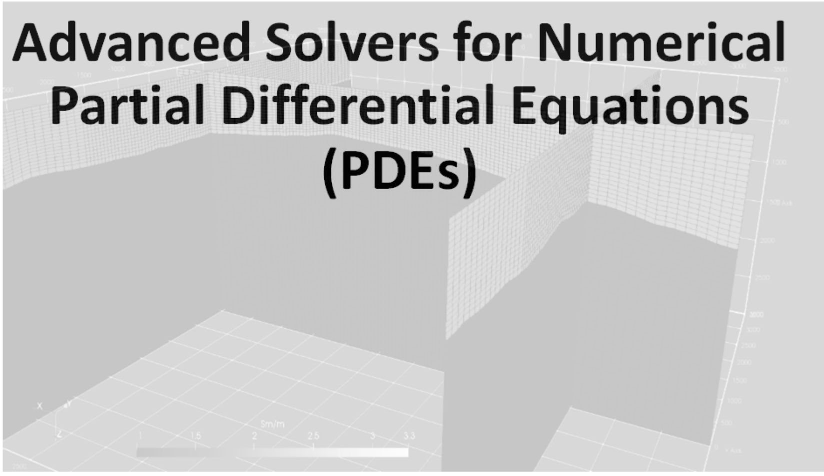
Advanced Solvers for Numerical Partial Differential Equations (PDEs)



Lecture 5

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Part 1
Discretization of Maxwell's equations

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Time-harmonic Maxwell's Equations

If we assume time-dependence $e^{-i\omega t}$, Maxwell's equations take the form:

Faraday's law of induction

$$curl\, \boldsymbol{E} = i\omega\mu_0 \boldsymbol{H}$$

Ampère's law

$$curl\, \boldsymbol{H} = (\sigma - i\omega\varepsilon)\boldsymbol{E} + \boldsymbol{J}$$

Gauss's law

$$div\, \boldsymbol{H} = \boldsymbol{0}$$

$$div\, (\tilde{\sigma}\boldsymbol{E}) = -div\, \boldsymbol{J}$$

complex conductivity, $\tilde{\sigma} = \sigma - i\omega\varepsilon$

We can eliminate the magnetic field and receive,

$$curl\, curl\, \boldsymbol{E} - i\omega\mu_0\tilde{\sigma}\, \boldsymbol{E} = i\omega\mu_0\, \boldsymbol{J}$$

Wave-number squared, $\kappa^2 = -i\omega\mu_0\tilde{\sigma}$

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Maxwell's Equations Modes

Depending on the wave-number, we can distinguish several modes

- $\sigma \approx 0$, $\kappa^2 = -\omega^2\mu_0\varepsilon < 0$ (negative)
  Radio-wave mode / high-frequency
- $\varepsilon \approx 0$, $\kappa^2 = -i\omega\mu_0\sigma$ (pure imaginary)
  Quasi-static / diffusive mode/ low-frequency
- $\kappa^2 > 0$ (positive)
  Implicit time-stepping / self-adjoint operator

Next, we will be mainly assume the low-frequency mode.

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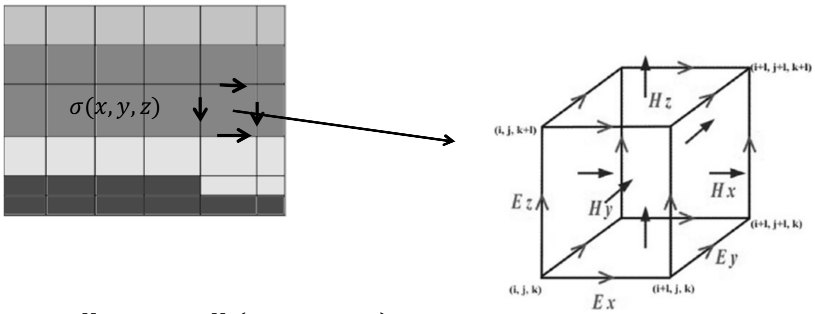
Staggered Grid Discretization

$curl\ curl\ \boldsymbol{E} - i\omega\mu_0\sigma\,\boldsymbol{E} = i\omega\mu_0\,\boldsymbol{J}$, in V
$\boldsymbol{E} \times \boldsymbol{\nu} = 0$, on ∂V

$$E_{i+\frac{1}{2}\,j\,k} \approx E_x(x_{i+\frac{1}{2}}, y_j, z_k),$$
$$E_{i\,j+\frac{1}{2}\,k} \approx E_y(x_i, y_{j+\frac{1}{2}}, z_k),$$
$$E_{i\,j\,k+\frac{1}{2}} \approx E_z(x_i, y_j, z_{k+\frac{1}{2}}).$$

K. Yee, 1966



$$H_{i+\frac{1}{2}\,j+\frac{1}{2}\,k} \approx H_z(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_k)$$

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Staggered Grid Discretization

Exercise 1
Express $H_{i+\frac{1}{2}\,j+\frac{1}{2}\,k}$ (i.e. discrete H_z) via discrete electric field

Exercise 2
Express $E_{i+\frac{1}{2}\,j\,k}$ (i.e. discrete E_x) via discrete magnetic field

Exercise 3
Prove that the discrete electric field is divergence-free in a source-less homogenous domain.

Exercise 4
Same for the discrete magnetic field

Vertex-based discretizations for E and H do not possess these properties, producing spurious solutions

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Staggered Grid Discretization

$$-\frac{\partial^2 E_x}{\partial y^2}-\frac{\partial^2 E_x}{\partial z^2}+\frac{\partial^2 E_y}{\partial x \partial y}+\frac{\partial^2 E_z}{\partial x \partial z}-i\omega\mu_0\sigma E_x = i\omega\mu_0 J_x,$$

$$\begin{aligned}
&\frac{E_{i+\frac{1}{2}\,j\,k}-E_{i+\frac{1}{2}\,j+1\,k}}{h^y_j h^y_{j+\frac{1}{2}}}+\frac{E_{i+\frac{1}{2}\,j\,k}-E_{i+\frac{1}{2}\,j-1\,k}}{h^y_j h^y_{j-\frac{1}{2}}}+\\
&\frac{E_{i+\frac{1}{2}\,j\,k}-E_{i+\frac{1}{2}\,j\,k+1}}{h^z_k h^z_{k+\frac{1}{2}}}+\frac{E_{i+\frac{1}{2}\,j\,k}-E_{i+\frac{1}{2}\,j\,k-1}}{h^z_k h^z_{k-\frac{1}{2}}}+\\
&\frac{E_{i+1\,j+\frac{1}{2}\,k}-E_{i\,j+\frac{1}{2}\,k}}{h^x_{i+\frac{1}{2}} h^y_j}+\frac{E_{i\,j-\frac{1}{2}\,k}-E_{i+1\,j-\frac{1}{2}\,k}}{h^x_{i+\frac{1}{2}} h^y_j}+\\
&\frac{E_{i+1\,j\,k+\frac{1}{2}}-E_{i\,j\,k+\frac{1}{2}}}{h^x_{i+\frac{1}{2}} h^z_k}+\frac{E_{i\,j\,k-\frac{1}{2}}-E_{i+1\,j\,k-\frac{1}{2}}}{h^x_{i+\frac{1}{2}} h^z_k}-\\
&\qquad -i\omega\mu_0\sigma_{i+\frac{1}{2}\,j\,k}E_{i+\frac{1}{2}\,j\,k} = i\omega\mu_0 J_{i+\frac{1}{2}\,j\,k}.
\end{aligned}$$

Staggered Grid Discretization

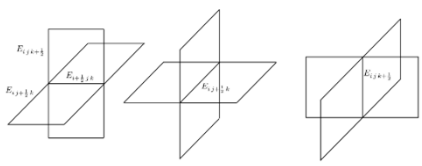
Let us form the unknown vector e of the discrete electric fields E_x, E_y, E_z,

- First we enumerate the electric fields assigned to the edges parallel to the x axis
- then those parallel to y, and
- finally those parallel to z.

Within each set of edges, we assume the lexicographic x − y − z order

- At most 13 non-zero entries per row
- Complex symmetric matrix, $A = R - i\omega\mu_0 S$
- Number of unknowns = number of edges

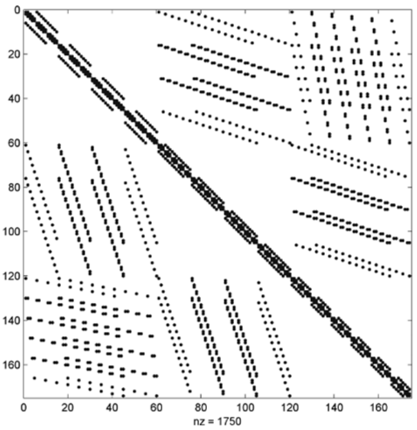
FD stencil



$A\,e = j$

$$cond(A) = \frac{|\lambda_{\max}|}{|\lambda_{\min}|} \leq \frac{13}{h^2_{min}\omega\,\mu_0\sigma_{min}}$$

Staggered Grid Discretization



System matrix structure for 4x4x6 grid

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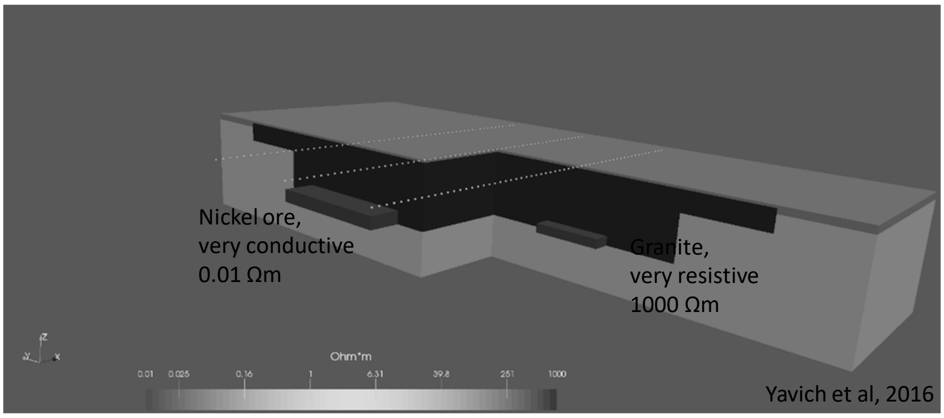
Example / Ore Exploration

Norilsk ore deposit conductivity structure
Incident plain wave



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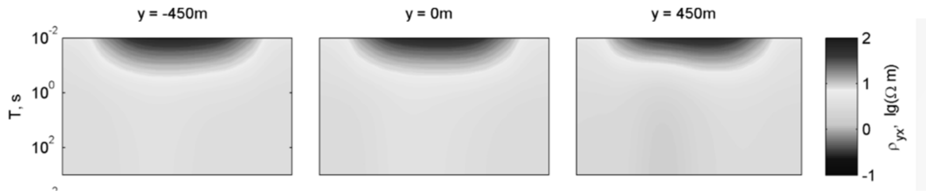
Example / Ore Exploration

Modeling at 21 periods, from 0.01 to 1000 s, four periods per decade.



Electric and magnetic field components transformed

Part 2
FEM for Maxwell's equations

Finite-element Discretization

$$curl\ curl\ \boldsymbol{E} - i\omega\mu_0\sigma\,\boldsymbol{E} = i\omega\mu_0\,\boldsymbol{J}$$
$$\boldsymbol{E} \times \boldsymbol{\nu} = 0$$

- Incorporation of complex geometrical features
- No conductivity averaging needed

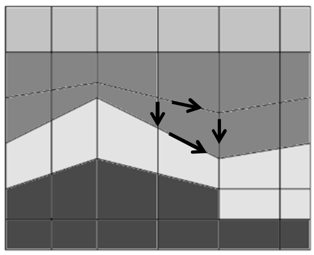
Exercise

$$\int_\Omega curl\,\boldsymbol{E} \cdot curl\,\boldsymbol{F} dV - i\omega\mu_0 \int_\Omega \sigma\,\boldsymbol{E} \cdot \boldsymbol{F} dV = i\omega\mu_0 \int_\Omega \boldsymbol{J} \cdot \boldsymbol{F} dV$$

$E, F \in H(curl, \Omega)$

$$\|\boldsymbol{v}\|^2 = \int_\Omega \boldsymbol{v}^2\,dx + \int_\Omega curl\,\boldsymbol{v}^{\,2}\,dx$$

Square-integrable vector-functions with square-integrable curl



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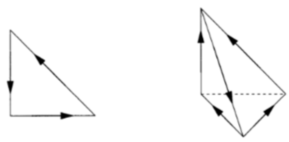
Finite-element Discretization



- Lowest-order Nédélec finite element constant tangential component

- Tangential flux continuity ensure conformity to $H(curl, \Omega)$

2D $\boldsymbol{v}_h = \begin{pmatrix} a \\ b \end{pmatrix} + c\begin{pmatrix} y \\ -x \end{pmatrix}$

3D $\boldsymbol{v}_h = \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \begin{pmatrix} d \\ e \\ f \end{pmatrix} \times \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

Finite-element (FE) system, lowest-order Nédélec FE

$$A\,e = g, \qquad A = R - i\omega\mu_0 S$$

Assembling procedure fairly similar to Lagrange finite elements

Exercise
Check $div\,\boldsymbol{v}_h$

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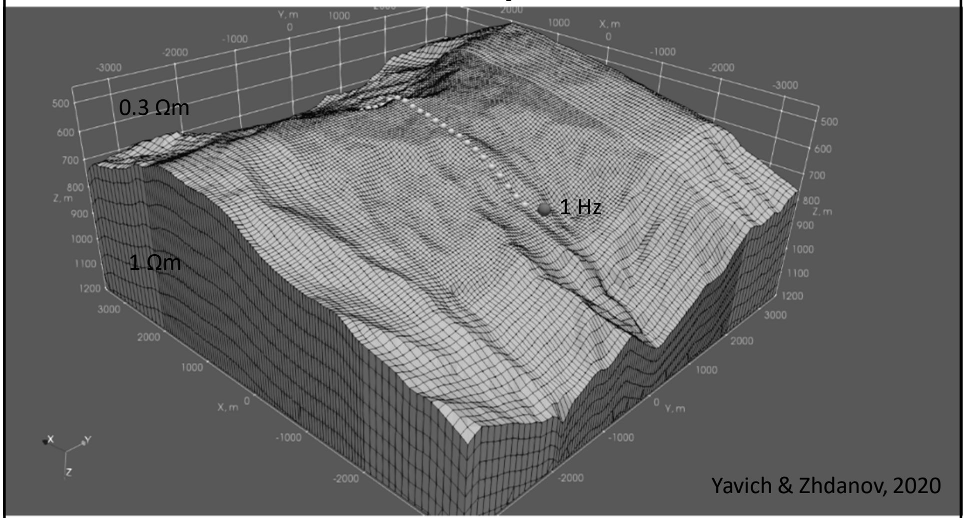
Example



Black Sea seafloor

115×100×55 nonuniform hexahedral grid
1.851 mln unknowns

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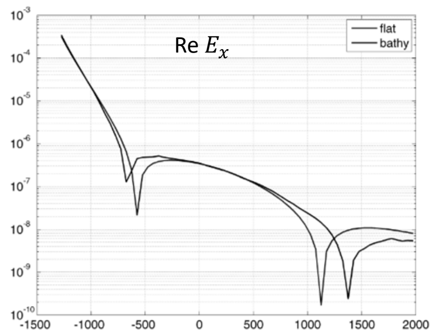
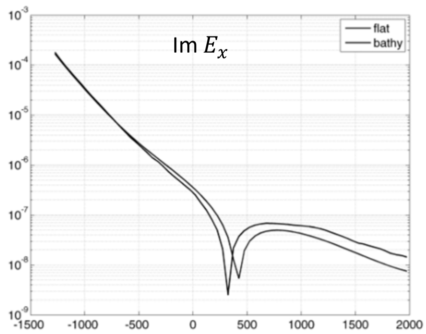
Electric Field Response

Real seafloor (bathy) vs flat





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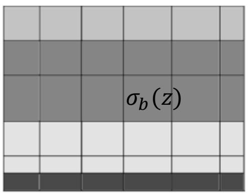
Part 3
Fast Solvers for
Maxwell's Equations

FFT-based solver



$$A_{b\,FD} = \begin{pmatrix} A_{xx} & A_{xy} & A_{xz} \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & A_{zz} \end{pmatrix}$$

$$A_{xx} = I_d^z \otimes A_d^y \otimes I_n^x + A_d^z \otimes I_d^y \otimes I_n^x - i\omega\mu_0\Sigma^x \otimes I_d^y \otimes I_n^x$$

$$A_{xy} = I_d^z \otimes F_{dn}^y \otimes F_{nd}^x$$

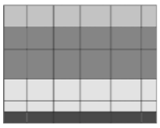
$$A_{xz} = F_{dn}^z \otimes I_d^y \otimes F_{nd}^x \qquad A_d^x \approx \frac{\partial^2}{\partial x^2} \qquad F_{nd}^x \approx \frac{\partial}{\partial x}$$

$$\cdots$$

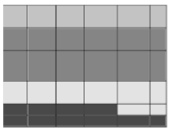
$$A_{zz} = I_n^z \otimes A_d^y \otimes I_d^z + I_n^z \otimes I_d^y \otimes A_d^x - i\omega\mu_0\Sigma^z \otimes I_d^y \otimes I_n^x$$

- $A_{b\,FD}^{-1}v$ can be computed in $O(N^{\frac{4}{3}})$ operations for **nonuniform grids** or in $O(Nlog\,N)$ operations for equidistant grids (with 2D FFT) Zaslavsky et al, 2011
- Evidently can be used as a preconditioner

FFT-based solver



$\sigma_b(z)$



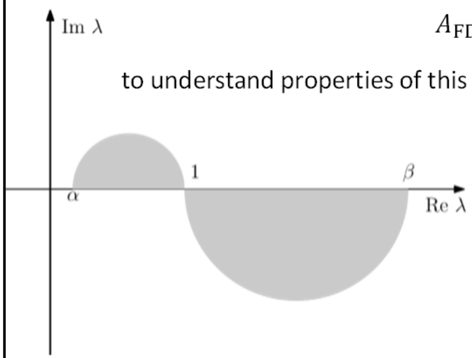
$\sigma(x, y, z)$

$\alpha\, \sigma_b(z) \leq \sigma(x, y, z) \leq \beta\, \sigma_b(z)$

We studied the respective eigenvalue problem,

$$A_{\mathrm{FD}}\, v = \lambda\, A_{FD\,b} v,$$

to understand properties of this preconditioner.



$$cond\left(A_{b\,FD}^{-1} A_{FD}\right) \leq \frac{\beta}{\alpha}$$

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Static Divergence Correction

Note the charge conservation law, $\mathrm{div}(\sigma E) = -\mathrm{div} J^{ext}$.

Let's enforce it within iterations:

$$E_n' = E_n - \nabla\psi \quad \text{with} \quad -\mathrm{div}(\sigma\nabla\psi) = \mathrm{div}(-J^{ext} - \sigma E_n).$$

This will imply, $\mathrm{div}(\sigma E_n') = -\mathrm{div} J^{ext}$.

Greatly improves convergence, requires solution of the DC equation on each iteration.

J.T. Smith (1993).

Heavily reused later, R. Mackie (1994), G. Newman (2002).

Note, we can also enforce the law locally rather than in the whole domain.

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Multigrid Framework

Based on sequential smoothing of the residual vector on a set of hierarchical grids.

Solution complexity $O(N\log(\varepsilon))$ if components are chosen appropriately.

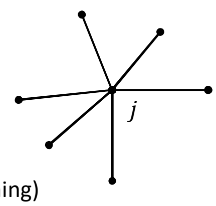
- Poisson equation, $-\Delta u = f$,
  R. Fedorenko (1961), A. Brandt (1973)

- Self-adjoint Maxwell's equations, curl curl$E + \alpha E = j$, $\alpha > 0$,
  R. Hiptamir (1998)
  Multigrid + divergence correction in the whole comp. domain Ω.

- Self-adjoint Maxwell's equations,
  D. Arnold et al (1999)
  Multigrid + local divergence correction (points, segments, planes) as a smoother.

Smoothing and Restriction

Patch of 6 edges



(smoothing)

Smoothing reduces null space components.

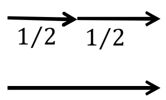
B_j 6x6 block of A, edges meeting at node j completed by the identity matrix

For j=0 to Nnodes-1

$$u_{j+1} = u_j + \eta\, B_j^{-1}(f - A\, u_j)$$

Restriction

E_x^h



E_x^{2h}

What would you do on stretched grids?

Example

$$rot\, rot\, E + i\omega\mu_0\sigma\, E = F \text{ в } V$$
$$E \times n = 0 \qquad \text{на } \Gamma$$

$$\sigma = \begin{cases} 10^{-7}, & z < 0 \\ 1, & z > 0 \end{cases} \text{ С/м}$$

Сетка	N	**Кол-во уровней**	**Число итераций**	**Время расчёт** (с)
20x20x24	29 тыс	2	9	1.6
40x40x48	230 тыс	3	9	15
80x80x96	1.85 млн	4	9	123

Yavich&Scholl, 2012