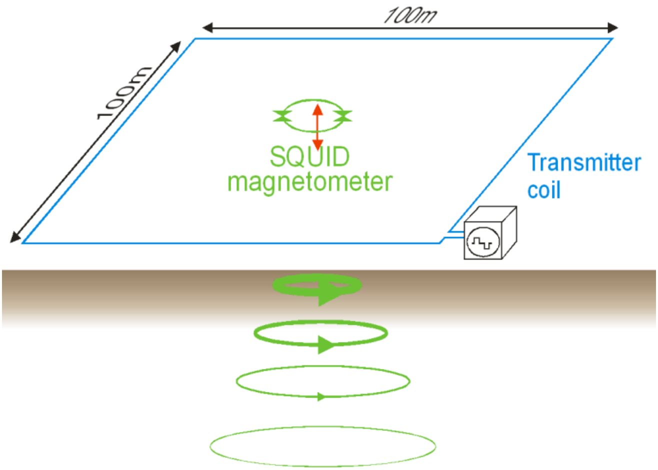
Our aim:

- Simulate propagation of transient electromagnetic fields (TEM) in the subsurface.
- Fields are a response to controlled electromagnetic sources.
  - Here: Vertical magnetic dipole.
- Solve the forward problem.

Practical aspects:

- TEM is an important method in geophysical exploration to infer properties of the subsurface.

Typical Setup



Governing Equations

Quasi-static Maxwell's equations:

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

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,
$\boldsymbol{j}^e=\boldsymbol{j}^e(\boldsymbol{x},t)$	is the impressed source current density

with $\boldsymbol{x}\in\Omega\subset\mathbb{R}^3$ and $t\in\mathbb{R}$.

Further Assumptions

- Typically, the spatial domain Ω is a parallelepiped with its upper boundary at ground level or above it.
- We assume the perfect conductor boundary condition $\boldsymbol{n} \times \boldsymbol{e} = \boldsymbol{0}$ on $\partial\Omega$.
- The impressed source current is typically of *shut-off type*, i.e. of the form

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

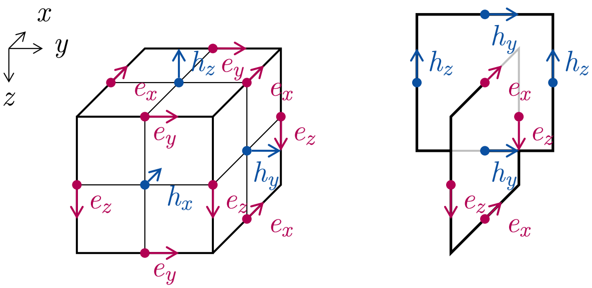
  with H denoting the Heaviside unit step function and the vector field $\boldsymbol{q}$ being the spatial current pattern.
  - In our case the right-hand side of (Maxwell) vanishes since we are looking at times $t > 0$.

Spatial Discretization

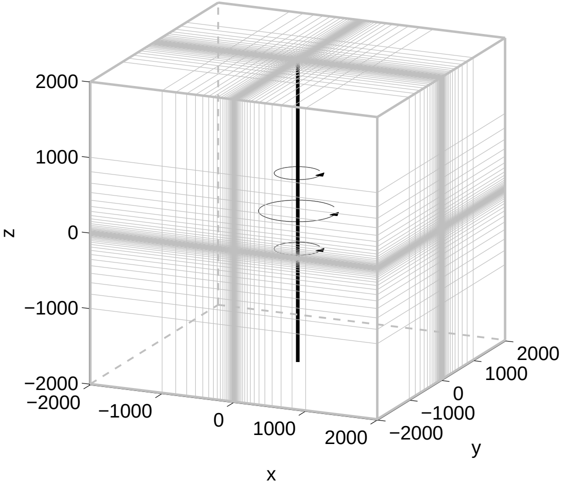
Spatial Discretization

Subdivision of spatial domain Ω:

- Graded grid.
- Increasing cell size as we move away from the source.
- Staggered grid (Yee grid).
  - Electric components $\boldsymbol{e}$ at the center of the edges.
  - Magnetic components $\boldsymbol{h}$ at the center of the faces.
  - System of elementary electric and magnetic loops.



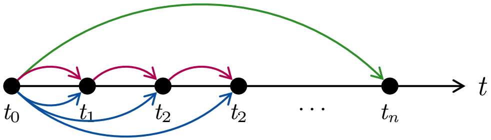
Example of a Graded Grid



Computational Strategies

Computational Strategies

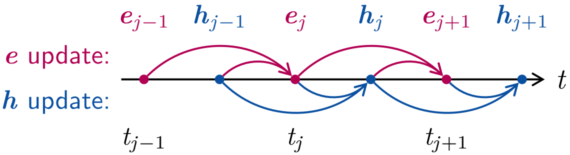
- We usually start with an initial solution to the electric field $\boldsymbol{e}_0$ at a time $t_0 > 0$. Our interest lies in computing $\boldsymbol{e}_j = \boldsymbol{e}(t_j)$ at few times t_j with $t_{j-1} < t_j$ for $0 < j \leq n$.
- Depending on the used method we have different possibilities:
  - Small steps calculating $\boldsymbol{e}_j$ from $\boldsymbol{e}_{j-1}$.
  - Steps of increasing size calculating $\boldsymbol{e}_j$ from $\boldsymbol{e}_0$.
  - One big step calculating $\boldsymbol{e}_n$ from $\boldsymbol{e}_0$.



Time-Stepping Methods

Du Fort-Frankel Method

- Proposed by [Wang & Hohmann, 1993].
- Explicit.
- Solves coupled first-order Maxwell's equations.
- Uses Yee grid for spatial dicretization.
- Computes time-interleaved electric fields $\boldsymbol{e}_j$ and magnetic fields $\boldsymbol{h}_j$ in a leap-frog type iteration.



Stability of the Du Fort-Frankel Method

This method was shown to be stable if

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

where

$\Delta x_{\min}$	is the smallest grid size,
$\mu_{\min}$	is the minimal magnetic permeability,
$\sigma_{\min}$	is the minimal electric conductivity.

Krylov Subspace Methods

Rewriting the Problem (I)

To apply Krylov subspace methods we have to rewrite our problem. Starting with (Maxwell) we get

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

This reduces to the solution of a linear first-order ordinary differential equation

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

where A represents the discrete action of $-{}^1\!/\!_\sigma \nabla \times ({}^1\!/\!_\mu \nabla \times \cdot)$ on the spatial discretization of the electric field $\boldsymbol{e}$.

Rewriting the Problem (II)

An explicit solution of (ODE) is given by

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

Thus, we have to evaluate the exponential function for a sparse matrix times a vector, which is what Krylov subspace methods are well suited for.

Arnoldi/Lanczos Procedure

- We define the m-th Krylov subspace as follows

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

- Generate an orthornormal 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/three-term recurrence relation satisfying

$$V_m^\top A V_m = H_m$$

with $H_m \in \mathbb{R}^{m\times m}$ upper Hessenberg/tridiagonal.

- Calculate the Arnoldi approximation of order m

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

Time-Stepping, Recycling, and Restarts (I)

- Remember: Given $\boldsymbol{e}_0$ at time t_0 we are interested in evaluating the electric fields $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n$ at times $t_1 < t_2 < \ldots < t_n$ from an interval $[t_0, t_n]$.
- Time-stepped Arnoldi
  - In each time step we compute

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

    with $\boldsymbol{f}_0^m = \boldsymbol{e}_0$ and $m = m(j) \sim \|(t_{j+1} - t_j)\, A\|^{1/2}$. Such a choice of $m(j)$ guarantees a certain relative error for our approximation.
  - This approach requires us to build a new Krylov subspace in every time step.

Time-Stepping, Recycling, and Restarts (II)

- Arnoldi with Recycling
  - Similarly to the time-stepped variant we compute in each step

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

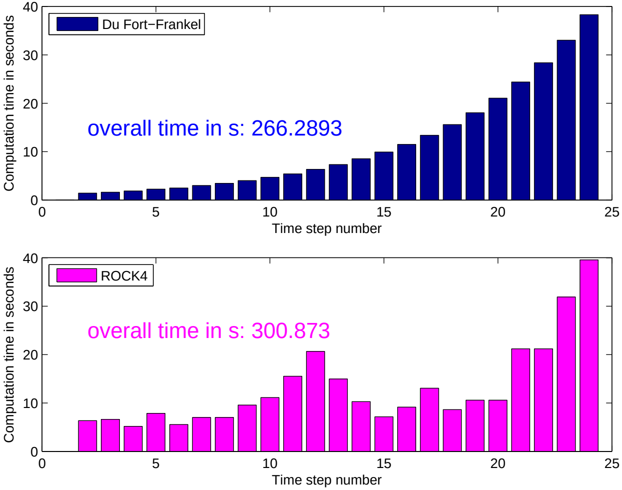
    with $m = m(j) \sim \|(t_j - t_0)\, A\|^{1/2}$. This allows us to reuse basis vectors from the $j-1$-th step and only compute the additional basis vectors $\boldsymbol{v}_{m(j)+1}, \boldsymbol{v}_{m(j)+2}, \ldots, \boldsymbol{v}_{m(j+1)}$.
- Restarted Arnoldi Method
  - If A cannot be symmetrized the unrestarted Arnoldi method might require a prohibitively high number of basis vectors. To overcome this problem a restared Arnoldi method was proposed in [Eiermann & Ernst, 2006] where we discard all but the last basis vector after every m steps and start to build a new Krylov subspace starting with this last vector.
  - See Stefan Güttel's talk today at 18:20 (same session).

Numerical Examples

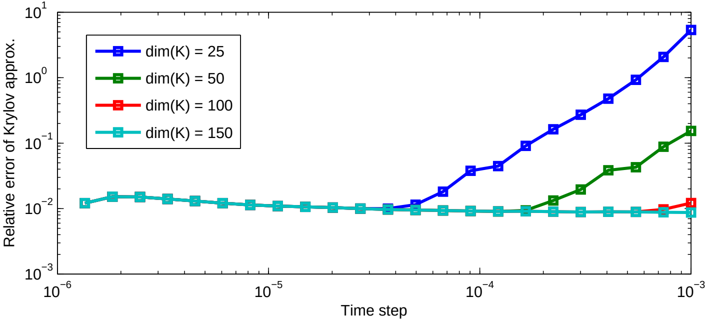
Setup

- Vertical magnetic dipole of unit strength located at the origin.
- Yee discretization of (PDE).
- Grid with $58 \times 58 \times 58$ cells, i.e. 565326 unknowns.
- Constant coefficients $\mu = 1.26 \cdot 10^{-6}$, $\sigma = 1.00 \cdot 10^{-1}$.
- 24 logarithmically equidistant time steps from the interval $[t_0, t_n] = [10^{-6}, 10^{-3}]$ seconds.
- Everything implemented in pure MATLAB (Release 2007a).

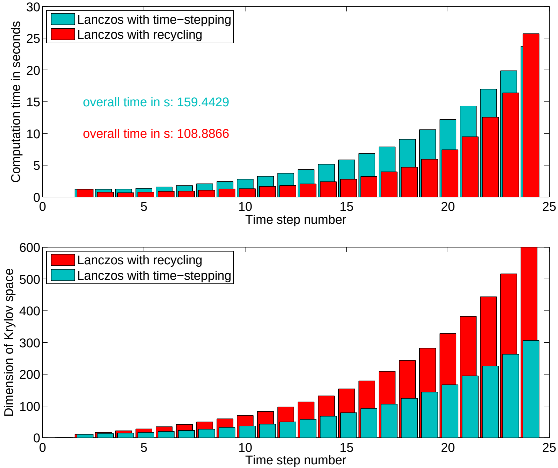
Du Fort-Frankel Method vs. ROCK4



Lanczos Method: Time-Stepping vs. Recycling (I)



Lanczos Method: Time-Stepping vs. Recycling (II)

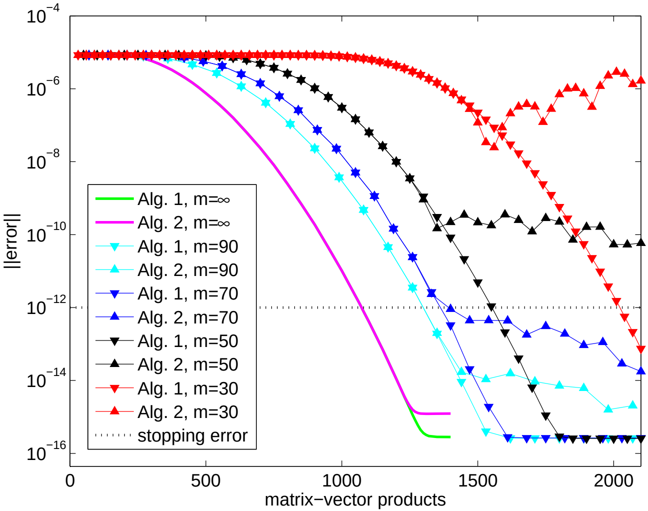


Restarted Arnoldi (I)

- Algorithm 1: Proposed in [Eiermann & Ernst, 2006].
- Algorithm 2: Improved variant of Algorithm 1.
- $m = \infty\ (I)$: Standard Lanczos (unrestarted).
- $m = \infty\ (II)$: Two-pass Lanczos (unrestarted).

	Algorithm 1			Algorithm 2		
m	time [s]	mvp	acc.	time [s]	mvp	acc.
$\infty\ (I)$	118	1072	9.93e-13	86	1072	9.93e-13
$\infty\ (II)$	176	2144	9.93e-13	144	2144	9.93e-13
90	273	1350	1.92e-13	118	1350	2.01e-13
70	339	1400	3.28e-13	112	1400	9.13e-13
50	613	1600	2.10e-13	very slow convergence		
30	2014	2040	5.64e-13	divergence		

Restarted Arnoldi (II)



Summary and Future Work

Summary and Future Work

- Summary
  - We successfully applied various methods to our model problem.
  - Restarted Krylov subspace methods might become a viable alternative to the well known Du Fort-Frankel and Spectral Lanczos Decomposition methods.
- Future work
  - Implicit time stepping.
  - FE discretization.
  - Heterogeneous materials.
  - Error estimates.
- References
  - Implementation of a Restarted Krylov Subspace Method for the Evaluation of Matrix Functions [A, Eiermann, Ernst, & Güttel, 2007].