Conceptual Design of PETSc Time Stepper for Flow and Transport

The generalized partial differential equation for groundwater flow is

$$\frac{\partial}{\partial t}\varphi\rho + \nabla\cdot\rho\boldsymbol{u} = \mathscr{S}, \tag{1}$$

with $\boldsymbol{u}$ given by Darcy's law

$$\boldsymbol{u} = -\frac{\kappa}{\mu}\nabla\big(p - W\rho g z\big), \tag{2}$$

with permeability κ, viscosity μ, molar fluid density ρ, formula weight of water W, acceleration of gravity g, and source/sink term $\mathscr{S}$. For full tensor permeability, permeability tensor κ takes the form

$$\kappa = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}, \tag{3}$$

and therefore, Equation 2 expands to

$$\boldsymbol{u} = \frac{1}{\mu}\begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}\cdot\begin{bmatrix} \dfrac{p}{\partial x} \\ \dfrac{p}{\partial y} \\ \dfrac{p - W\rho g z}{\partial z} \end{bmatrix}. \tag{4}$$

Since $\boldsymbol{u}$ is the flux vector across the cells interface, $\boldsymbol{u}$ could also be described as a scalar-vector product

$$\boldsymbol{u} = \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix} = u\cdot\boldsymbol{n} = u\cdot\begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix}, \tag{5}$$

where $\boldsymbol{n}$ is a unit vector normal to the cell surface as shown in Figure 1. Therefore,

$$u\cdot\begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} = \frac{1}{\mu}\begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}\cdot\begin{bmatrix} \dfrac{p}{\partial x} \\ \dfrac{p}{\partial y} \\ \dfrac{p - W\rho g z}{\partial z} \end{bmatrix}. \tag{6}$$

The magnitude of the flux normal to the surface (u) is obtained by multiplying through by $\boldsymbol{n}^T$

$$u = \frac{1}{\mu}\begin{bmatrix} n_x & n_y & n_z \end{bmatrix}\cdot\begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}\cdot\begin{bmatrix} \dfrac{p}{\partial x} \\ \dfrac{p}{\partial y} \\ \dfrac{p - W\rho g z}{\partial z} \end{bmatrix}. \tag{7}$$

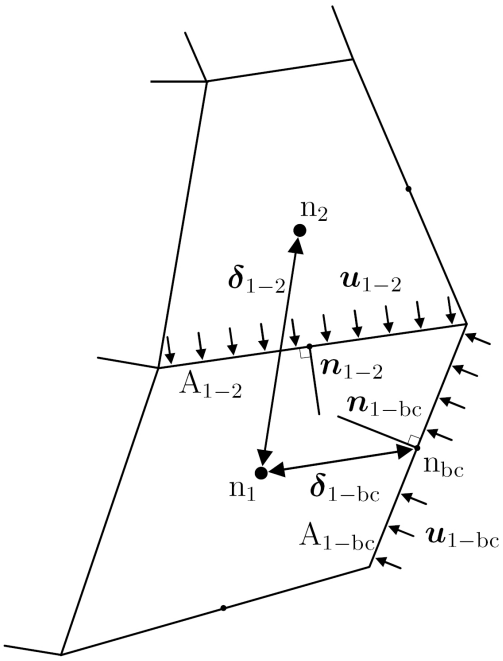

Figure 1: Schematic of unstructured grid.

The scalar "u" would be the flux applied across the boundary and intercellular fluxes in PFLOTRAN.