# Numerical Simulation Methods in Geophysics, Part 2: Finite Differences

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

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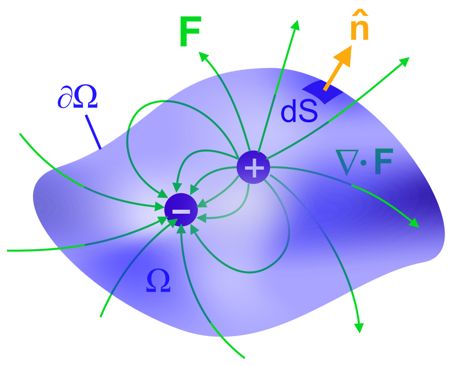
# Some mathematical background

# 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 $\boldsymbol{\nabla} \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$

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

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



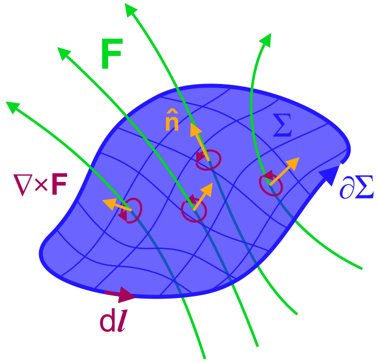

Gauss's theorem in EM

# 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*

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




Stokes' 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

# Partial differential equations (PDEs)

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

PDE Types ($u$-function, $f$-source, $a/c$-parameter):

- 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

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

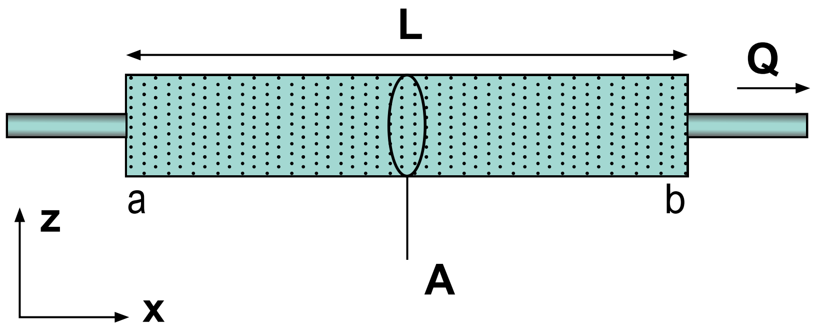
# Darcy's law

volumetric flow rate $Q$ caused by gradient of pressure $p$

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

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

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




Darcy's law

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

# Navier-Stokes equation

Stokes equation

$$\mu \nabla^2 \mathbf{v} - \boldsymbol{\nabla} p + f = 0$$

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0$$

Navier-Stokes equation (incompressible, uniform viscosity)

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} = \nu \nabla^2 \mathbf{u} - 1/\rho \boldsymbol{\nabla} p + f$$

# 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

$$\nabla^2 \mathbf{F} + k^2 \mathbf{F} = f$$

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 ($s$)

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

# The Finite Difference Method (FDM)

# Taylor expansion

Assume the Poisson equation

$$\nabla \cdot (a\nabla u) = f$$

Taylor expansion

$$f(x) = f(x_0) + f'(x0)(x - x_0) + f''(x_0)(x - x_0)^2/2$$

# Finite differences

**Approximate derivative operators by differences**

$$\frac{\partial u}{\partial x} \approx \frac{\Delta u}{\Delta x}$$

and solution $u$ by finite values $u_i$ at points $x_i$, e.g.

$$\mathrm{d}u/\mathrm{d}x_{2.5} := (u_3 - u_2)/(x_3 - x_2)$$

$$\frac{\partial^2 u_3}{\partial x^2} \approx \frac{\mathrm{d}u/\mathrm{d}x_{3.5} - \mathrm{d}u/\mathrm{d}x_{2.5}}{(x_4 - x_2)/2} = \frac{(u_4 - u_3)/(x_4 - x_3) - (u_3 - u_2)/}{(x_4 - x_2)/2}$$

# Difference stencil

Assumption: equidistant discretization $\Delta x$, conductivity 1

1st derivative: $[-1, +1]/dx$, 2nd derivative $[+1, -2, +1]/dx^2$

Matrix-Vector product $\mathbf{A} \cdot \mathbf{u} = \mathbf{f}$ with

$$\mathbf{A} = \begin{bmatrix} +1 & -2 & +1 & 0 & \dots & \\ 0 & +1 & -2 & +1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ \dots & \dots & 0 & +1 & -2 & +1 \end{bmatrix}$$

# FDM on the general Poisson equation

Assume the Poisson equation

$$\boldsymbol{\nabla} \cdot (a \boldsymbol{\nabla} u) = f$$

$$\frac{\partial (a \, \mathrm{d}/\mathrm{d}u)}{\partial z} = a \frac{\partial^2 u}{\partial z^2} + \frac{\partial a}{\partial z} \frac{\partial u}{\partial z}$$

# Boundary conditions

Dirichlet conditions: $u_0 = u_B$ (homogeneous if 0)

Neumann conditions (homogeneous if 0)

$$\partial u / \partial x_0 = g_B$$

Mixed boundary conditions $u_0 + \alpha du_0/dx = \gamma$

# Dirichlet BC implementation way 1

$$u_0 = u_B$$

$$\begin{bmatrix} +1 & 0 & 0 & \dots & & \\ +1 & -2 & +1 & 0 & \dots & \\ \vdots & \vdots & \ddots & \vdots & & \\ \dots & \dots & 0 & +1 & -2 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} u_B \\ f_1 \\ \vdots \\ f_N \end{bmatrix}$$

# Dirichlet BC implementation way 2

$$u_B - 2u_1 + u_3 = f_1$$

$$\begin{bmatrix} -2 & +1 & 0 & \dots & \\ +1 & -2 & +1 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \\ \dots & 0 & +1 & -2 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_1 - u_B \\ f_2 \\ \vdots \\ f_N \end{bmatrix}$$

# Neumann BC implementation way 1

$$u_1 - u_0 = g_B$$

$$\begin{bmatrix} -1 & +1 & 0 & \dots & \\ +1 & -2 & +1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \dots & \dots & +1 & -2 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_0 + g_B \\ f_1 \\ \vdots \\ f_N \end{bmatrix}$$

# Neumann BC implementation way 2

$$u_0 - 2u_1 + u_2 = f_1 \qquad u_1 - u_0 = g_B \Rightarrow u_2 - u_1 = f_1 + g_B$$

$$\begin{bmatrix} -1 & +1 & 0 & \dots & & \\ +1 & -2 & +1 & 0 & \dots \\ \vdots & \vdots & \ddots & \vdots & \\ \dots & 0 & +1 & -2 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_1 + g_B \\ f_2 \\ \vdots \\ f_N \end{bmatrix}$$

# Parabolic PDEs

# Heat transfer in 1D

$$\frac{\partial T}{\partial t} - a\frac{\partial^2 T}{\partial z^2} = 0$$

with the periodic boundary conditions:

- $T(z = 0, t) = T_0 + \Delta T \sin \omega t$ (daily/yearly cycle)
- $\frac{\partial T}{\partial z}(z = z_1) = 0$ (no change at depth)

and the initial condition $T(z, t = 0) = \sin \pi z$ has the analytical solution

$$T(z, t) = \Delta T e^{-\pi^2 t} \sin \pi z$$

# Explicit methods

$$\frac{\partial T}{\partial t} - a\frac{\partial^2 T}{\partial z^2} = 0$$

Solve Poisson equation $\boldsymbol{\nabla} \cdot (a\boldsymbol{\nabla} u) = f$

for every time step $i$ (using FDM, FEM, FVM etc.)

Finite-difference step in time: update field by

$$T_{i+1} = T_i + a\frac{\partial^2 u}{\partial z^2} \cdot \Delta t$$

# Implicit methods

next lecture

# Mixed methods