Numerical Simulation Methods in Geophysics, Part 2: Finite Differences

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

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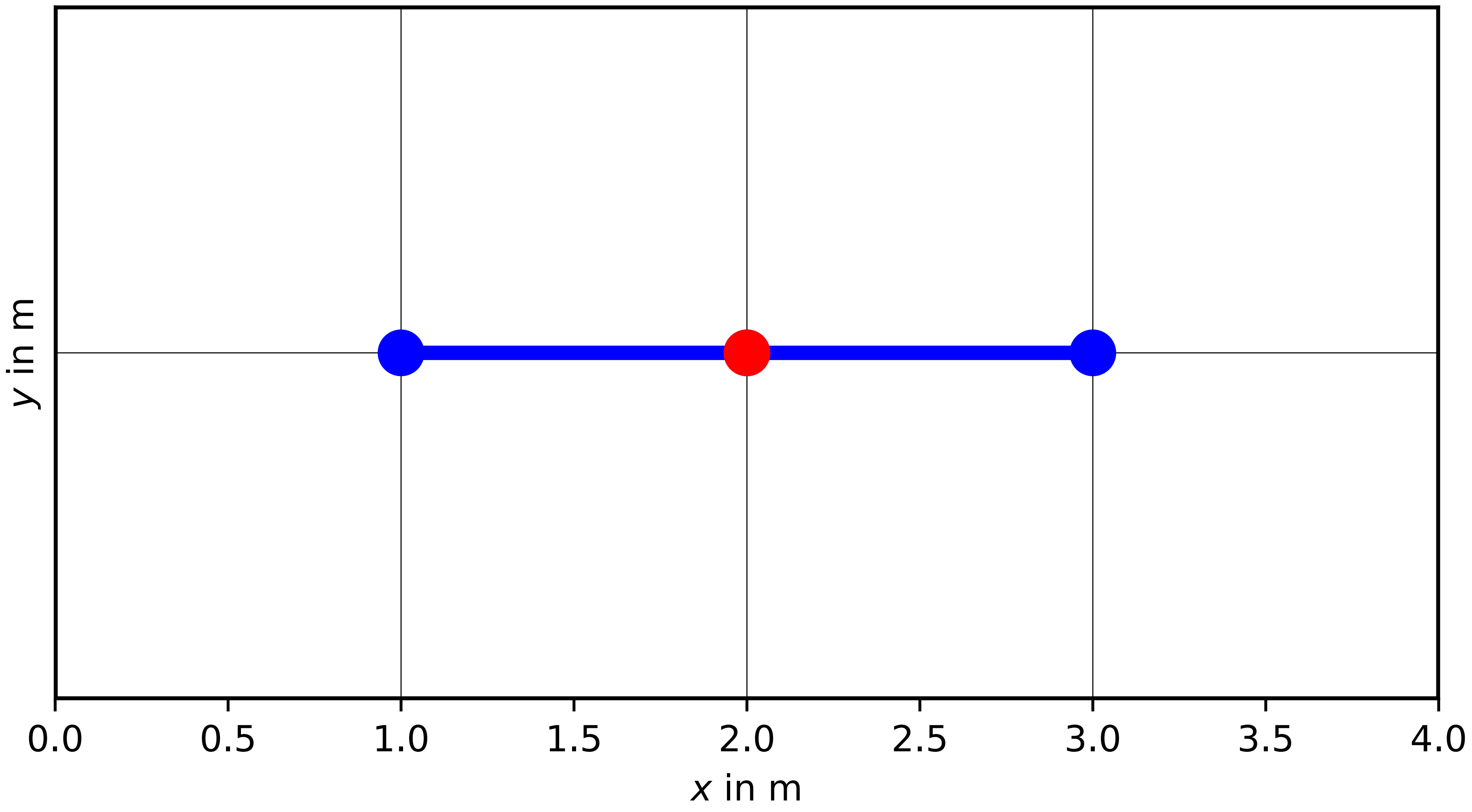
What have we learned?

- Poisson equation better with - (source leads to maximum)

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

- Finite Difference (FD) easy to implement
- source leads to maximum (negative curvature)
- piece-wise linear solution for source-free regions
- quadratic solution for constant source
- boundary conditions fix potential (Dirichlet) or gradient (Neumann)

Finite Differences (FD)



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

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.

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

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

Summarize in a matrix

Assumption: equidistant discretization Δx=1, conductivity a=1

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

Matrix-Vector product $\mathbf{A} \cdot \mathbf{u} = \mathbf{f}$ with matrix $A \in R^{N-2 \times N}$

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

Boundary conditions

$A \in R^{N-2 \times N}$ is not enough information to compute N potentials

- add 2 rows in matrix (or remove columns!)
- 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

$u_0 = u_L$ & $u_N = u_R$

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

Dirichlet BC implementation way 2

$$-u_L + 2u_1 - u_2 = f_1 \Rightarrow 2u_1 - u_2 = f_1 + u_L$$

$$\begin{bmatrix} +2 & -1 & 0 & \dots & & \\ -1 & +2 & -1 & 0 & \dots & \\ 0 & -1 & +2 & -1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ \dots & \dots & 0 & -1 & +2 & -1 \\ \dots & \dots & \dots & 0 & -1 & +2 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_1 + u_L \\ f_2 \\ f_3 \\ \vdots \\ f_{N-2} \\ f_{N-1} + u_R \end{bmatrix}$$

Neumann BC implementation way 1

$$u_1 - u_0 = g_L$$

$$\begin{bmatrix} +1 & -1 & 0 & \dots & & & \\ -1 & +2 & -1 & 0 & \dots & & \\ 0 & -1 & +2 & -1 & 0 & \dots & \\ \vdots & \vdots & \vdots & \ddots & \vdots & & \\ \dots & \dots & 0 & -1 & +2 & -1 & \\ \dots & \dots & \dots & 0 & -1 & +1 & \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} g_L \\ f_1 \\ f_2 \\ \vdots \\ f_{N-1} \\ g_R \end{bmatrix}$$

Neumann BC implementation way 2

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

$$\begin{bmatrix} +1 & -1 & 0 & \dots & & \\ -1 & +2 & -1 & 0 & \dots & \\ 0 & -1 & +2 & -1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \\ \dots & \dots & 0 & -1 & +2 & -1 \\ \dots & \dots & \dots & 0 & -1 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_1 + g_L \\ f_2 \\ f_3 \\ \vdots \\ f_{N-1} \\ f_{N-1} + g_R \end{bmatrix}$$

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?

Solution for f=1

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

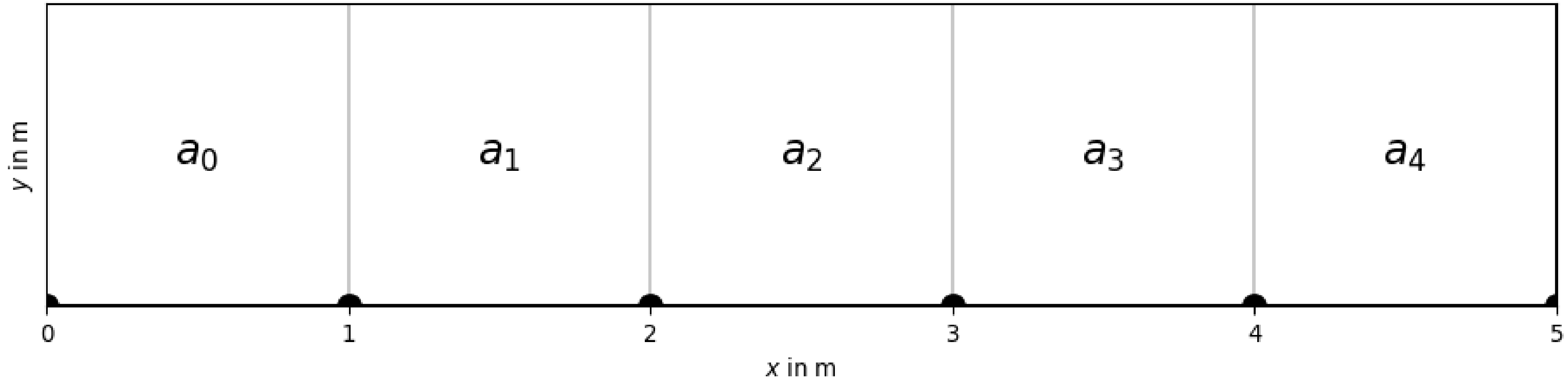
BC x=0	**BC $x = X$**	C_0	C_1
Dirichlet	Dirichlet	u_0	$X/2 + (u_X - u_0)/X$
Dirichlet	Neumann	u_0	$u'_X + X$
Neumann	Dirichlet	u'_0	$u_X - u'_0 X + X^2/2$

Tasks

1. Create a system matrix for unit quantities
2. Implement Dirichlet BC on one and Neumann on other side
3. Solve system for different right-hand sides:
    - no source at all
    - single source in the middle or at the boundary
    - several sources with different strengths (& signs)
    - source on part of the domain
4. Alwas plot the solution and its Laplacian

The general case

$\Delta x \neq 1$ & $a \neq 1$ with $\mathbf{x} \in \mathbf{R}^{\mathbf{N}}$ and $a \in R^{N-1}$ (in-between)



$\frac{\partial u}{\partial x}$ live on .5 space like $a \Rightarrow$ `a/np.diff(x)`

second derivative: `np.diff(a*np.diff(x))/...`

Coupling coefficients

$$A_{i,i-1} = C_i^{left} = -a_{i-1}/(x_i - x_{i-1})/(x_{i+1} - x_{i-1}) \cdot 2$$

$$A_{i,i+1} = C_i^{right} = -a_i/(x_{i+1} - x_i)/(x_{i+1} - x_{i-1}) \cdot 2$$

$$\begin{bmatrix} +1 & 0 & 0 & \dots & & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots & \\ \vdots & \vdots & \ddots & \vdots & & \\ \dots & \dots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \dots & \dots & & 0 & -1 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} u_B \\ f_1 \\ \vdots \\ f_N \\ g_B \Delta \end{bmatrix}$$

Symmetry

$$A_{i+1,i} = C_{i+1}^{left} = a_i/(x_{i+1} - x_i)/(x_{i+2} - x_i) \cdot 2$$

$$A_{i,i+1} = C_i^{right} = a_i/(x_{i+1} - x_i)/(x_{i+1} - x_{i-1}) \cdot 2$$

only symmetric if Δx is constant around x_i, better take $a_i/(\Delta x_i)^2$

$$A_{i,i-1} = C_i^{left} = a_{i-1}/(x_i - x_{i-1})^2$$

$$A_{i,i+1} = C_i^{right} = a_i/(x_{i+1} - x_i)^2$$

$\Rightarrow$ inaccuracies expected for non-equidistant discretization

A closer look at the Dirichlet boundary

$$\begin{bmatrix} +1 & 0 & 0 & \dots & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots \end{bmatrix} \begin{bmatrix} u_B \\ f_1 \end{bmatrix}$$

1. C can be differently scaled from 1 $\Rightarrow$ multiply with C_i^L
2. Matrix is non-symmetric

$$\begin{bmatrix} C_1^L & 0 & 0 & \dots & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots \end{bmatrix} \begin{bmatrix} u_B C_i^L \\ f_1 \end{bmatrix}$$

A closer look at the Neumann boundary

$$\begin{bmatrix} \cdots & \cdots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \cdots & \cdots & & 0 & -1 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_N \\ g_B \Delta x_N \end{bmatrix}$$

1. C can be differently scaled from 1 $\Rightarrow$ multiply with C_N^R
2. Matrix is non-symmetric $\Rightarrow$ multiply with -1

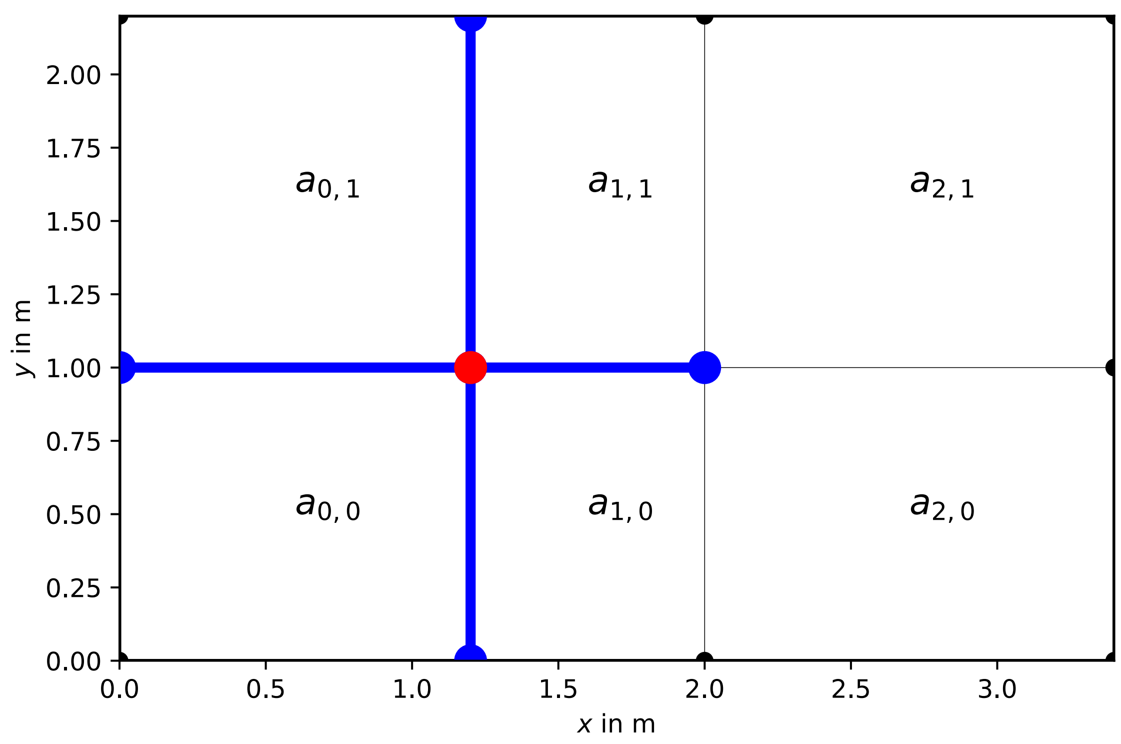
$$\begin{bmatrix} \cdots & \cdots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \cdots & \cdots & & 0 & C_N^R & -C_N^R \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_N \\ -g_B \Delta x_N C_N^R \end{bmatrix}$$

Tasks

1. Derive the coefficients for the general case
2. Write a function implementing the general case
3. Divide the “subsurface” in regions with different a
4. Compute the solution for different source fields
5. Use a non-equidistant discretisation
6. Always plot solution along with source and Laplacian

Higher dimensions

FD in 2D: discretization



Simple 2D conductivity grid with FD stencil

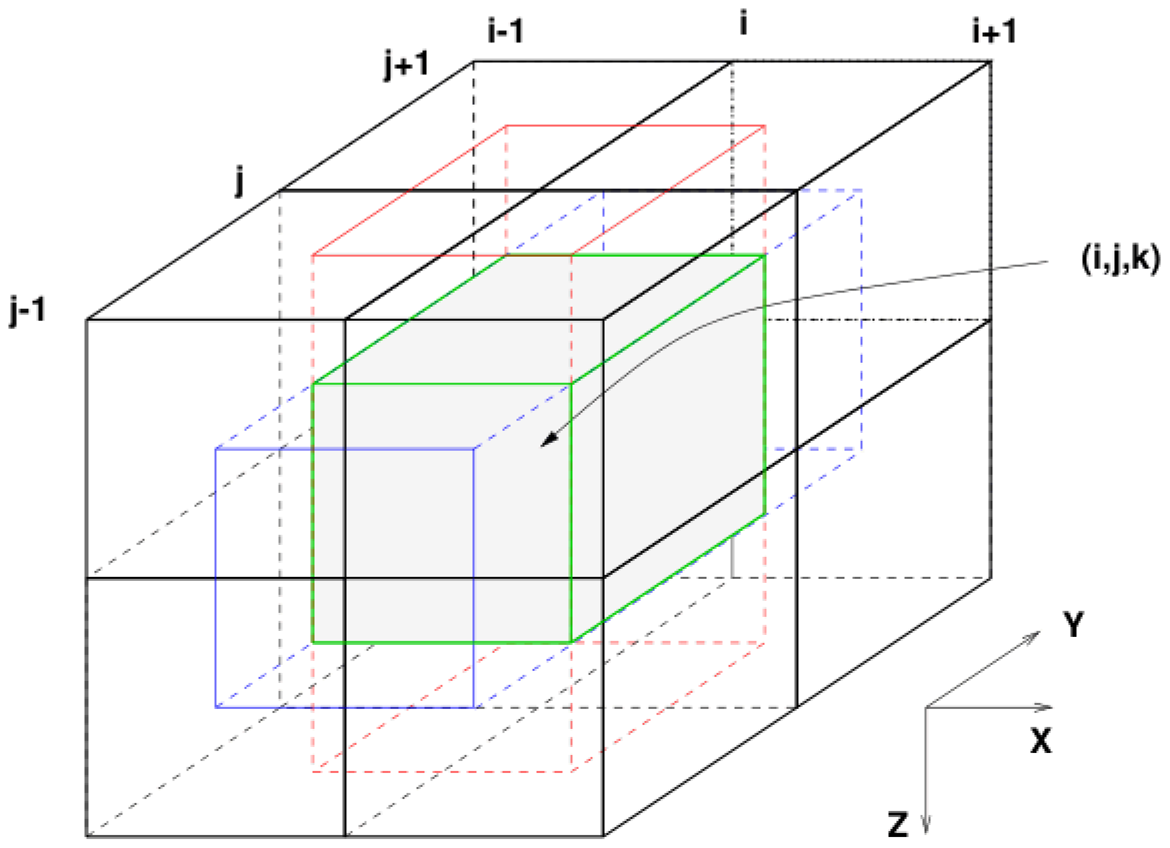
$$C_{i,j}^{right} = a_{i,j-1/2}/(x_{i+1} - x_i)^2$$

$$a_{i,j-1/2} = (a_{i,j-1} + a_{i,j})/2 \text{ ?}$$

harmonic, geometric? weighting?

$$a_{i,j-1/2} = \frac{a_{i,j-1}\Delta y_{j-1} + a_{i,j}\Delta y_j}{y_j + 1 - y_{j-1}} \text{ ?}$$

FD in 2D: discretization



3D discretization

$$C_{top} = -\frac{1}{\Delta z_{k-1}}\left(\sigma_{i-1,j,k-1}\frac{\Delta x_{i-1}\Delta y_j}{4} + \sigma_{i,j,k-1}\frac{\Delta x_i \Delta y_j}{4} + \right.$$

$$\left. + \sigma_{i-1,j-1,k-1}\frac{\Delta x_{i-1}\Delta y_{j-1}}{4} + \sigma_{i,j,k-1}\frac{\Delta x_i \Delta y_j}{4}\right)$$

coupling coefficient