Discrete operators

demo_testing-ops m

Best to discretize eqn in conservation form

$$\nabla \cdot q = 0$$
$$q = -K \nabla h$$

Highlights the two basic linear operators in vector calculus.

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

All eqns in flow and transport in porous media are built from these two operators!

If we had <u>discrete</u> analogs of these operators:

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

A <u>linear</u> differential operator $\mathcal{L}$ takes a function and returns a different function, e.g derivative: $\dot{f} = \mathcal{D}(f)$

The discrete equivalent of a function $f(x)$ is a vector $\underline{f}$

$\Rightarrow$ discrete linear operator takes a vector and returns a vector

because it is linear a discrete operator is a matrix.

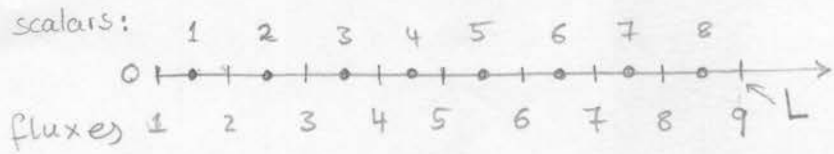
$$\dot{f} = \mathcal{D}(f) \longrightarrow \dot{\underline{f}} = \underline{\underline{D}}\,\underline{f}$$

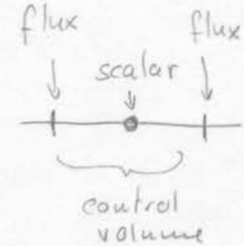
We are looking for two matrices $\underline{\underline{D}}$ and $\underline{\underline{G}}$ so that

$$\left.\begin{array}{lcl} \nabla \cdot q = \underline{f} & \longrightarrow & \underline{\underline{D}}\, q = \underline{f} \\ q = -\nabla h & \longrightarrow & q = -\underline{\underline{G}}\,\underline{h} \end{array}\right\} -\nabla^2 h = f \longrightarrow -\underline{\underline{D}}\,\underline{\underline{G}}\, h = f$$

Discrete divergence, gradient and Laplacian in 1D

Consider the following D staggered grid



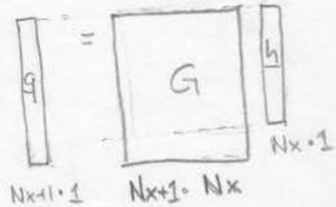


Divide domain $x \in [0, L]$ into $N_x = 8$ control volumes. Any scalar independent variable is evaluated at the $N_x = 8$ cell centers. All fluxes of the independent variables are evaluated at the $N_x + 1 = 9$ cell interfaces.

Gradient operator

Gradient takes a scalar and returns a flux vector: $\underline{q} = -\nabla h \quad (K=1)$
In 1D the discrete scalar, $\underline{h}$, is a N_x by 1 vector and the discrete flux q is a N_x+1 by 1 vector. The discrete gradient is a N_x+1 by N_x matrix $\underline{\underline{G}}$.

$$\underset{N_x+1 \cdot 1}{\underline{q}} = -\underset{N_x+1 \cdot N_x}{\underline{\underline{G}}} \cdot \underset{N_x \cdot 1}{\underline{h}}$$



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

- assume no flow across boundaries
- central difference approx.

Continuous. $\nabla h = \frac{\partial h}{\partial x}$

Discrete. $\frac{\partial h}{\partial x} = \frac{h(i) - h(i-1)}{\Delta x}$ (← $\frac{1}{\Delta x}$

(2nd order accurate)

$$-\underline{\underline{G}} \cdot \underline{h} = \underline{q}$$

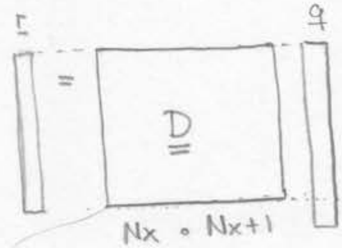
$$-\frac{1}{\Delta x}\;
\begin{array}{c|cccccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\hline
1 & 0 & & & & & & & \\
2 & -1 & 1 & & & & & & \\
3 & & -1 & 1 & & & & & \\
4 & & & -1 & 1 & & & & \\
5 & & & & -1 & 1 & & & \\
6 & & & & & -1 & 1 & & \\
7 & & & & & & -1 & 1 & \\
8 & & & & & & & -1 & 1 \\
9 & & & & & & & & 0 \\
\hline
\end{array}
\cdot
\begin{bmatrix} h(1) \\ h(2) \\ h(3) \\ h(4) \\ h(5) \\ h(6) \\ h(7) \\ h(8) \end{bmatrix}
=
\begin{bmatrix} 0 \\ [h(2)-h(1)]/\Delta x \\ \\ \\ \\ \\ \\ \\ 0 \end{bmatrix}$$

Divergence operator.

Divergence takes a flux vector and returns a scalar: $\nabla \cdot \underline{q} = \underline{r}$

In 1D the discrete divergence is therefore a Nx by Nx+1 matrix $\underline{\underline{D}}$.

$$\underset{Nx \cdot 1}{\underline{r}} = \underset{Nx \cdot Nx+1}{\underline{\underline{D}}} \cdot \underset{Nx+1 \cdot 1}{\underline{q}}$$



Definition of $\underline{\underline{D}}$:

- central difference approximation

Continous $\nabla \cdot q = \frac{\partial q}{\partial x}$

Discrete. $\frac{\partial q}{\partial x} \approx \frac{q(i+1) - q(i)}{\Delta x}$

(2nd order)

$$\underline{\underline{D}} \cdot \underline{q} = \underline{r}$$

$$\frac{1}{\Delta x}\begin{array}{c|ccccccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
1 & -1 & 1 & & & & & & & \\
2 & & -1 & 1 & & & & & & \\
3 & & & -1 & 1 & & & & & \\
4 & & & & -1 & 1 & & & & \\
5 & & & & & -1 & 1 & & & \\
6 & & & & & & -1 & 1 & & \\
7 & & & & & & & -1 & 1 & \\
8 & & & & & & & & -1 & 1 \\
\hline
\end{array}
\begin{bmatrix} q(1) \\ q(2) \\ q(3) \\ q(4) \\ q(5) \\ q(6) \\ q(7) \\ q(8) \\ q(9) \end{bmatrix}
=
\begin{bmatrix} [q(2)-q(1)]/\Delta x \\ [q(3)-q(2)]/\Delta x \\ [q(4)-q(3)]/\Delta x \\ \\ \\ \\ \\ \\ \end{bmatrix}$$

Laplacian operator.

The Laplacian operator is defined as $\nabla^2(\cdot) = \nabla \cdot \nabla(\cdot)$

The Laplacian takes a scalar and returns a scalar: $\nabla^2 h = r$

The discrete Laplacian should be a Nx by Nx matrix $\underline{\underline{L}}$.

$$\underset{Nx \cdot 1}{r} = \underset{Nx \cdot Nx}{\underline{\underline{L}}} \; \underset{Nx \cdot 1}{\underline{h}}$$

Discrete composition of the Laplacian $\underset{Nx \cdot Nx}{\underline{\underline{L}}} = \underset{Nx \cdot Nx+1}{\underline{\underline{D}}} * \underset{Nx+1 \cdot Nx}{\underline{\underline{G}}}$

$$\underline{\underline{L}} = \frac{1}{\Delta x^2}\begin{bmatrix}
-1 & 1 & & & & & & \\
1 & -2 & 1 & & & & & \\
 & 1 & -2 & 1 & & & & \\
 & & 1 & -2 & 1 & & & \\
 & & & 1 & -2 & 1 & & \\
 & & & & 1 & -2 & 1 & \\
 & & & & & & -2 & 1 \\
 & & & & & & 1 & -1
\end{bmatrix}$$

Relation between div & grad

Simple motivation:

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

$$\nabla \cdot g = \left(\frac{\partial}{\partial x}\ \frac{\partial}{\partial y}\ \frac{\partial}{\partial y}\right) \cdot \begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} = \frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} + \frac{\partial g_z}{\partial z}$$

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

$\Rightarrow$ divergence is ~~ike~~ a transpose of gradient $\nabla \cdot = \nabla^T$

If we look at $\underline{\underline{D}}$ and $\underline{\underline{G}}$ matrices we observe

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

At the boundaries the natural BC's on $\underline{\underline{G}}$ eliminate some entries

This relationship between div & grad is related to the fact that they are adjoint operators in continuum theory

The cleanest way to assemble the discrete divergence and then obtain gradient by transpose.