Numerical Simulation Methods in Geophysics, Part 1: Equations & Finite Differences

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

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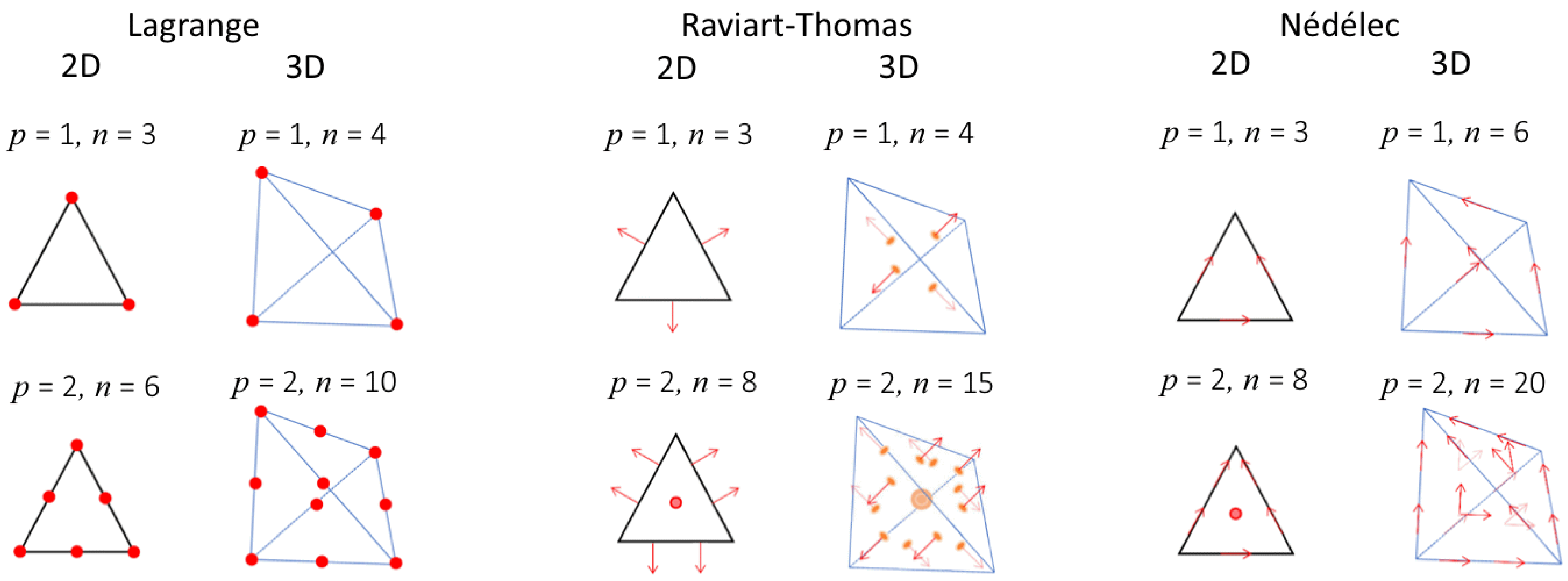
Introduction



$$\mathcal{H}^1(\Omega) \quad := \quad \{v \in L^2(\Omega) : \nabla v \in [L^2(\Omega)]^3\}$$

$$\mathcal{H}(\text{div};\Omega) \quad := \quad \{v \in [L^2(\Omega)]^3 : \nabla \cdot v \in L^2(\Omega)\}$$

$$\mathcal{H}(\text{curl};\Omega) \quad := \quad \{v \in [L^2(\Omega)]^3 : \nabla \times v \in [L^2(\Omega)]^3\}$$

Content

Schedule

Lectures Thursday, 09:45-11:15, MEI-0150

14 slots: 23.10., 30.10., 06.11., 13.11., 20.11., 27.11., 04.12., 11.12., 18.12., 08.01., 22.01., 28.01., 05.02., 06.02. (15.01. dies)

Exercises Wednesday, 09:45-11:15, CIP pool MEI1203a

14 slots: 22.10., 29.10., 05.11., 12.11., 26.11., 03.12., 10.12., 17.12., 07.01., 14.01., 21.01., 28.01., 04.02., 11.02. (19.11. holiday)

Grade: submitting two reports including codes

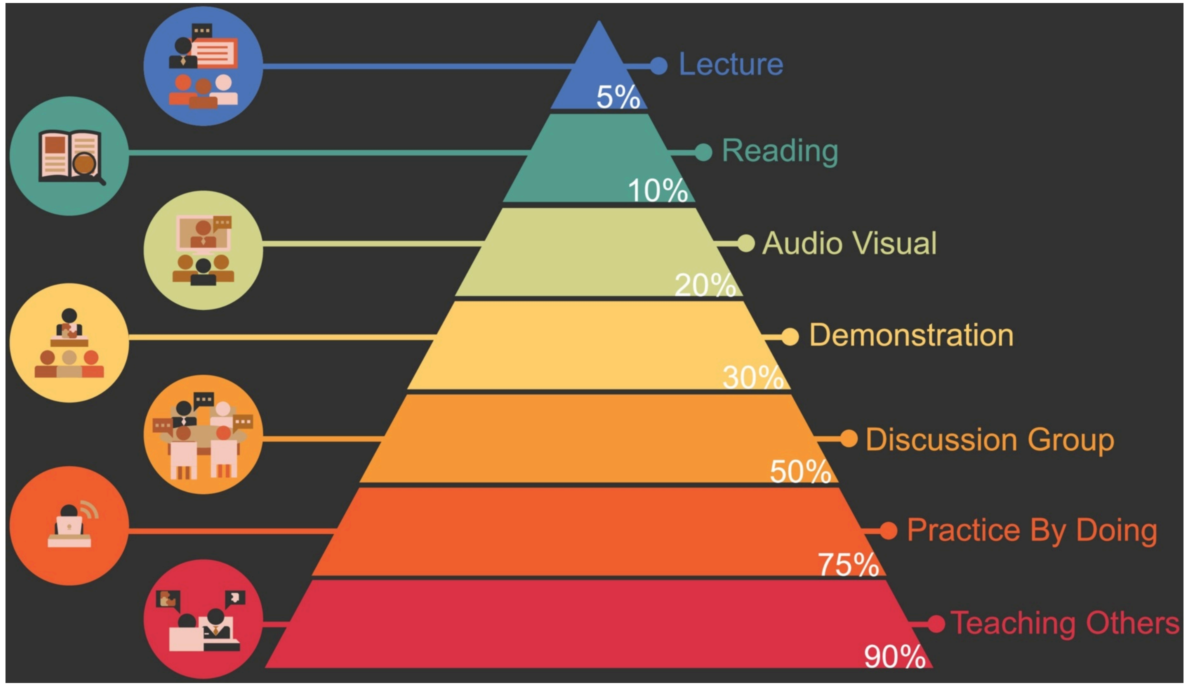
What should you know already?

- 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
- 2D electromagnetic fields in the Earth
- (3D DC modelling - see 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

Learning goal



- basic understanding of the common modelling techniques
- feeling for strengths and weaknesses of numerical solutions
- ability to write your own modelling codes in Python

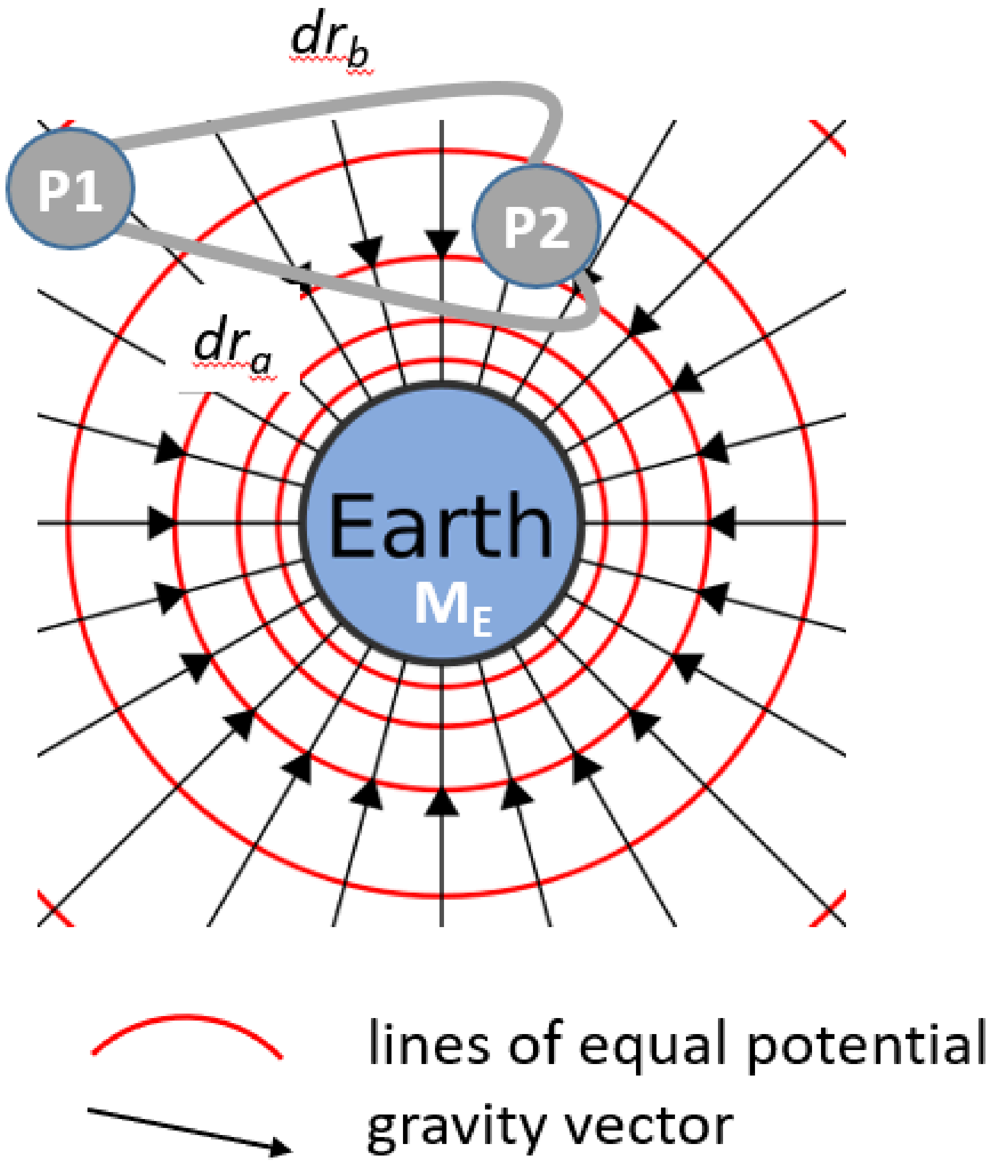
Literature

- Morra (2018): Pythonic Geodynamics - Implementations for fast computing, frei verfügbar, Dive into Python programming
- Warnick: Numerical Methods for Engineering : An Introduction Using MATLAB® and Computational Electromagnetics Examples
- Igel (2007): Numerical modelling in geophysics, short course
- Logg et al. (2011): Automated Solution of Differential Equations by the Finite Element Method: Link
- Press (2007): Numerical recipes: the art of scientific computing
- Haber (2015): Computational methods geophysical electromagnetics

Further links

- Course notes
- pyGIMLi: Python Geophysical Inversion and Modelling Library
- Homepage of Oskar package
- Geoscience.XYZ
- Fenics handbook
- Theory of electromagnetics

Numerical Simulation

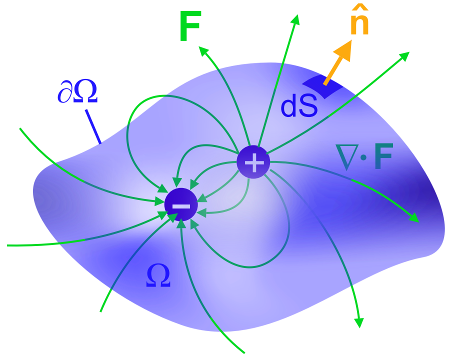


Differential operators

- 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)*

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



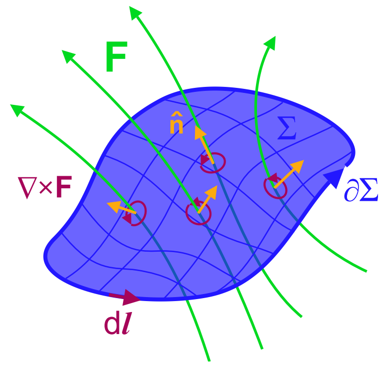
Gauss's theorem in EM

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 $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} u) = 0$

Partial differential equations (PDEs)

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

derived by $\boldsymbol{\nabla} \cdot \mathbf{F} = f$ with potential field $\mathbf{F} = -a\nabla u$

Assume the Poisson equation (source f, conductivity a)

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

solution u: potential, e.g. temperature T, gravity or electric potential, hydraulic head

PDE Types in geophysics

(u-function, f-source, a/b/c-parameter):

- elliptic PDE: $\nabla^2 u = f$ or $\nabla^2 u + k^2 u = f$
- parabolic PDE $\nabla^2 u - b\frac{\partial u}{\partial t} = f$
- hyperbolic $\nabla^2 u - c^2\frac{\partial^2 u}{\partial t^2} = f$
  - or $\nabla^2 u - b\frac{\partial u}{\partial t} - c^2\frac{\partial^2 u}{\partial t^2} = f$
- nonlinear $(\nabla u)^2 = s^2$ (Eikonal equation - first arrivals)

Poisson equation

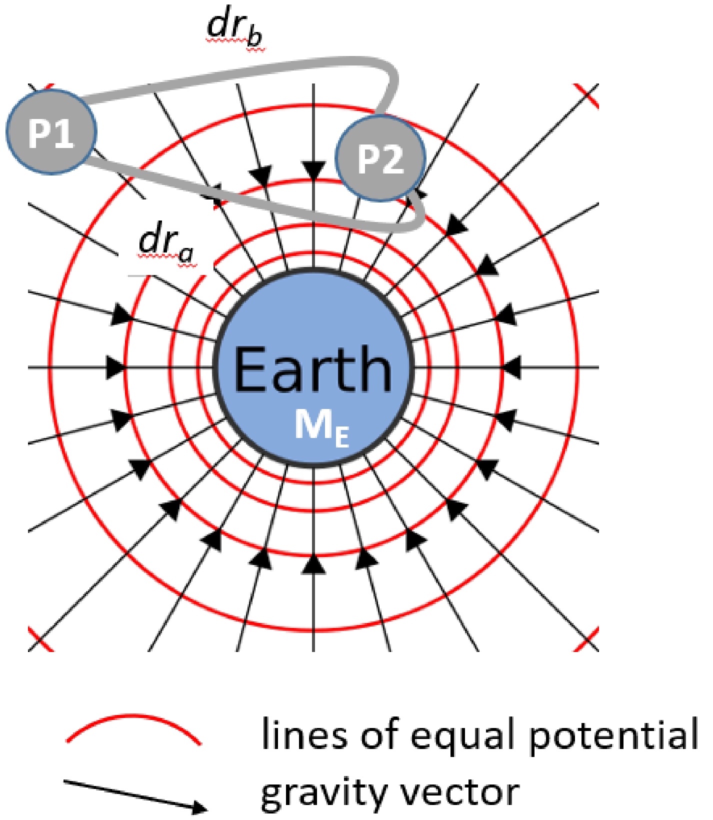
potential field u generates field $\mathbf{F} = -\nabla u$

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

a: conductivity (electric, hydraulic, thermal)

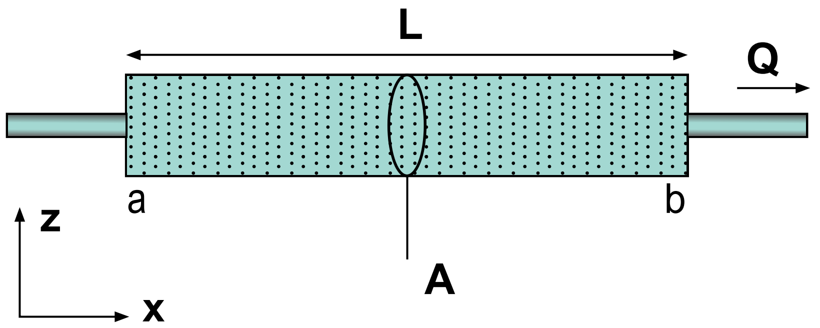
continuity of flow: divergence of total current $\mathbf{j} + \mathbf{j}_s$ is zero

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



Darcy's law

volumetric flow rate Q caused by gradient of pressure p



Darcy's law

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

k permeability

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

μ viscosity

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

The heat equation

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)

Stoke equations

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

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

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 $\mathbf{B} = \mu\mathbf{H}$

Helmholtz equations

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

results from wavenumber decomposition of diffusion or wave equations

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

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

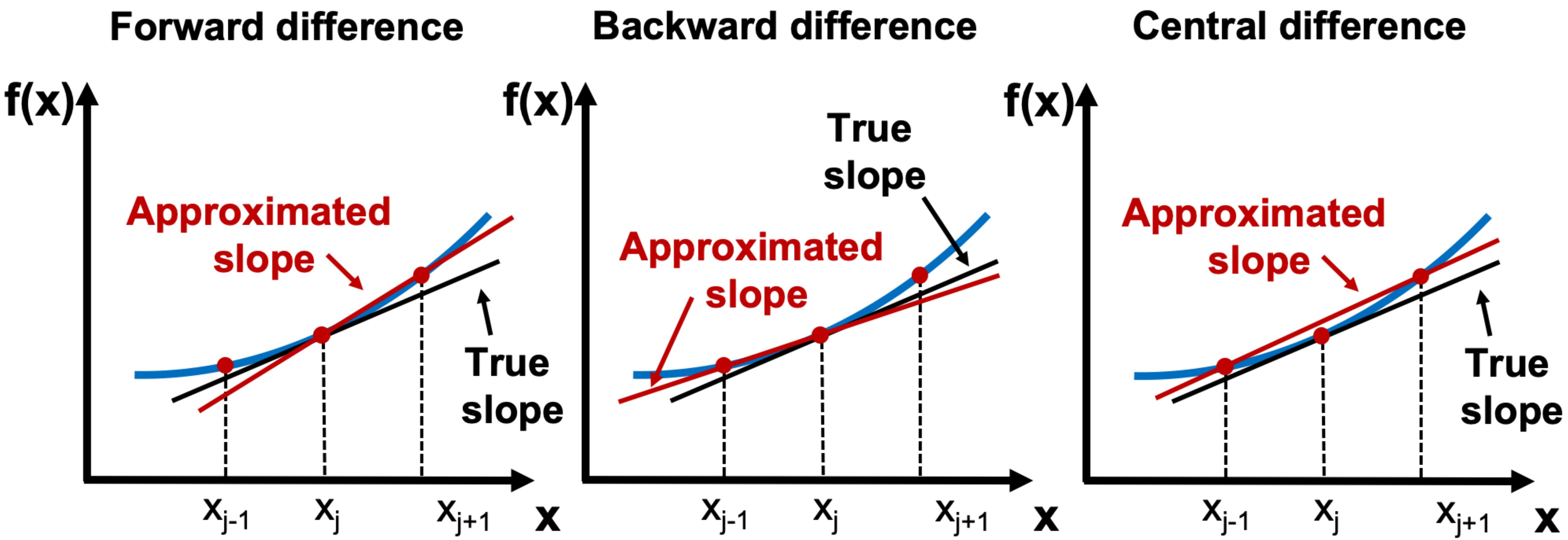
$$\Rightarrow \nabla^2 \mathbf{F} - a\imath\omega\mathbf{F} + c^2\omega^2\mathbf{F} = 0$$

The eikonal equation

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

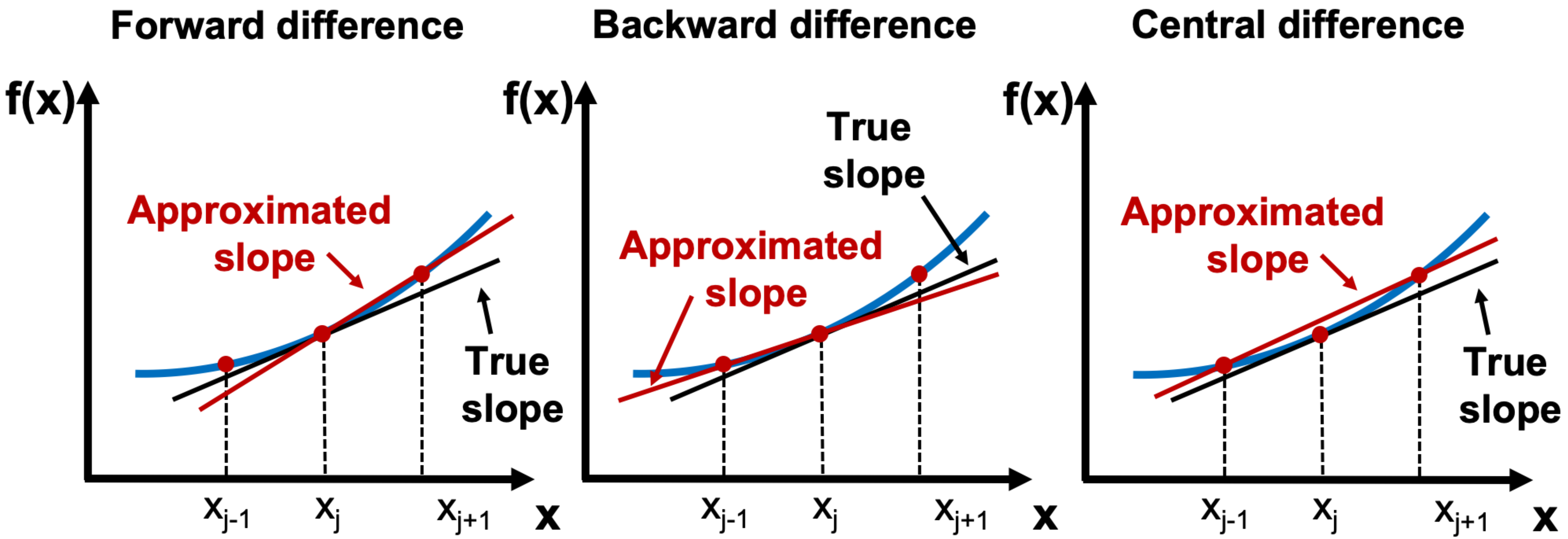
$$|\boldsymbol{\nabla} t| = s = 1/v$$

Finite Differences (FD)



Taylor expansion

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



Forward, backward and central difference for 1D FD grid

Poisson equation in 1D

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

reads in 1D as

$$-\frac{\partial (a \frac{\partial u}{\partial x})}{\partial x} = f$$

Approximate derivative operators by differences

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

Finite differences

Approximate derivative operators by differences

$$\frac{\partial u}{\partial x} \approx \frac{\delta u}{\delta x} \qquad \frac{\partial^2 u}{\partial x^2} \approx \frac{\delta \frac{\delta u}{\delta x}}{\delta x} \qquad \frac{\partial}{\partial x}\left(a \frac{\partial u}{\partial x}\right) \approx \frac{\delta a}{\delta x}\frac{\delta u}{\delta x} + a \frac{\delta \frac{\delta u}{\delta x}}{\delta x}$$

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

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

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

Summarize in a matrix

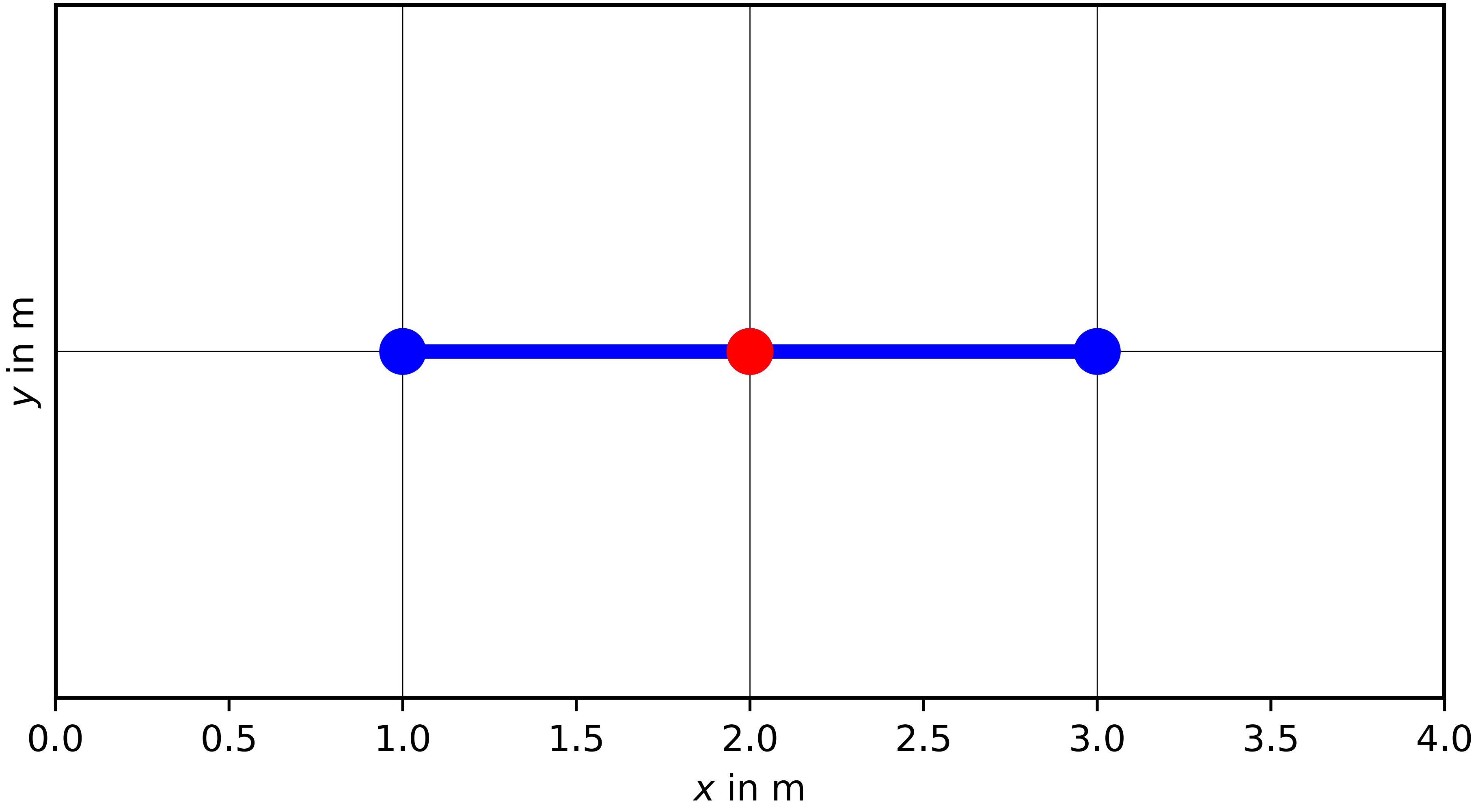
Assumption: equidistant discretization Δx, conductivity 1

1st derivative: $[-1, +1]/\Delta x$, 2nd derivative $[+1, -2, +1]/\Delta x^2$

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

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

Finite difference stencil



compute each value (red) using its neighbors (blue)

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 $u_0 + \alpha\, \partial u / \partial x = \gamma$

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

$$u_B - 2u_1 + u_2 = f_1$$

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

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

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

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

Accuracy: analytical solution

Assume a=1 & $f(x) = 1 \Rightarrow -\frac{\partial^2 u}{\partial x^2} = 1$ can be integrated twice:

$$\frac{\partial u}{\partial x} = -x + C_1$$

$$u(x) = -\frac{1}{2}x^2 + C_1 x + C_0$$

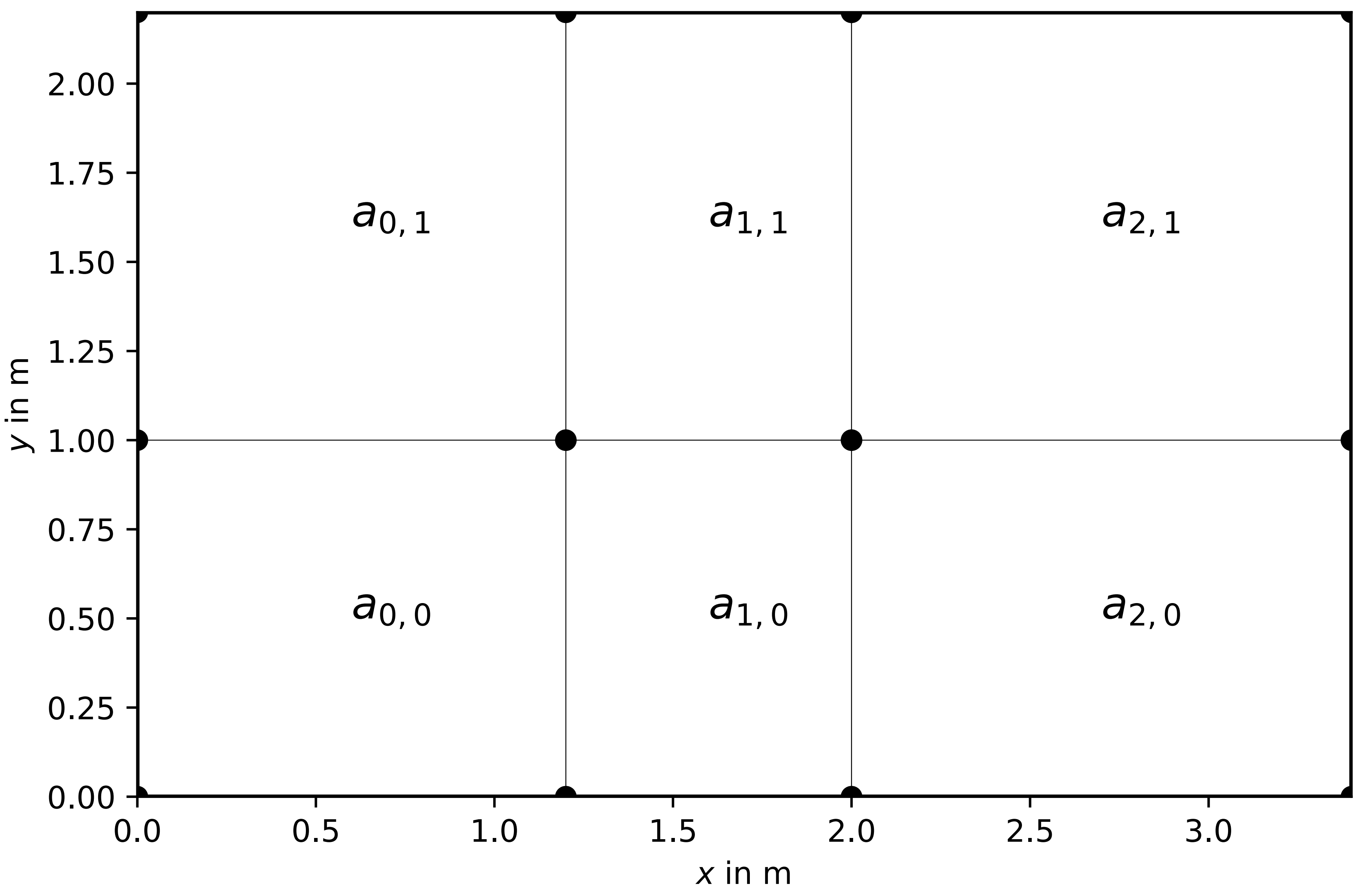
For x=0, $u_0 = C_0$, for x=X?

Solutions

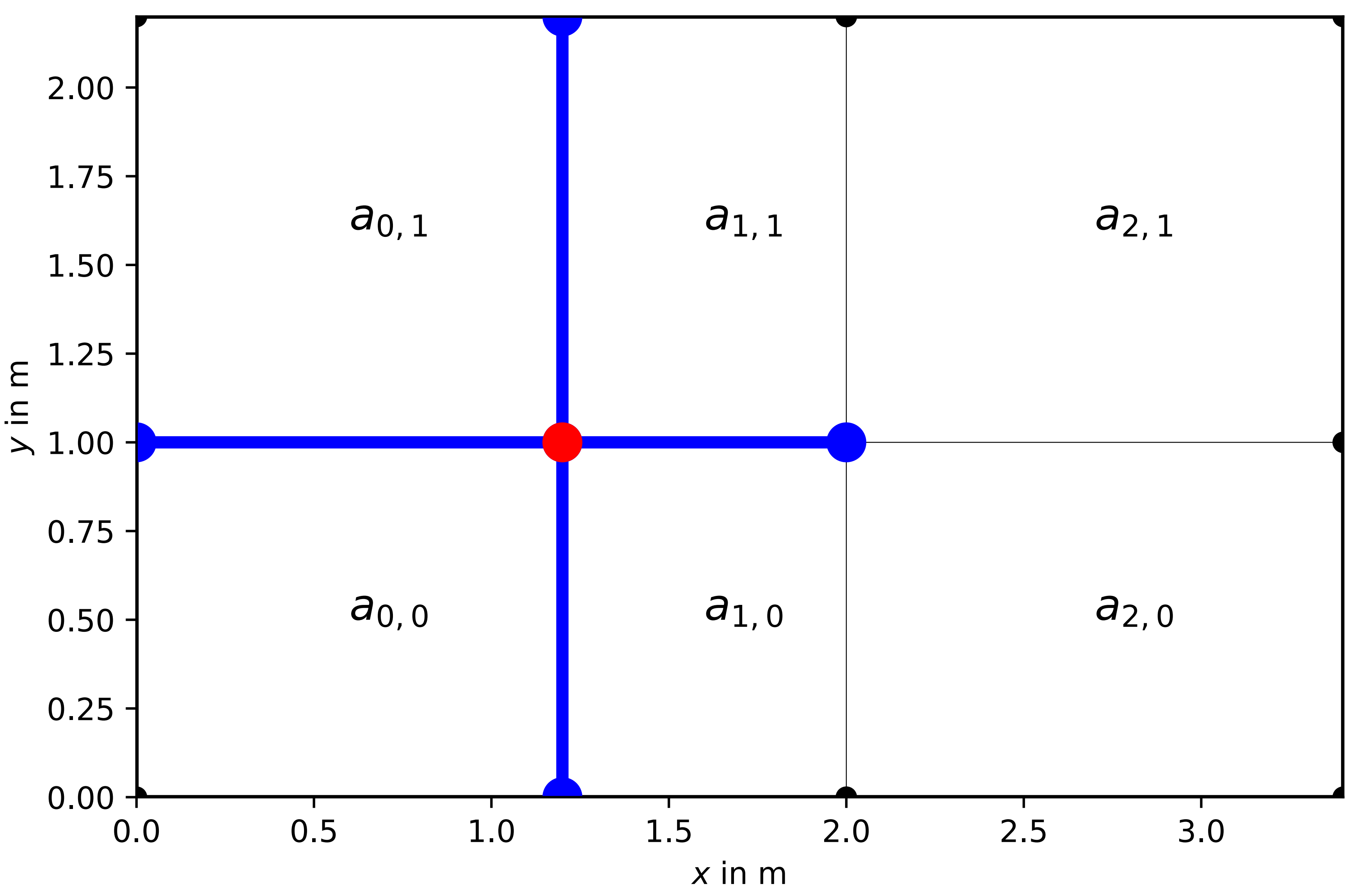
$$u(x) = -\frac{1}{2}x^2 + C_1 x + C_0$$

BC x**=0**	**BC** $x = X$	C_0	C_1
Dirichlet	Dirichlet	u_0	$X/2 + (u_X - u_0)/X$
Dirichlet	Neumann	u_0	$u'_X + X$
Neumann	Dirichlet	u'_0	$u_X - u'_0 X + X^2/2$

FD in 2D: discretization



FD in 2D: difference stencil



The end