Lecture 4: Discrete Operators

Logistics: - HW 1 is due Feb 3

- make use of office hours & piazza

Last time: Introduction to numerics

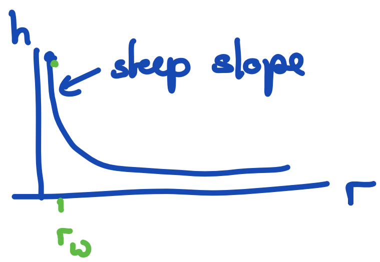
- Finite Differences $\left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$
- Differentiation matrix

$$\underline{df} = \underline{\underline{D}}\,\underline{f} \qquad \underline{ddf} = \underline{\underline{D}}^2\,\underline{f}$$

- Example of flow around well

$$\nabla \cdot (r K \nabla h)$$

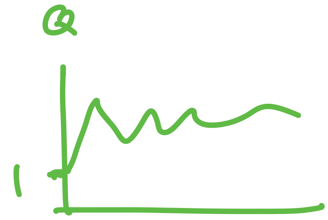
$$\frac{d}{dr}\left(K r \frac{dh}{dr}\right) = 0$$



- Attempt 1: Expand

$$K r \frac{d^2h}{dr^2} + \frac{dh}{dr} = 0$$

$$\left(K \underline{\underline{R}}\,\underline{\underline{D}}^2 + \underline{\underline{D}}\right)\underline{h} = 0$$



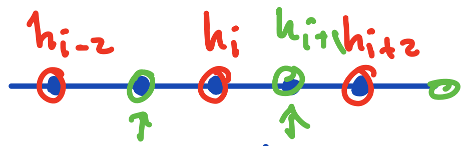
→ very bad approx.

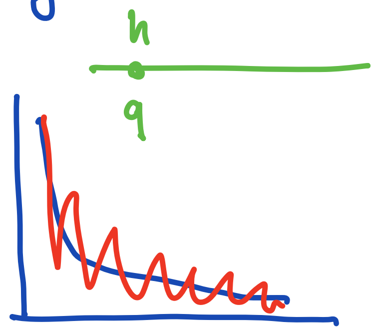
→ mass is not conserved

- Attempt 2: keep divergence

$$\frac{d}{dr}\left(K r \frac{dh}{dr}\right) = 0$$

$$\underline{\underline{D}}\,(K\,\underline{\underline{R}}\,\underline{\underline{D}})\,\underline{h} = 0$$





even-odd decoupling $\Rightarrow$ oscillations

Today: - Staggered grid
- Conservative differences
- Discrete operators
- coding basics
- boundary conditions

Discrete operators

Best to discretize in conservation form

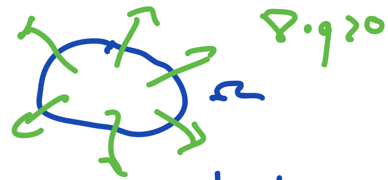
1) $\nabla \cdot \underline{q} = f_s$

2) $\underline{q} = -K \nabla h$

Highlights two basic operators we need

to approximate.

1) Divergence of a flux
2) Gradient of a scalar



Almost all PDE in continuum physics are composed of these two operators ($\nabla \times$ = curl)

If we have <u>discrete</u> analogs of these operators.

- solve different equations
- clean & readable implementation
- dimension & coordinate system independent

Ideas are from "mimetic finite differences"

Both divergence & gradient are <u>linear</u> diff. operators $\Rightarrow$ the discre operator is a matrix.

Looking for 2 matrices $\underline{\underline{D}}$ and $\underline{\underline{G}}$ so that

$$\nabla \cdot q = f \quad \rightarrow \quad \underline{\underline{D}}\, \underline{q} = \underline{f}$$

$$q = -K \nabla h \quad \rightarrow \quad \underline{q} = -K\, \underline{\underline{G}}\, \underline{h}$$

Want to be able to compose these

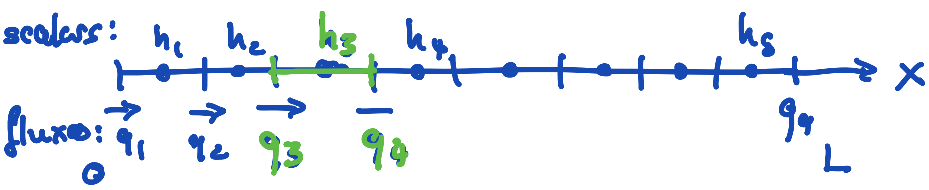
$$-\nabla \cdot [K \nabla h] = f \quad \rightarrow \quad -\underline{\underline{D}}\,[K\, \underline{\underline{G}}]\, \underline{h} = \underline{f}$$

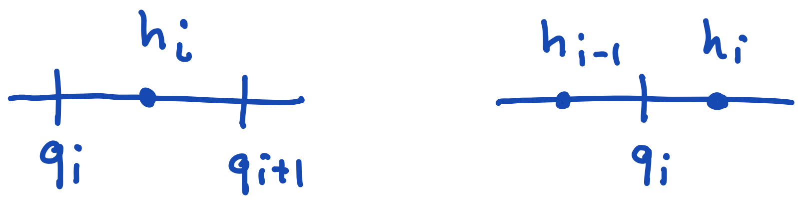
$$k=1: \quad \nabla \cdot \nabla = \nabla^2 \quad \rightarrow \quad \underline{\underline{L}} = \underline{\underline{D}}\, \underline{\underline{G}}$$

Discrete Divergence and Gradient in 1D

Consider staggered grid

$N_x = 8$





Gradient operator

Gradient takes a scalar and returns a vector: $\underline{q} = -\nabla h$

$\Rightarrow$ $\underline{\underline{G}}$ is <u>not</u> square matrix

In 1D the discre scalar $\underline{h}$ is Nx by 1

but the flux is on faces so that q Nx+1 by 1

$$\underset{Nx+1 \cdot 1}{q} = \underset{Nx+1 \cdot Nx}{G} \; \underset{Nx \cdot 1}{h}$$

$\Rightarrow$ discrete gradient $\underline{\underline{G}}$ is Nx+1 by Nx

Entries of $\underline{\underline{G}}$:

$$\underline{dh} = \frac{1}{\Delta x} \; \underline{\underline{G}} \; \underline{h}$$

$$\begin{bmatrix} \\ \\ dh_3 = \frac{h_3 - h_2}{\Delta x} \\ \\ \\ \\ \\ \\ \\ \end{bmatrix} = \frac{1}{\Delta x} \begin{array}{c|cccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & 0 & & & & & & & \\ 2 & -1 & 1 & & & & & & \\ 3 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 4 & & & -1 & 1 & & & & \\ 5 & & & & -1 & 1 & & & \\ 6 & & & & & -1 & 1 & & \\ 7 & & & & & & -1 & 1 & \\ 8 & & & & & & & -1 & 1 \\ 9 & & & & & & & & 0 \end{array} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \\ h_7 \\ h_8 \end{bmatrix}$$

0

-1

$$dh_4 = \frac{h_4 - h_3}{\Delta x}$$

h_{i-1} h_i

q_i

dh_i

$$q = -K \, \underline{dh}$$

$$dh_i = \frac{h_i - h_{i-1}}{\Delta x}$$

$$dh_3 = \frac{h_3 - h_2}{\Delta x}$$

Set gradient on boundary to zero! (choice)

$\Rightarrow$ No flow/flux boundaries are built in.

(natural boundary conditions)

Discrete divergence operator

Divergence takes a flux and returns a scalar

$\nabla \cdot \mathbf{q} = f$

1D discrete div. matrix $\underline{\underline{D}}$ is N_x by N_x+1

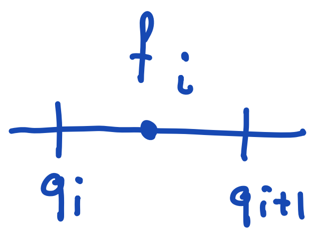
$$\underset{N_x \cdot 1}{f} = \underset{N_x \cdot N_x+1}{\underline{\underline{D}}} \; \underset{N_x+1 \cdot 1}{\mathbf{q}}$$

Entries of divergence matrix

$$\underline{f} \qquad\qquad \underline{\underline{D}} \qquad\qquad \underline{q}$$

$0 \quad +1$

$$\begin{bmatrix} f_1 \\ \\ \\ \\ \\ \\ \\ \\ \end{bmatrix} = \frac{1}{\Delta x} \begin{bmatrix} -1 & 1 & & & & & & & \\ & -1 & 1 & & & & & & \\ & & -1 & 1 & & & & & \\ & & & -1 & 1 & & & & \\ & & & & -1 & 1 & & & \\ & & & & & -1 & 1 & & \\ & & & & & & -1 & 1 & \\ & & & & & & & -1 & 1 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ \\ \\ \\ \\ \end{bmatrix}$$



$$\frac{q_{i+1} - q_i}{\Delta x} = f_i$$

$$\frac{q_2 - q_1}{\Delta x} = f_1$$

$\underline{\underline{D}}$ does not need special treatment on boundary

Relation between $\underline{\underline{G}}$ and $\underline{\underline{D}}$

Continuous case:

$$\nabla f = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z} \end{pmatrix}$$

$$\nabla \cdot q = \left(\frac{\partial}{\partial x} \;\; \frac{\partial}{\partial y} \;\; \frac{\partial}{\partial z} \right) \cdot \begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix} = \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}$$

$$\nabla \cdot \nabla = \nabla^2 = \left(\frac{\partial}{\partial x} \;\; \frac{\partial}{\partial y} \;\; \frac{\partial}{\partial z} \right) \cdot \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

divergence is row vector (of partial deriv.)

gradient is column vector (of partial deriv.)

$\nabla \cdot = \nabla^T$ (operators are adjoints)

If we look at the discrete matrices

$\boxed{\underline{\underline{G}} = -\underline{\underline{D}}^T}$ in the interior of domain

$\Rightarrow$ still need to impose natural BC's on $\underline{\underline{G}}$

This is true in all dimensions in cartesian coordinate systems.

In homework this will be implemented

in function build_ops.m

$[D, G, C, I, M] = \text{build\_grid}(Grid)$

$-\nabla^2 h + h = f$

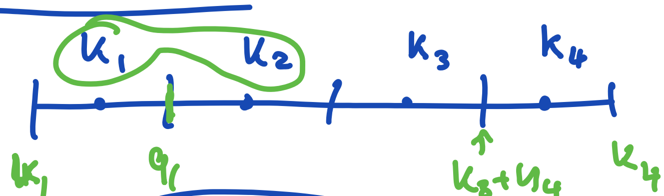
$(-DG + I)\underline{h} = \underline{f}$

$D = \text{div} \quad G = \text{grad} \quad C = \text{curl} \quad I = \text{identity}$

M = arithm. mean from cell centers to cell faces

on bnd face put value from bnd cell !

Mean matrix



$\underset{\text{face}}{q} = -K \; \underset{\text{face}}{\nabla h} \qquad \underline{\underline{M}}\,\underline{K}$

$\underline{q} = -(\underline{\underline{M}}\,\underline{K})\,\underline{\underline{G}}\,\underline{h}$

$N_{x+1} \cdot 1 \quad (N_{x+1}) \cdot 1$

Kd = spdiags(MK, 0,

$=$ [illegible]

$\sqrt{x+1} \cdot \sqrt{x+1}$