Die Ressourcenuniversität. Seit 1765.

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3D MT Simulation using

(1) Vector Finite Elements on Unstructured Grids

(2) Finite Differences (Ralph-Uwe Börner)

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March 30 - April 1, 2011

Outline

1. Finite Element Approach
   - MT Boundary Value Problem for the Magnetic Vector Potential
   - Finite Element Method
2. Finite Difference Approach
   - MT Boundary Value Problem for the Secondary Electric Field
   - Finite Difference Method
3. MT3DINV-2 forward model

Maxwell's Equations

- harmonic time dependency $e^{i\omega t}$

$$\begin{aligned} \nabla \times \mathbf{H} &= \mathbf{j} + i\omega\mathbf{D} \\ \nabla \times \mathbf{E} &= -i\omega\mathbf{B} \\ \nabla \cdot \mathbf{D} &= \rho \\ \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

- constitutive relations, Ohm's law

$$\mathbf{D} = \varepsilon\mathbf{E}, \quad \mathbf{B} = \mu\mathbf{H}, \quad \mathbf{j} = \sigma\mathbf{E}$$

Electromagnetic potentials

- magnetic vector potential $\mathbf{A}$, electric scalar potential V

$$\mathbf{H} = \mu^{-1}(\nabla \times \mathbf{A}) \qquad \mathbf{E} = -\nabla V - i\omega\mathbf{A}$$

Equation of Induction and Equation of Continuity

$$\begin{aligned} \nabla \times \mu^{-1} \nabla \times \mathbf{A} + (i\omega\sigma - \omega^2\varepsilon)\mathbf{A} + (\sigma + i\omega\varepsilon)\nabla V &= 0 \\ -\nabla \cdot \Big((i\omega\sigma - \omega^2\varepsilon)\mathbf{A} + (\sigma + i\omega\varepsilon)\nabla V \Big) &= 0 \end{aligned}$$

Gauge Condition

Choosing

- $\tilde{\mathbf{A}} = \mathbf{A} - \nabla\Psi$, $\tilde{V} = V - \dot{\Psi}$

and the gauge condition

- $\Psi = -iV/\omega$

yield

- $\tilde{\mathbf{A}} = \mathbf{A} - \frac{i}{\omega}\nabla V, \quad \tilde{V} = 0.$

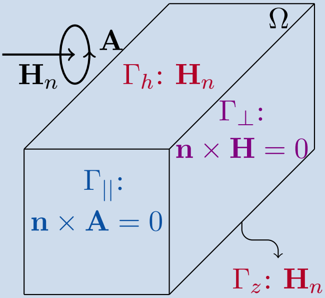
Boundary Value Problem for the Magnetic Vector Potential $\mathbf{A}$

Find $\mathbf{A}$ such that

$$\nabla \times \mu^{-1} \nabla \times \mathbf{A} + (i\omega\sigma - \omega^2\varepsilon)\mathbf{A} = 0 \quad \text{in} \quad \Omega$$

with

$$\begin{aligned} \mathbf{n} \times \mathbf{H} &= 0 \quad \text{on} \quad \Gamma_\perp \\ \mathbf{n} \times \mathbf{A} &= 0 \quad \text{on} \quad \Gamma_{||} \\ \mathbf{H} &= \mathbf{H}_n(z) \quad \text{on} \quad \Gamma_h, \Gamma_z \\ \mathbf{n}_1 \times \mathbf{H}_1 - \mathbf{n}_2 \times \mathbf{H}_2 &= 0 \quad \text{on} \quad \Gamma_i. \end{aligned}$$



Weak formulation

Find $\mathbf{A} \in U$ such that

$$\int_\Omega (\mu^{-1}\nabla \times \mathbf{A} \cdot \nabla \times \mathbf{v} \quad + \quad (i\omega\sigma - \omega^2\varepsilon)\,\mathbf{A} \cdot \mathbf{v})\; d\mathbf{x} = \int_{\Gamma_h} (\mathbf{n} \times \bar{\mathbf{v}}) \cdot \mathbf{H}_n \; d\mathbf{x} \quad + \quad \int_{\Gamma_z} (\mathbf{n} \times \bar{\mathbf{v}}) \cdot \mathbf{H}_n \; d\mathbf{x} \quad \forall \mathbf{v} \in V$$

where

$$\begin{aligned} U &:= \{\mathbf{A} \in H(\text{curl}, \Omega) : \mathbf{n} \times \mathbf{A} = 0 \quad \text{on} \quad \Gamma_{||}\}, \\ V &:= \{\mathbf{v} \in H(\text{curl}, \Omega) : \mathbf{n} \times \mathbf{v} = 0 \quad \text{on} \quad \Gamma_{||}\} \quad \text{and} \\ H(\text{curl}, \Omega) &:= \{\mathbf{v} \in (L^2(\Omega))^3, \nabla \times \mathbf{v} \in (L^2(\Omega))^3\}. \end{aligned}$$

Finite Element Analysis

A discrete approximation $\mathbf{A}^h \in U_h$ of $\mathbf{A} \in U$

$$\mathbf{A}^h = \sum_{i=1}^{N} a_i \boldsymbol{\phi}_i$$

and discrete test functions $\mathbf{v}_i = \boldsymbol{\phi}_i$ yield the discretized boundary value problem

$$\begin{aligned} \mathbf{KA} &= \mathbf{L} \quad \text{with} \\ K_{i,j} &= \int_\Omega (\mu^{-1}(\nabla \times \boldsymbol{\phi}_i) \cdot \nabla \times \bar{\boldsymbol{\phi}}_j + (i\omega\sigma - \omega^2\epsilon)\boldsymbol{\phi}_i \cdot \bar{\boldsymbol{\phi}}_j) dV, \\ L_i &= \int_{\Gamma_h} (\mathbf{n} \times \bar{\boldsymbol{\phi}}_i) \cdot \mathbf{H}_n \, d\mathbf{x} + \int_{\Gamma_z} (\mathbf{n} \times \bar{\boldsymbol{\phi}}_i) \cdot \mathbf{H}_n \, d\mathbf{x}. \end{aligned}$$

To solve the system of equations we apply the PARDISO-package (http://www.pardiso-project.org).

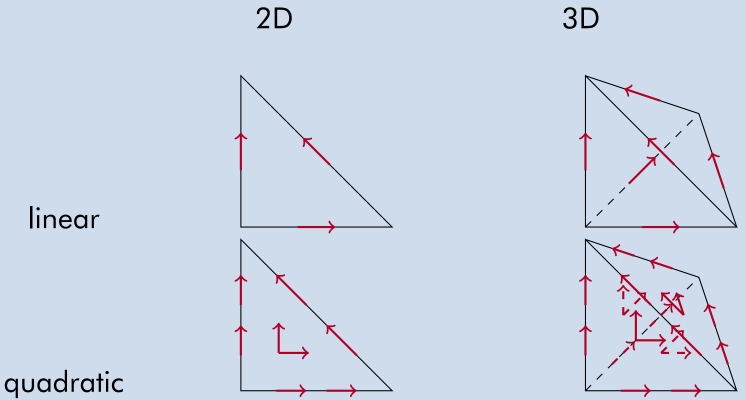
The basis functions

... ϕ_i are polynomials of arbitrary degree, mostly linear or quadratic. To the so-called degrees of freedom (DOF) l_n

$$l_n(\boldsymbol{\phi}_j) = \delta_{n,j},$$

applies.

Nédélec Elements



DOF: Integrals over $\mathbf{A}$ along edges and over faces

Challenges

- large effort to administer the unstructured tetrahedral grids
- optimum trade-off between fitting the boundary conditions and minimizing the discretization error
  $\rightarrow$ smart distribution of DOF is needed

Advantages of the FE method in conjunction with unstructured grids

- precise parametrization of arbitrary model geometries including surface and seafloor topography
- adaptive mesh refinement based on *a posteriori* error estimators
- convergence studies yield estimates of accuracy even if the analytical solution is unknown

Boundary Value Problem for the Secondary Electric Field $\mathbf{E}_s$

Find $\mathbf{E}_s$ such that

$$\nabla \times \nabla \times \mathbf{E}_s + i\omega\mu\sigma\mathbf{E}_s \quad = \quad -i\omega\mu\sigma_s\mathbf{E}_p \quad \text{in} \quad \Omega$$

with

$$\mathbf{E}_s = 0 \quad \text{on} \quad \Gamma$$

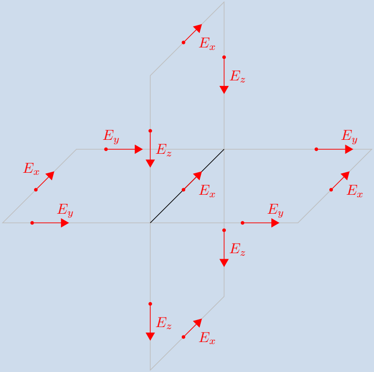
and

$$\mathbf{E} = \mathbf{E}_s + \mathbf{E}_p, \quad \sigma = \sigma_s + \sigma_p$$

where σ_p represents the conductivity distribution of a layered half-space model and $\mathbf{E}_p$ the appropriate electric fields that are computed analytically.

Finite Difference Method

$$\nabla \times \nabla \times \mathbf{E} \rightarrow \mathbf{C}^H \cdot \mathbf{C}^E \cdot \mathbf{E}^h$$
$$i\omega\mu\sigma\mathbf{E} \rightarrow i\omega\mu\mathbf{S} \cdot \mathbf{E}^h$$

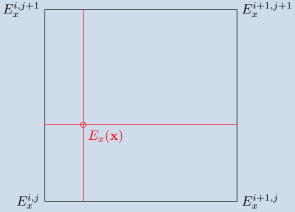


$$\mathbf{C}^H = \begin{pmatrix} 0 & -\mathbf{G}_z^H & \mathbf{G}_y^H \\ \mathbf{G}_z^H & 0 & -\mathbf{G}_x^H \\ -\mathbf{G}_y^H & \mathbf{G}_x^H & 0 \end{pmatrix}$$
$$\mathbf{C}^E = \begin{pmatrix} 0 & -\mathbf{G}_z^E & \mathbf{G}_y^E \\ \mathbf{G}_z^E & 0 & -\mathbf{G}_x^E \\ -\mathbf{G}_y^E & \mathbf{G}_x^E & 0 \end{pmatrix}$$

$$\mathbf{C}^E : V^E \rightarrow V^H,$$
$$\mathbf{C}^H : V^H \rightarrow V^E,$$
$$\mathbf{S} : V^\sigma \rightarrow V^E \text{(area weighted)}$$

Interpolation operator $\mathbf{Q}$

- continuous approximate solution $\mathbf{E}(\mathbf{x})$ obtained by application of interpolation operator $\mathbf{Q} : V^E \rightarrow V^D$
- columns of $\mathbf{Q}$ provide linear combinations of $\mathbf{E}^h$ or $\mathbf{C}^E \cdot E^h$
- Elements of $\mathbf{Q}$ obtained by e.g. bilinear interpolation



MT3DINV-2 forward model

FE approach

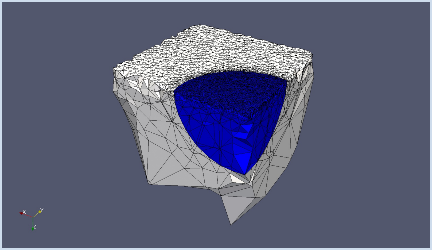
- one model per decade: $60 \times 60 \times 60\,\text{km}^3$ ... $3000 \times 3000 \times 3000\,\text{km}^3$
- edge length: $\Delta_{\text{min}} = 33\,\text{m}$, $\Delta_{\text{max}} = 16\,\text{km}$ ... $\Delta_{\text{min}} = 738\,\text{m}$, $\Delta_{\text{max}} = 872\,\text{km}$
- no. of unknowns: $2 \cdot 10^6$
- computing time: 5 h 40 min
- 8 nodes (2.4 GHz), 64 GB shared memory
- COMSOL Multiphysics®, MATLAB®, PARDISO*

FD approach

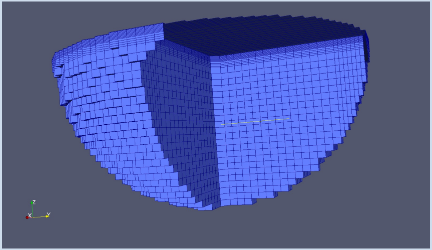
- model size: $214 \times 214 \times 296\,\text{km}^3$
- $\Delta x_{\text{min}} = 125\,\text{m}$, $\Delta x_{\text{max}} = 32\,\text{km}$, $\Delta y_{\text{min}} = 125\,\text{m}$, $\Delta y_{\text{max}} = 32\,\text{km}$, $\Delta z_{\text{min}} = 5\,\text{m}$, $\Delta z_{\text{max}} = 100\,\text{km}$
- no. of unknowns: $1.2 \cdot 10^6$
- computing time: 6 h 20 min
- 16 nodes (2.4 GHz), 128 GB shared memory
- MATLAB®, PARDISO*

* http://www.pardiso-project.org

Discretized MT3DINV-2 forward model



FE discretization
for $0.01\,\mathrm{s} \leq T < 0.1\,\mathrm{s}$



FD discretization of the hemisphere