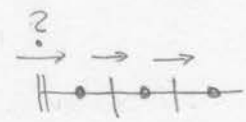
Computing Fluxes of Gradient Fields

We are concerned with fluxes that are the gradients of scalar potential fields: $\underline{v} = -\nabla u$ or $\underline{q} = -K\nabla h$

The discrete approximation is $\underline{v} = -\underline{\underline{G}}\,\underline{u}$, which is computed easily using the existing discrete gradient.

This works well in the interior of the domain, but on the boundary the discrete gradient is zero by construction.

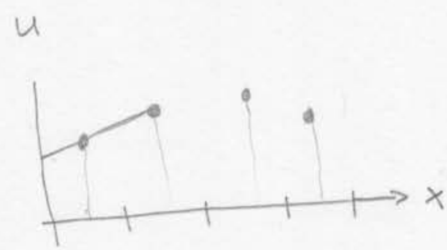
$\Rightarrow$ $\underline{v} = \underline{q} = 0$ on boundary



This is due to the difficulty of approximating bnd derivative on staggered mesh.

$\Rightarrow$ Need to reconstruct flux/velocity on boundary:

Option 1:



Extrapolate unknown to boundary equivalent to using one-sided FD

Problem: loose discrete conservation

"Sum of fluxes and sources/sinks in the boundary cell is not zero"

Option 2: Use balance law in the boundary cell to compute the exact flux that is required for discrete conservation.

Residual of the discretization of a linear PDE

PDE : $\left.\begin{array}{l} -\nabla^2 u = f_s \\ -\nabla^2 u + \underline{u} = f_s \end{array}\right\} \quad \underline{\underline{L}}\,\underline{u} = \underline{f}_s$

residual. $\underline{r} = \underline{\underline{L}}\,\underline{u} - \underline{f}_s$

If the discrete equations are satisfied $\underline{r} = \underline{0}$.

In the boundary cells $\underline{r} \neq 0$, because the gradient on the boundary is arbitrarily set to zero!

$\Rightarrow$ non-zero residual contains the information about the boundary flux:

If dof-cells is a vector containing all boundary cells and dof-face is a vector containing all associated bnd faces

residual on bnd cells is: r(dof-cells)
unknown bnd fluxes are: q(dof-face)

Note: Assume each bnd cell has on face with non-zero flux! In 1D always true but in higher dimensions cells in corners and along edges have multiple faces. We'll assume all but one have zero flux.

If there are non-zero boundary fluxes the linear system is

$$\underline{\underline{L}}\,\underline{u} = \underline{f}_s + \underline{f}_D + \underline{f}_N$$

so that $\underline{r} = \underline{f}_D + \underline{f}_N$

On the Neumann boundary ($f_D = 0$) we have computed f_n by converting flux through the face into a volumetric source term: $\underline{f_n = A\, q_b / V}$

We can reverse that argument to get the flux from the source term: $\underline{q_b = f_n V / A}$

On Neumann bnd $f_n = r \Rightarrow \underline{q_b = r\, V/A}$

The same works on the Dirichlet boundary so that we can generally reconstruct the unknown boundary fluxes as:

$$\boxed{\texttt{q(dof-face) = }\underline{\texttt{sign}}\texttt{.* }\underline{\texttt{r}}\texttt{(dof-cells,u).* }\underline{\texttt{V}}\texttt{(dof-cells)./A(dof-face);}}$$

where $\underline{\text{sign}} = \begin{cases} 1, & \text{dof-face} \in [\text{dof-xmin}, \text{dof-ymin}] \\ -1, & \text{dof-face} \in [\text{dof-xmax}, \text{dof-ymax}] \end{cases}$

The negative sign on the xmax, ymax boundary simply indicates that positive flux on those boundaries is an outflow!