Numerical Modelling for Geophysical Electromagnetic Methods

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The Plan

- Five “lectures”, each of approximately 1 hour duration.
- Informal, so questions and comments are welcomed at any time.
- Timing is flexible, and can be adjusted as needed.
- Some exercises will be provided, with Fortran source code available.
- We can have tutorials, or similar, if desired.

Outline

I. 1-D

II. EM rules & regulations

III. Finite difference

IV. Finite element

V. Integral equation

I. 1-D

1. An example: Set-up

Derive a partial differential equation (PDE) from Maxwell's equations, Ohm's law, etc., in frequency domain, in quasi-static régime:

Maxwell/Faraday $\longrightarrow$	$\nabla \times \mathbf{E} = i\omega \mathbf{B}$
curl $\longrightarrow$	$\nabla \times \nabla \times \mathbf{E} = i\omega \nabla \times \mathbf{B}$
$\mathbf{B} = \mu_0 \mathbf{H} \longrightarrow$	$\nabla \times \nabla \times \mathbf{E} = i\omega\mu_0 \nabla \times \mathbf{H}$
Maxwell/Ampère $\longrightarrow$	$\nabla \times \nabla \times \mathbf{E} = i\omega\mu_0 \mathbf{J}$
Ohm, $\sigma(\mathbf{r}) \longrightarrow$	$\nabla \times \nabla \times \mathbf{E} = i\omega\mu_0 \sigma \mathbf{E}$

Hence:

$$\nabla \times \nabla \times \mathbf{E} - i\omega\mu_0 \sigma \mathbf{E} = 0$$

Assume . . .

1-D spatial variation of conductivity: $\sigma = \sigma(z)$

1-D spatial variation of electric field: $\mathbf{E} = \mathbf{E}(z)$ and $\frac{\partial}{\partial x} = \frac{\partial}{\partial y} = 0$

electric field in x-direction only: $\mathbf{E}(z) = E_x(z)\,\hat{\mathbf{x}}$

(That is, source of infinite extent in x- & y-directions to generate electric field with only one component, and no spatial structure to break this symmetry. Looking like 1-D MT.)

(And further assume that the “source” of the electric field can be implemented via boundary conditions. This is 1-D MT.)

So:

$$\nabla \times \mathbf{E} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 0 & \frac{\partial}{\partial z} \\ E_x & 0 & 0 \end{vmatrix} = \frac{\partial E_x}{\partial z}\,\hat{\mathbf{y}}$$

and

$$\nabla \times \nabla \times \mathbf{E} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 0 & \frac{\partial}{\partial z} \\ 0 & \frac{\partial E_x}{\partial z} & 0 \end{vmatrix} = -\frac{\partial^2 E_x}{\partial z^2}\,\hat{\mathbf{x}}$$

Hence, the 1-D PDE is:

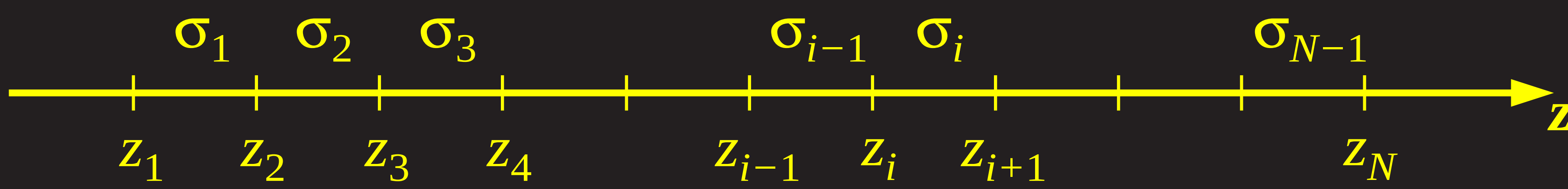
$$-\frac{\partial^2 E_x}{\partial z^2} - i\omega\mu_0\sigma(z)\,E_x = 0$$

(with some boundary conditions).

2. Discretize the Earth

For numerical solution, need to get everything in terms of numbers so that a computer can do the arithmetic.

Discretize the Earth, e.g., into layers of uniform conductivity:



z-coordinates of layer interfaces: $z_1, z_2, \ldots, z_N$

conductivities of layers: $\sigma_1, \sigma_2, \ldots, \sigma_{N-1}$

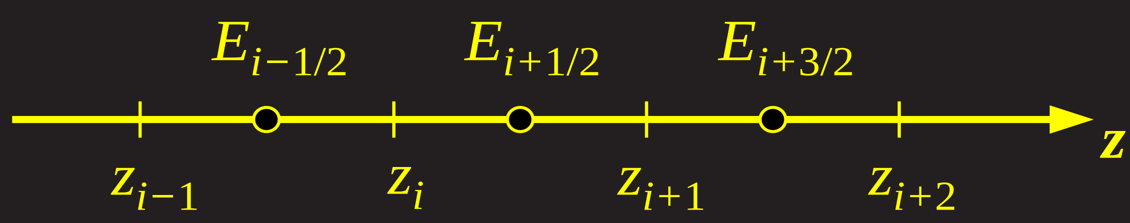
3. Discretize the electric field

Continue to get everything in terms of lists of numbers.

Sliding towards the *finite-difference* method . . .

Let's specify an approximate electric field in terms of its values at nodes, and . . .

. . . let's locate these nodes at the centres of the layers:



(The subscript x in E_x has been dropped; the subscript now represents to which node a value of the approximate electric field corresponds.)

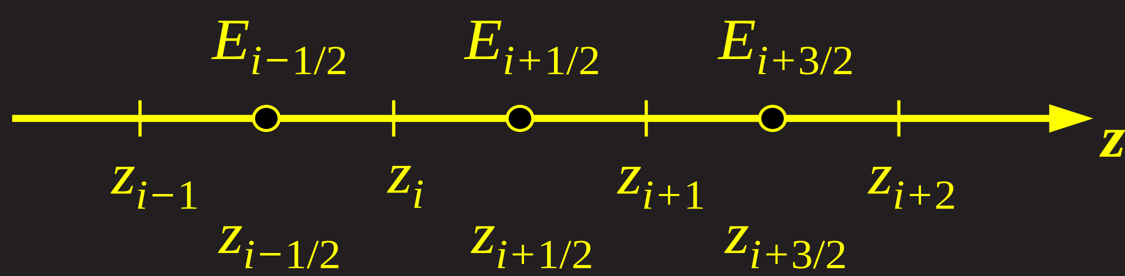
4. Discretize the PDE

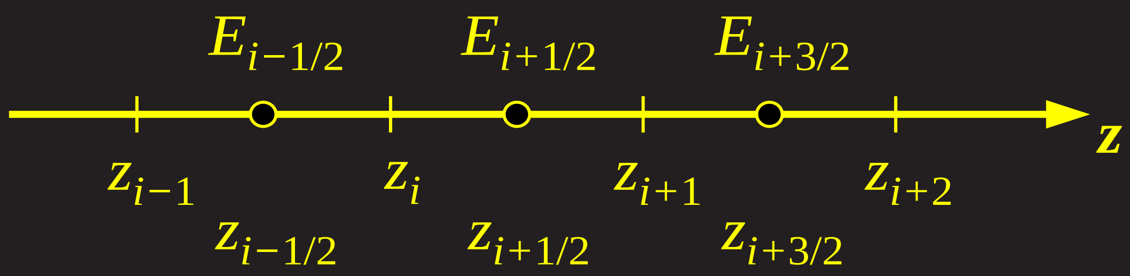
Returning to the PDE:

$$\frac{\partial^2 E_x}{\partial z^2} + i\omega\mu_0\sigma(z)\, E_x = 0$$

What do we do about the z-derivatives now that we're in our discretized realm?

Consider the $(i+\frac{1}{2})$th node and its neighbours:



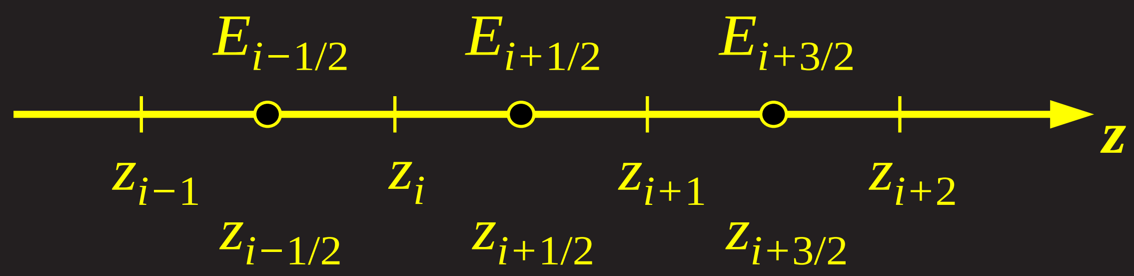


Approximating derivatives by finite differences:

$$\left.\frac{\partial E}{\partial z}\right|_{z_i} \approx \frac{E_{i+\frac{1}{2}} - E_{i-\frac{1}{2}}}{z_{i+\frac{1}{2}} - z_{i-\frac{1}{2}}} \quad \text{and} \quad \left.\frac{\partial E}{\partial z}\right|_{z_{i+1}} \approx \frac{E_{i+\frac{3}{2}} - E_{i+\frac{1}{2}}}{z_{i+\frac{3}{2}} - z_{i+\frac{1}{2}}}$$

Let's assume layers of equal thickness, Δz, for ease of writing:

$$\left.\frac{\partial E}{\partial z}\right|_{z_i} \approx \frac{E_{i+\frac{1}{2}} - E_{i-\frac{1}{2}}}{\Delta z} \quad \text{and} \quad \left.\frac{\partial E}{\partial z}\right|_{z_{i+1}} \approx \frac{E_{i+\frac{3}{2}} - E_{i+\frac{1}{2}}}{\Delta z}$$

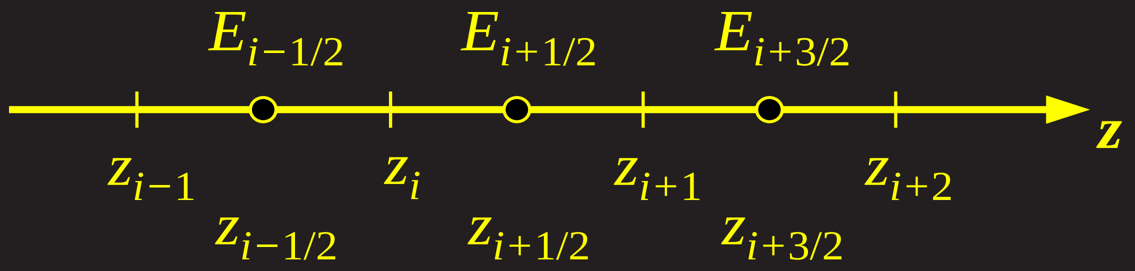


And similarly for the second-order derivative:

$$\frac{\partial^2 E}{\partial z^2}\bigg|_{z_{i+\frac{1}{2}}} = \frac{\partial}{\partial z}\left\{\frac{\partial E}{\partial z}\right\}\bigg|_{z_{i+\frac{1}{2}}} \approx \frac{1}{\Delta z}\left\{\frac{\partial E}{\partial z}\bigg|_{z_{i+1}} - \frac{\partial E}{\partial z}\bigg|_{z_i}\right\}$$

$$= \frac{1}{\Delta z}\left\{\frac{E_{i+\frac{3}{2}} - E_{i+\frac{1}{2}}}{\Delta z} - \frac{E_{i+\frac{1}{2}} - E_{i-\frac{1}{2}}}{\Delta z}\right\}$$

$$= \frac{1}{\Delta z^2}\left\{E_{i+\frac{3}{2}} - 2E_{i+\frac{1}{2}} + E_{i-\frac{1}{2}}\right\}$$

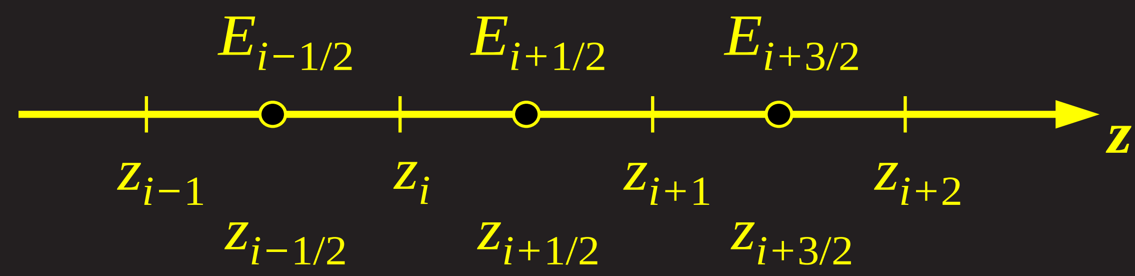


So, an approximation of the PDE that is centred on the $(i + \frac{1}{2})$th node is:

$$\frac{1}{\Delta z^2} \left\{ E_{i+\frac{3}{2}} - 2E_{i+\frac{1}{2}} + E_{i-\frac{1}{2}} \right\} + \; i\omega\mu_0\sigma_i \, E_{i+\frac{1}{2}} \; = \; 0$$

(where σ_i is the conductivity of the ith layer, i.e., between z_i and z_{i+1}.)

Rearranging the above expression to gather together the various electric field terms …



$$\frac{1}{\Delta z^2} E_{i-\frac{1}{2}} + \left(i\omega\mu_0\sigma_i - \frac{2}{\Delta z^2} \right) E_{i+\frac{1}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{3}{2}} \;=\; 0$$

The PDE can be approximated in a similar manner in the neighbourhood of each "interior" node, e.g.,

$$\frac{1}{\Delta z^2} E_{i-\frac{3}{2}} + \left(i\omega\mu_0\sigma_{i-1} - \frac{2}{\Delta z^2} \right) E_{i-\frac{1}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{1}{2}} = 0 \quad \text{for } z_{i-\frac{1}{2}}$$

$$\frac{1}{\Delta z^2} E_{i+\frac{1}{2}} + \left(i\omega\mu_0\sigma_{i+1} - \frac{2}{\Delta z^2} \right) E_{i+\frac{3}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{5}{2}} = 0 \quad \text{for } z_{i+\frac{3}{2}}$$

Showing again these discrete approximations of the PDE, this time in order:

$$\frac{1}{\Delta z^2} E_{i-\frac{3}{2}} + \left(i\omega\mu_0\sigma_{i-1} - \frac{2}{\Delta z^2} \right) E_{i-\frac{1}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{1}{2}} = 0 \quad \text{for } z_{i-\frac{1}{2}}$$

$$\frac{1}{\Delta z^2} E_{i-\frac{1}{2}} + \left(i\omega\mu_0\sigma_{i} - \frac{2}{\Delta z^2} \right) E_{i+\frac{1}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{3}{2}} = 0 \quad \text{for } z_{i+\frac{1}{2}}$$

$$\frac{1}{\Delta z^2} E_{i+\frac{1}{2}} + \left(i\omega\mu_0\sigma_{i+1} - \frac{2}{\Delta z^2} \right) E_{i+\frac{3}{2}} + \frac{1}{\Delta z^2} E_{i+\frac{5}{2}} = 0 \quad \text{for } z_{i+\frac{3}{2}}$$

If we can find E's that mean all three of these equations are satisfied, we will have a solution to our discretized, approximate PDE ...

... in the neighbourhood of $z_{i-\frac{1}{2}}$, $z_{i+\frac{1}{2}}$ and $z_{i+\frac{3}{2}}$.

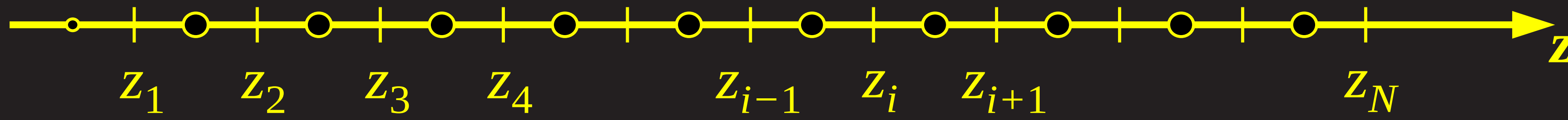
Showing yet again these discrete approximations of the PDE, this time lining things up:

$$\begin{array}{ccccccc} \blacksquare E_{i-\frac{3}{2}} & \blacksquare E_{i-\frac{1}{2}} & \blacksquare E_{i+\frac{1}{2}} & 0 & 0 & = & 0 \\ 0 & \blacksquare E_{i-\frac{1}{2}} & \blacksquare E_{i+\frac{1}{2}} & \blacksquare E_{i+\frac{3}{2}} & 0 & = & 0 \\ 0 & 0 & \blacksquare E_{i+\frac{1}{2}} & \blacksquare E_{i+\frac{3}{2}} & \blacksquare E_{i+\frac{5}{2}} & = & 0 \end{array}$$

where the $\blacksquare$'s correspond to the coefficients of the E's.

In matrix notation:

$$\begin{pmatrix} \blacksquare & \blacksquare & \blacksquare & 0 & 0 \\ 0 & \blacksquare & \blacksquare & \blacksquare & 0 \\ 0 & 0 & \blacksquare & \blacksquare & \blacksquare \end{pmatrix} \begin{pmatrix} E_{i-\frac{3}{2}} \\ E_{i-\frac{1}{2}} \\ E_{i+\frac{1}{2}} \\ E_{i+\frac{3}{2}} \\ E_{i+\frac{5}{2}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$



Collecting the discrete, approximate PDE bits for nodes $(2+\frac{1}{2})$ to $(N-2+\frac{1}{2})$:

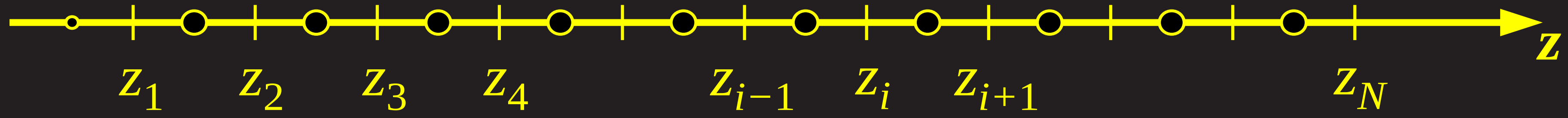
$$\begin{pmatrix} \blacksquare & \blacksquare & \blacksquare & 0 & \dots & 0 \\ 0 & \blacksquare & \blacksquare & \blacksquare & \dots & 0 \\ \vdots & & & & & \vdots \\ 0 & \dots & 0 & \blacksquare & \blacksquare & \blacksquare \end{pmatrix} \begin{pmatrix} E_{1+\frac{1}{2}} \\ \\ \vdots \\ \\ E_{N-1+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \vdots \\ 0 \\ \vdots \end{pmatrix}$$

This is a discretization of the 1-D electric field PDE.

This is a system of $N-3$ equations in $N-1$ unknowns.

5. Discretize the boundary conditions

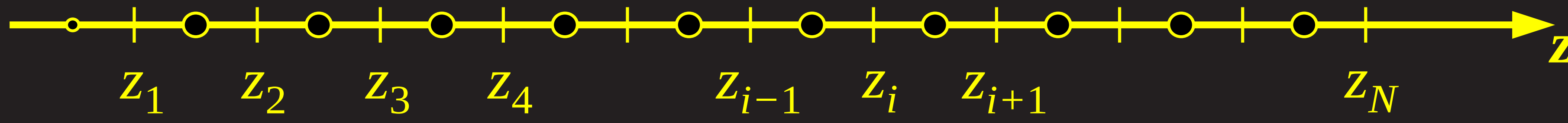
Okay, so we need two more equations. Let's now consider what's happening at the "boundary" nodes.



Firstly, at $z_{N-\frac{1}{2}}$ and thereabouts.

Assume that our boundary condition here is that the electric field has decayed to nothing, as an MT electric field would deep in the Earth.

Let's try to get this boundary condition into our approximate realm. The best we can do (in this particular discretization) is to set $E_{N-\frac{1}{2}} = 0$.

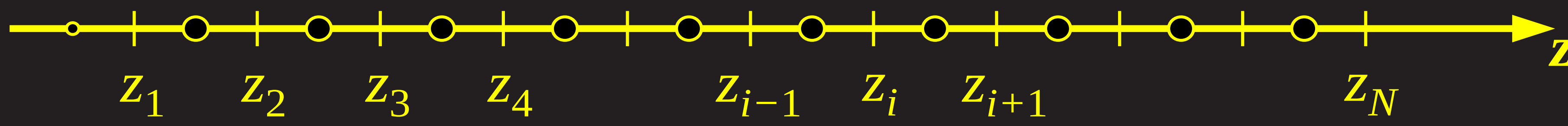


Putting this into our system of equations gives:

$$\begin{pmatrix} \blacksquare & \blacksquare & \blacksquare & 0 & \dots & 0 \\ 0 & \blacksquare & \blacksquare & \blacksquare & \dots & 0 \\ \vdots & & & & & \vdots \\ 0 & \dots & 0 & \blacksquare & \blacksquare & \blacksquare \\ 0 & & \dots & & 0 & 1 \end{pmatrix} \begin{pmatrix} E_{1+\frac{1}{2}} \\ \\ \vdots \\ \\ E_{N-1+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

This is now a system of $N-2$ equations in $N-1$ unknowns.

Consider the boundary condition at the other end, i.e., at z_1 and thereabouts.



Assume that our boundary condition here represents a non-zero magnetic field. This mimics the effect of the simple plane-wave source of MT.

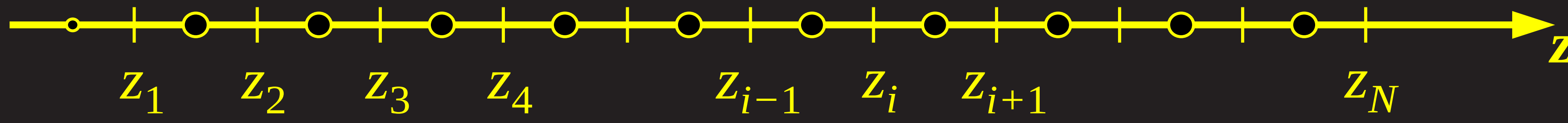
In our nice 1-D scenario, $i\omega\mu_0 H_y = \partial E_x / \partial z$.

Let's choose $H_y = 1$ at z_1, that is, $\partial E_x / \partial z = i\omega\mu_0$.

In our discretized world, we can approximate this boundary condition as:

$$\frac{1}{\Delta z}\left(E_{1+\frac{1}{2}} - E_{1-\frac{1}{2}}\right) = i\omega\mu_0.$$

This involves the approximate electric field at the "ghost" node at $z_{1-\frac{1}{2}}$.

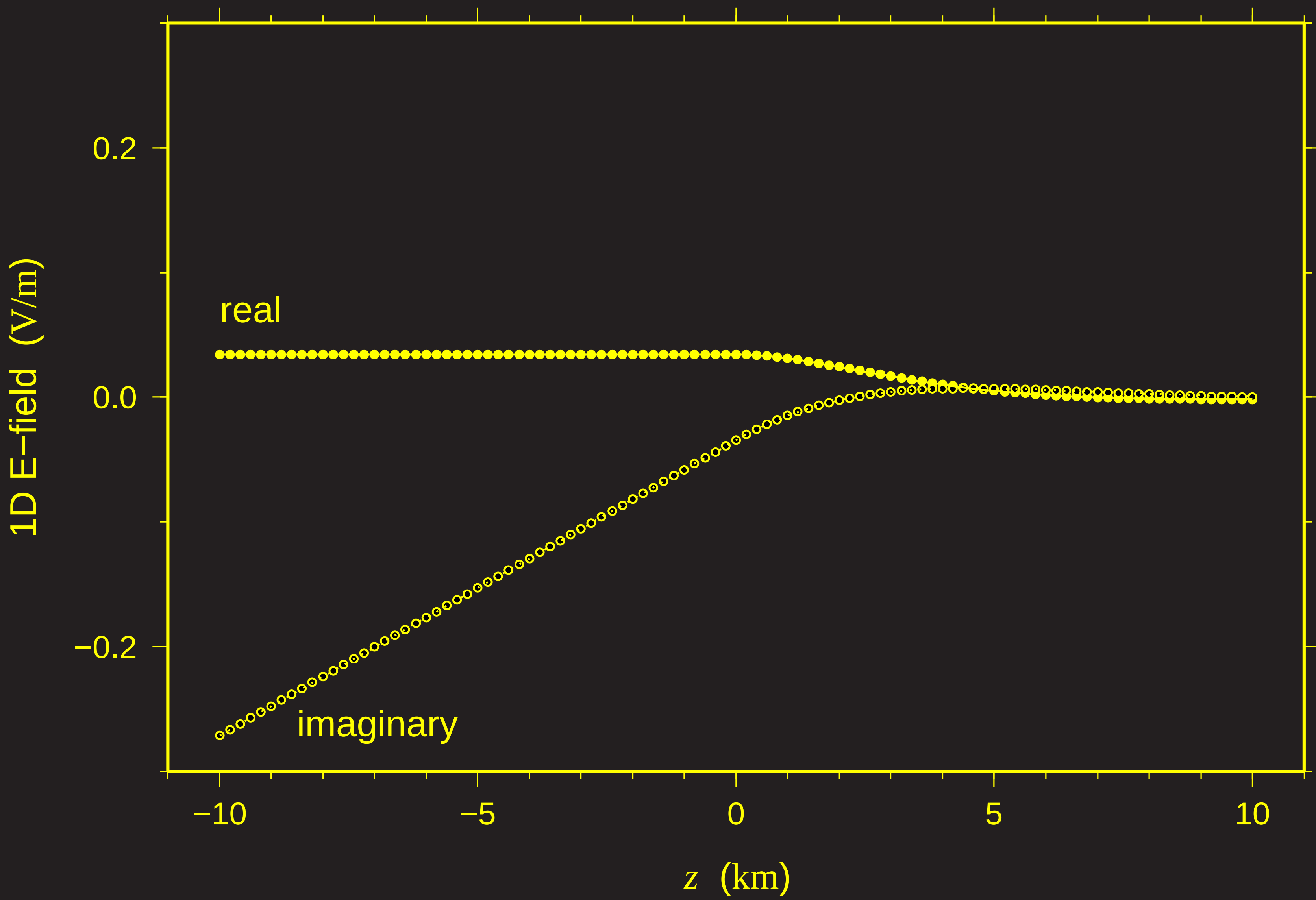


Including the preceding equation in our system, AND the discrete approximation to the PDE that is centred on $z_{1+\frac{1}{2}}$ gives:

$$
\begin{pmatrix}
\frac{-1}{\Delta z} & \frac{1}{\Delta z} & 0 & & \dots & 0 \\
\blacksquare & \blacksquare & \blacksquare & 0 & \dots & 0 \\
0 & \blacksquare & \blacksquare & \blacksquare & \dots & 0 \\
\vdots & & & & & \vdots \\
0 & \dots & 0 & \blacksquare & \blacksquare & \blacksquare \\
0 & & \dots & & 0 & 1
\end{pmatrix}
\begin{pmatrix}
E_{1-\frac{1}{2}} \\
E_{1+\frac{1}{2}} \\
\\
\vdots \\
\\
E_{N-1+\frac{1}{2}}
\end{pmatrix}
=
\begin{pmatrix}
i\omega\mu_0 \\
\vdots \\
0 \\
\vdots \\
0
\end{pmatrix}
$$

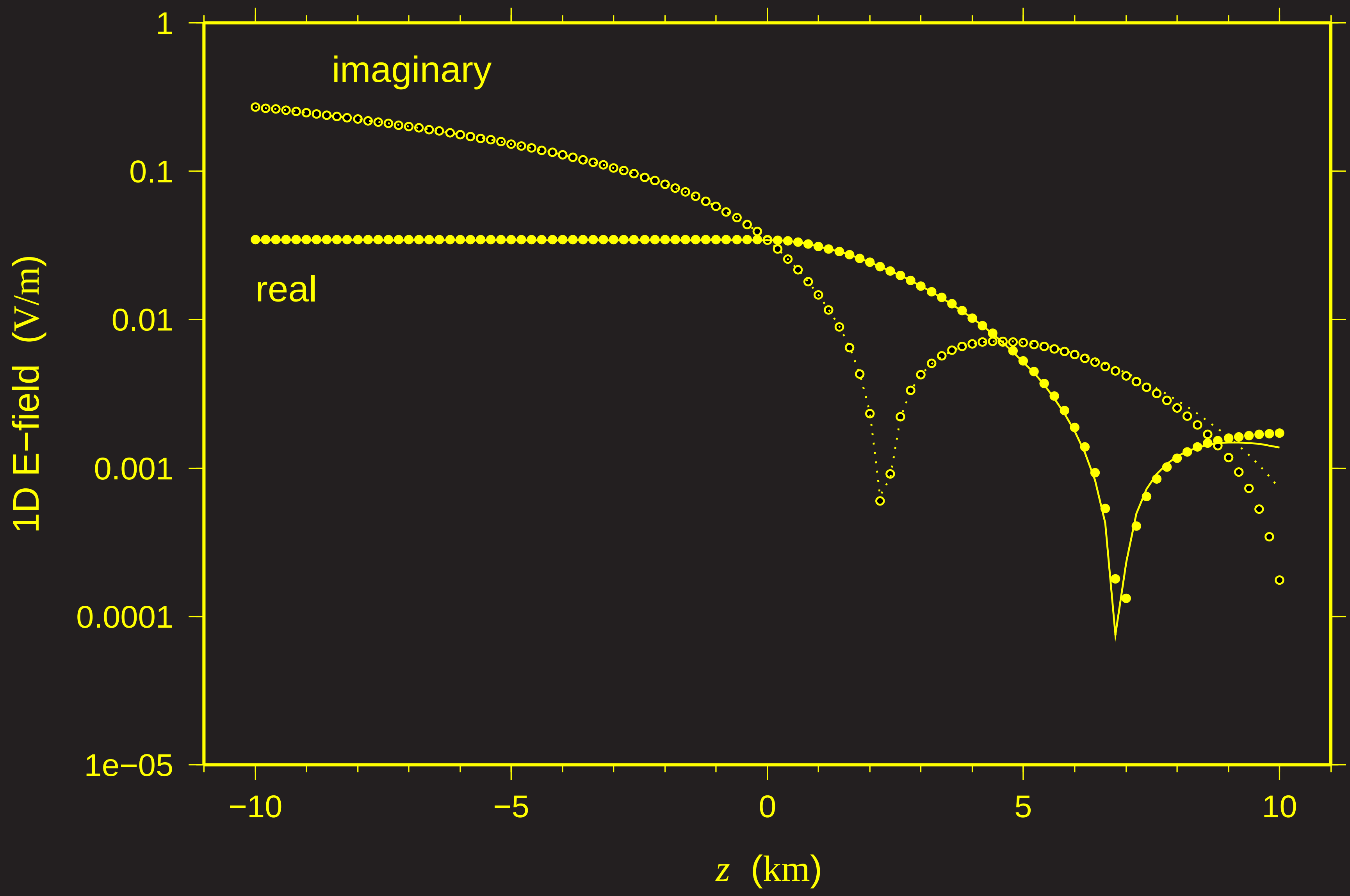
This is now a system of N equations in N unknowns. Woo-hoo!

Form system, and solve ...



It works!

(Homogeneous halfspace of 0.01 S/m; “air” of 10^{-8}S/m; 3 Hz.)



Same again (homogeneous halfspace of 0.01 S/m, 3 Hz), using logarithmic vertical axis.

6. The system of equations

Backing up a bit.

The system of equations for the PDE, which was written out before as:

$$\begin{pmatrix} \blacksquare & \blacksquare & 0 & & \dots & 0 \\ \blacksquare & \blacksquare & \blacksquare & 0 & \dots & 0 \\ 0 & \blacksquare & \blacksquare & \blacksquare & \dots & 0 \\ \vdots & & & & & \vdots \\ 0 & \dots & 0 & \blacksquare & \blacksquare & \blacksquare \\ 0 & & \dots & & 0 & 1 \end{pmatrix} \begin{pmatrix} E_{1-\frac{1}{2}} \\ E_{1+\frac{1}{2}} \\ \\ \vdots \\ \\ E_{N-1+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} i\omega\mu_0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

can be written more neatly as:

$$(\,\underline{\mathbf{L}} + i\omega\mu_0\,\underline{\mathbf{S}}\,)\,\tilde{\mathbf{E}} = \mathbf{r}$$

$$(\underline{\mathbf{L}} + i\omega\mu_0\underline{\mathbf{S}})\,\tilde{\mathbf{E}} = \mathbf{r}$$

where

$\mathbf{r}$ is the right-hand side vector (dimension N);

$\tilde{\mathbf{E}}$ is the vector containing the values of the approximate electric field at the nodes (including the ghost node) (dimension N);

$\underline{\mathbf{S}}$ is the $N \times N$ diagonal matrix whose elements are the conductivities of the layers, i.e., $S_{ii} = \sigma_i$;

and $\underline{\mathbf{L}}$ is $\ldots$

$\underline{\mathbf{L}}$ is the finite-difference approximation of the $\partial^2/\partial z^2$ operator, i.e.,

$$\underline{\mathbf{L}} = \frac{1}{\Delta z}\begin{pmatrix} 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & \dots & 1 & -2 & 1 \end{pmatrix}$$

(Assuming the boundary conditions are implemented somehow in the system of equations, perhaps like the way described.)

The matrices $\underline{\mathbf{L}}$ and $\underline{\mathbf{S}}$ are real-valued.

However, the vectors $\tilde{\mathbf{E}}$ and $\mathbf{r}$ are complex-valued. So is the coefficient $i\omega\mu_0$ of the conductivity matrix.

Splitting the matrix equation into real and imaginary parts gives:

$$\begin{pmatrix} \underline{\mathbf{L}} & \omega\mu_0\underline{\mathbf{S}} \\ -\omega\mu_0\underline{\mathbf{S}} & \underline{\mathbf{L}} \end{pmatrix} \begin{pmatrix} \Re\tilde{\mathbf{E}} \\ \Im\tilde{\mathbf{E}} \end{pmatrix} = \begin{pmatrix} \Re\mathbf{r} \\ \Im\mathbf{r} \end{pmatrix}$$

This is a completely real system which can be solved with any number of good-quality, free, library routines.

7. Sparse matrices

The matrix $\underline{\mathbf{S}}$ is diagonal. It therefore only contains N non-zero numbers. It would be amazingly inefficient to store the whole matrix complete with all its zeros (N^2 numbers). Much more efficient to just store the non-zero values and their locations in the matrix.

The matrix $\underline{\mathbf{L}}$ is not diagonal (it is tri-diagonal), but it is also amazingly sparse. Again, it is way more efficient in terms of computer memory requirements to store only the non-zero values and their locations.

There are good-quality, freely available libraries that have all the necessary routines to work with sparse matrices, including matrix-vector products, matrix-matrix products, iterative solvers, preconditioners, format conversions. For example, Sparskit.

8. Matrix equation solvers

The classic "Gaussian elimination", or "LU decomposition" (L for lower and U for upper triangular).

Given the matrix equation $\underline{\mathbf{A}}\mathbf{x} = \mathbf{b}$, decompose $\underline{\mathbf{A}}$ into lower and upper triangular matrices:

$$\underline{\mathbf{A}} = \underline{\mathbf{L}}\,\underline{\mathbf{U}}.$$

The solution procedure is then:

$$\underline{\mathbf{A}}\mathbf{x} = \mathbf{b} \quad \rightarrow \quad \underline{\mathbf{L}}\,\underline{\mathbf{U}}\mathbf{x} = \mathbf{b} \quad \rightarrow \quad \mathbf{y} = \underline{\mathbf{U}}\mathbf{x} = \underline{\mathbf{L}}^{-1}\mathbf{b}$$

$$\mathbf{x} = \underline{\mathbf{U}}^{-1}\mathbf{y} = \underline{\mathbf{U}}^{-1}\underline{\mathbf{L}}^{-1}\mathbf{b}$$

$$\underline{\mathbf{A}}\mathbf{x} = \mathbf{b} \quad \rightarrow \quad \underline{\mathbf{L}}\,\underline{\mathbf{U}}\mathbf{x} = \mathbf{b} \quad \rightarrow \quad \mathbf{y} = \underline{\mathbf{U}}\mathbf{x} = \underline{\mathbf{L}}^{-1}\mathbf{b}$$

$$\mathbf{x} = \underline{\mathbf{U}}^{-1}\mathbf{y} = \underline{\mathbf{U}}^{-1}\underline{\mathbf{L}}^{-1}\mathbf{b}$$

The decomposition takes time and memory ($\underline{\mathbf{L}}$ and $\underline{\mathbf{U}}$ will be full and dense irrespective of whether or not $\underline{\mathbf{A}}$ is sparse).

However, the lower- and upper-triangular solves are fast.

Disadvantages: doesn't work well with sparse matrices; decomposition expensive in memory (and time).

Advantages: once you have the decomposition, solving for many different right-hand sides (for the same matrix) is very efficient.

Iterative solvers, e.g., conjugate gradients, ...

They work by producing a sequence of approximate solutions, i.e., $\{\mathbf{x}^{(k)}\}$, which hopefully converges to an $\mathbf{x}^{(K)}$ that adequately satisfies the matrix equation, specifically

$$\|\underline{\mathbf{A}}\,\mathbf{x}^{(K)} - \mathbf{b}\| \; < \; \tau$$

where τ is some small-ish number.

The only significant operations are products of the matrix (or its transpose) with vectors. This means iterative solvers work perfectly happily with sparse matrices.

Advantages: memory efficient because they preserve sparsity.

Disadvantages: require a whole new solution for every new right-hand side.

9. An exercise

Write code, in your favourite programming language or environment, to assemble the matrix equation shown earlier. Solve to get the MT electric field in a 1-D Earth model.

10. “Take-home” points

- ⋆ Basic (intuitive) finite-difference approximation of derivatives.

- ⋆ Use of such finite differences to approximate locally a differential equation.

- ⋆ Simultaneous system of such equations to approximate the differential equation over the whole domain.