Numerical Simulation Methods in Geophysics, Part 1: Foundations

1. MGPY+MGIN, 3. MDRS+MGEX-CMG

Thomas Günther, thomas.guenther@geophysik.tu-freiberg.de

Introduction

Content

Schedule

Lectures Wednesday, 11:30, MEI-2122 $\Rightarrow$ Meeting room MEI-211

14 slots : 16.10., 23.10., 30.10., 06.11., (13.11.), 27.11., 04.12., 11.12., 18.12., 08.01., 15.01., 22.01., 28.01., 05.02.

Exercises Thursday, 08:00-09:30, CIP pool MEI1203a

14 slots : 17.10., 24.10., 07.11., 14.11., 21.11., 28.11., 05.12., 12.12., 19.12., 09.01., 16.01., 23.01., 29.01., 06.02.

Grade: submitting a report including codes

What should you know already?

- Higher mathematics: differential equations, algebra (1.-2. BSc)
- Experimental and theoretical physics: governing equations
- Numerics for engineers (2. BSc)
- Programming (1. BSc), Software development (3. BSc)
- Geophysics: feeling for physical fields & methods
- Electromagnetics (5. BSc), Theory EM,
- now: Scientific programming, HPC, seismic imaging

Topics to be covered

- recap on partial differential equations
- (1D) heat equation: stationary and instationary (Geothermics course)
- 2D: magnetotellurics
- 3D DC modelling (content of Spitzer videos)
- 2D ground-penetrating radar (EM) and pressure waves (seismics)
- excurse to hydrodynamic modelling
- modelling the Eikonal equation (the travelling saleman)
- exercises: code FD & FE by hand, use packages to obtain feeling

Literature

- Haber (2015): Computational methods geophysical electromagnetics
- Morra (2018): Pythonic Geodynamics - Implementations for fast computing, frei verfügbar unter https://doi.org/10.1007/978-3-319-55682-6, zum Eintauchen ins Programmieren (MSc)
- Warnick: Numerical Methods for Engineering : An Introduction Using MATLAB® and Computational Electromagnetics Examples Link
- Igel (2007): Numerical modelling in geophysics, short course https://www.geophysik.uni-muenchen.de/~igel/nmg-short/ https://www.geophysik.uni-muenchen.de/~igel/downloads/
- Logg et al. (2011): Automated Solution of Differential Equations by the Finite Element Method: Link
- Press (2007): Numerical recipes: the art of scientific computing,

Further links

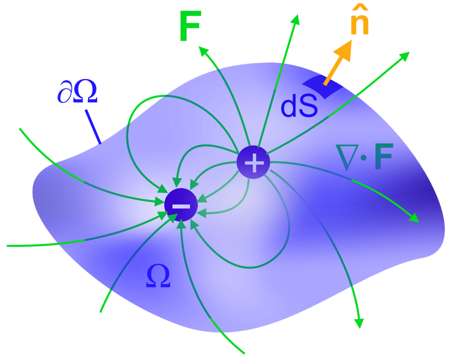
- pyGIMLi: Python Geophysical Inversion and Modelling Library https://pygimli.org
- Geoscience.XYZ: https://geosci.xyz
- Fenics handbook
- Theory of electromagnetics https://ruboerner.github.io/ThEM/

Differential operators

- single derivative in space $\frac{\partial}{\partial x}$ or time $\frac{\partial}{\partial t}$
- gradient $\boldsymbol{\nabla} = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})^T$
- divergence $\boldsymbol{\nabla} \cdot \mathbf{F} = (\frac{\partial F_x}{\partial x}, \frac{\partial F_y}{\partial y}, \frac{\partial F_z}{\partial z})^T = \begin{pmatrix} \frac{\partial F_x}{\partial x} \\ \frac{\partial F_y}{\partial y} \\ \frac{\partial F_z}{\partial z} \end{pmatrix}$

Gauss': *what's in (volume) comes out (surface)*

$$\int_V \boldsymbol{\nabla} \cdot \mathbf{F} \, dV = \iint_S \mathbf{F} \cdot \mathbf{n} \, dS$$



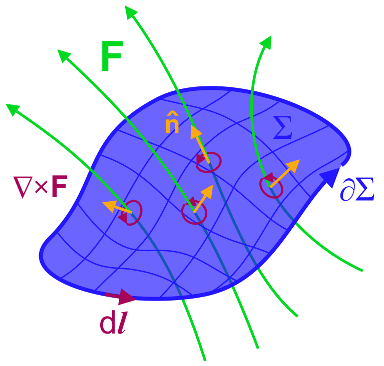
Gauss's theorem in EM

Curl (rotation)

- curl $\boldsymbol{\nabla} \times \mathbf{F} = (\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}, \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}, \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y})^T$

Stoke: *what goes around comes around*

$$\int_S \boldsymbol{\nabla} \times \mathbf{F} \cdot \mathbf{d}S = \iint_S \mathbf{F} \cdot \mathbf{d}l$$



Stoke's theorem in EM

- curls have no divergence: $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) = 0$
- potential fields have no curl $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} u) = 0$

Numerical simulation

Mostly: solution of partial differential equations (PDEs) for either scalar (potentials) or vectorial (fields) quantities

PDE Types:

- elliptic PDE: $\nabla^2 u = f$
- parabolic PDE $\nabla^2 u - a\frac{\partial u}{\partial t} = f$
- hyperbolic $\nabla^2 u - c^2\frac{\partial^2 u}{\partial t^2} = f$ (plus diffusive term)

$$\frac{\partial^2\, u}{\partial x^2} - c^2\frac{\partial^2 u}{\partial t^2} = 0$$

- coupled $\nabla \cdot u = f$ & $u = K\nabla p = 0$ (Darcy flow)
- nonlinear $(\nabla u)^2 = s^2$ (Eikonal equation)

Poisson equation

potential field u generates field $\vec{F} = -\nabla u$

causes some flow $\vec{j} = a\vec{F}$

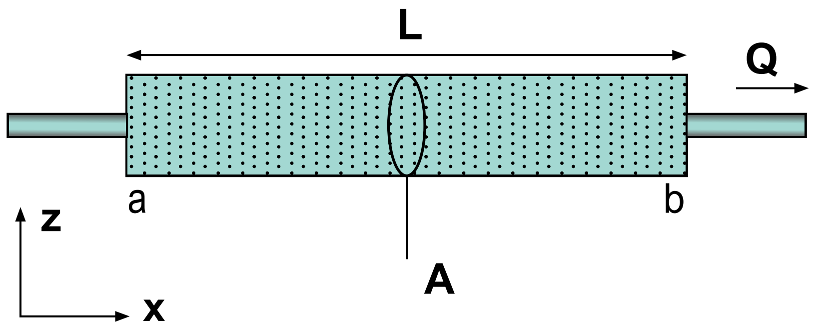
a is some sort of conductivity (electric, hydraulic, thermal)

continuity of flow: divergence of total current $\mathbf{j} + \mathbf{j}_s$ is zero

$$\boldsymbol{\nabla} \cdot (a\nabla u) = -\boldsymbol{\nabla} \cdot \mathbf{j}_s$$

Darcy's law

volumetric flow rate Q caused by gradient of pressure p



Darcy's law

$$Q = \frac{kA}{\mu L}\Delta p$$

$$\mathbf{q} = -\frac{k}{\mu}\nabla p$$

$$\boldsymbol{\nabla}\cdot\mathbf{q} = -\boldsymbol{\nabla}\cdot(k/\mu\boldsymbol{\nabla}p) = 0$$

The heat equation in 1D

sought: Temperature T as a function of space and time

heat flux density $\mathbf{q} = \lambda \boldsymbol{\nabla} T$

q in W/m², λ - heat conductivity/diffusivity in W/(m.K)

Fourier’s law: $\frac{\partial T}{\partial t} - a \nabla^2 T = s$ (s - heat source)

temperature conduction $a = \frac{\lambda}{\rho c}$ (ρ - density, c - heat capacity)

Maxwell's equations

- Faraday's law: currents & varying electric fields $\Rightarrow$ magnetic field

$$\boldsymbol{\nabla} \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{j}$$

- Ampere's law: time-varying magnetic fields induce electric field

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

- $\boldsymbol{\nabla} \cdot \mathbf{D} = \varrho$ (charge $\Rightarrow$), $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$ (no magnetic charge)
- material laws $\mathbf{D} = \epsilon\mathbf{E}$ and $\vec{B} = \mu\mathbf{H}$

Helmholtz equations

$$\nabla^2 u + k^2 u = f$$

results from wavenumber decomposition of diffusion or wave equations

approach: $\mathbf{F} = \mathbf{F_0} e^{\imath\omega t} \quad \Rightarrow \quad \frac{\partial \mathbf{F}}{\partial t} = \imath\omega\mathbf{F} \quad \Rightarrow \quad \frac{\partial^2 \mathbf{F}}{\partial t^2} = -\omega^2 \mathbf{F}$

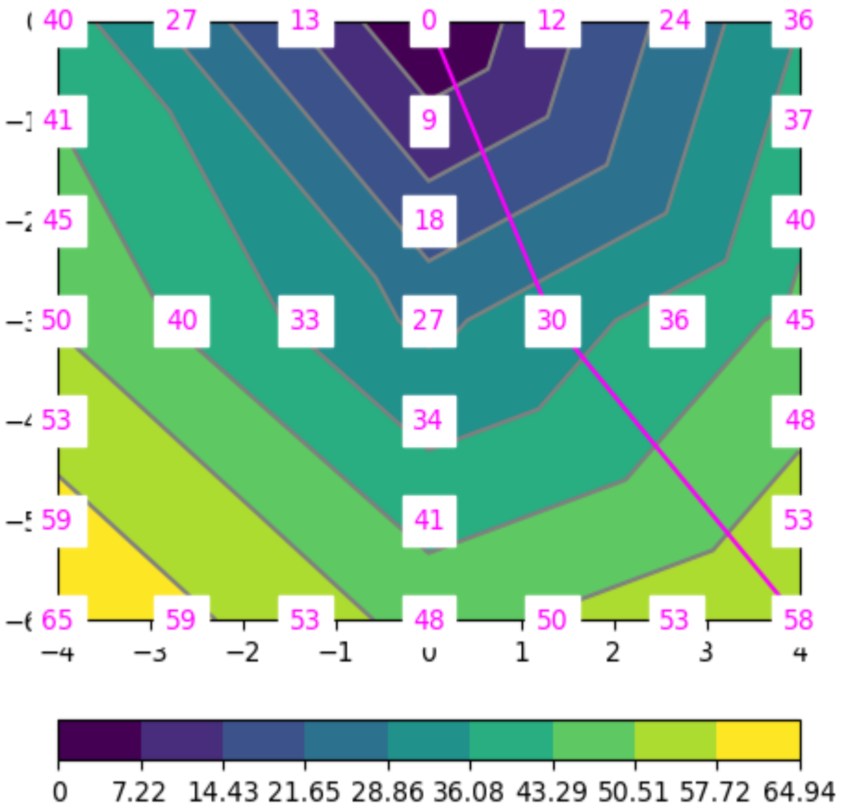
$$\nabla^2 \mathbf{F} - a\nabla_t \mathbf{F} - c^2 \nabla_t^2 \mathbf{F} = 0$$

$$\Rightarrow \nabla^2 \mathbf{F} - a\imath\omega\mathbf{F} + c^2\omega^2\mathbf{F} = 0$$

The eikonal equation

Describes first-arrival times t as a function of velocity (v) or slowness (s)

$$|\boldsymbol{\nabla} t| = s = 1/v$$



Taylor expansion