Analytic Jacobian Richards Equation

We want to solve

$$\frac{\partial \theta}{\partial t} - \nabla \cdot [D_H(\theta) \nabla \theta] = f$$

form of a general non-linear diffusion eqn.

Discretization with backward Euler

$$\boxed{\underline{r} = \theta^{n+1} - \theta^{n} - \Delta t \, \underline{\underline{D}} * [\{\underline{\underline{M}} \, \underline{D}_H(\underline{\theta}^{n+1})\}_f \underline{\underline{G}} \, \underline{\theta}^{n+1}] - \Delta t \, f_s = \underline{0}}$$

where $\underline{D}_H(\underline{\theta})$ is vector of D_H at cell centers

and $\{\underline{\underline{M}} \, \underline{\underline{D}}_H(\underline{\theta}^{n+1})\}_f$ is a Nf by Nf matrix of arithmetic averages on the faces

$\underline{\theta}^{n+1} \equiv \underline{\theta}$ unknown we find using Newton-Raphson

$n =$ superscript for time step

$k =$ superscript for N-R iteration

Linearize residual as before at $\underline{\bar{\theta}}$

$$\underline{\underline{L}}_{\underline{\bar{\theta}}}\, \underline{r} = \underline{r}(\underline{\bar{\theta}}) + \nabla_{\underline{\bar{\theta}}}\, \underline{r} \cdot \underline{\Delta\theta} \qquad \underline{\Delta\theta} = \epsilon\, \underline{\hat{\theta}}$$

$$= \underline{r}(\underline{\bar{\theta}}) + \epsilon\, \nabla_{\underline{\bar{\theta}}}\, \underline{r} \cdot \underline{\hat{\theta}}$$

$\uparrow$ dir. of update

Directional derivative of $\underline{r}$ at $\underline{h}$ in direction $\underline{\hat{\theta}}$

$$\boxed{\nabla_{\underline{\bar{\theta}}}\, \bar{r}\, \underline{\hat{\theta}} = \frac{d}{d\varepsilon}\, \underline{r}(\underline{\bar{\theta}} + \epsilon \underline{\hat{h}})\Big|_{\varepsilon=0}}$$

Simple example: Scalar-valued vector function

$$f(\underline{x}) = x + y^2 \qquad \nabla f = \begin{pmatrix} 1 \\ 2y \end{pmatrix}$$

Given some direction $\underline{\hat{x}} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}$ and location $\underline{\bar{x}} = \begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix}$

a) $$\nabla f\big|_{\underline{\bar{x}}} \cdot \underline{\hat{x}} = (1 \quad 2\bar{y}) \cdot \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} = \underline{\hat{x} + 2\bar{y}\hat{y}}$$

b) $$\frac{d}{d\varepsilon} f(\underline{\bar{x}} + \epsilon \underline{\hat{x}})\Big|_{\epsilon=0} = \frac{d}{d\varepsilon}\, \bar{x} + \epsilon\hat{x} + (\bar{y} + \epsilon\hat{y})^2 \Big|_{\epsilon=0}$$

$$= \frac{d}{d\varepsilon}\, \bar{x} + \epsilon\hat{x} + \bar{y}^2 + 2\epsilon\bar{y}\hat{y} + \epsilon^2\hat{y}^2 \Big|_{\epsilon=0}$$

$$= \hat{x} + 2\bar{y}\hat{y} + 2\epsilon\hat{y}^2 \Big|_{\epsilon=0}$$

$$= \underline{\hat{x} + 2\bar{y}\hat{y}}$$

Directional derivative of residual

To linearize our discrete system we need directional derivative of a vector-valued vector function.

$$\nabla \underline{r}\big|_{\underline{\bar{\theta}}}\, \underline{\hat{\theta}} = \frac{d}{d\varepsilon}\, \underline{r}\left(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}\right)\Big|_{\epsilon=0}$$

$$\underline{r}(\underline{\theta}) = \underline{\theta} - \underline{\theta}^{n} - \Delta t\, \underline{\underline{D}} * \left[\left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\theta}) \right\}_f \underline{\underline{G}}\, \underline{\theta} \right] - \Delta t\, \underline{f}_s = \underline{0}$$

where $\underline{\theta} = \underline{\theta}^{n+1}$!

$$\frac{d}{d\epsilon} r(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}})\Big|_{\varepsilon=0} = \frac{d}{d\varepsilon}\Big[\cancel{\underline{\bar{\theta}}}^{c} + \epsilon \underline{\hat{\theta}} - \cancel{\underline{\theta}^{n}}^{c} - \Delta t\, \underline{\underline{D}} * \left[\left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f \underline{\underline{G}} (\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right] - \Delta t\, \cancel{\underline{f}}^{c} \Big]\Big|_{\varepsilon=0}$$

$$= \underline{\hat{\theta}} - \Delta t\, \underline{\underline{D}} * \frac{d}{d\epsilon}\left[\left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f \underline{\underline{G}} (\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right]\Big|_{\epsilon=0}$$

$$= \underline{\hat{\theta}} - \Delta t\, \underline{\underline{D}} \left[\underbrace{\frac{d}{d\epsilon} \left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f} \underline{\underline{G}} (\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) + \left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f \underline{\underline{G}}\, \underline{\hat{\theta}} \right]$$

$$\frac{d}{d\epsilon} \left\{ \underline{\underline{M}}\, \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f = \left\{ \underline{\underline{M}} \frac{d}{d\epsilon} \underline{D}_H(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f$$

$$= \left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \frac{d}{d\epsilon}(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}}) \right\}_f$$

$$= \left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\underline{\bar{\theta}} + \epsilon \underline{\hat{\theta}})\, \underline{\hat{\theta}} \right\}_f$$

substitute and evaluate at $\epsilon = 0$

$$= \hat{\underline{\theta}} - \Delta t\, \underline{\underline{D}} * \left[\left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\bar{\underline{\theta}})\, \hat{\underline{\theta}} \right\}_f \underline{\underline{G}}\, \bar{\underline{\theta}} + \underbrace{\left\{ \underline{\underline{M}}\, D_H(\bar{\underline{\theta}}) \right\}_f}_{\underline{\underline{Kd}}(\bar{\underline{\theta}})} \underline{\underline{G}}\, \hat{\underline{\theta}} \right]$$

$\underline{\underline{G}}\,\bar{\underline{\theta}}$ = known vector = $\underline{\underline{GU}}$ diagonal matrix

$$\left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\bar{\underline{\theta}})\, \hat{\underline{\theta}} \right\}_f \underline{\underline{GU}} = \underline{\underline{GU}} \left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\bar{\underline{\theta}})\, \hat{\underline{\theta}} \right\}_f \qquad \text{switch}$$

$$\left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\bar{\underline{\theta}})\, \hat{\underline{\theta}} \right\}_f = \underbrace{\left\{ \underline{\underline{M}} \frac{dD_H}{d\theta}(\bar{\underline{\theta}}) \right\}_f}_{\underline{\underline{dKd}}(\bar{\underline{\theta}})} \hat{\underline{\theta}} = \underline{\underline{dKd}}(\bar{\underline{\theta}})\, \hat{\underline{\theta}}$$

substituting

$$\frac{d}{d\epsilon} \underline{r}(\bar{\underline{\theta}} + \epsilon \hat{\underline{\theta}}) \Big|_{\epsilon=0} = \hat{\underline{\theta}} - \Delta t\, \underline{\underline{D}} * \left[\underline{\underline{GU}} * \underline{\underline{dKd}}\, \hat{\underline{\theta}} + \underline{\underline{dK}} * \underline{\underline{G}}\, \hat{\underline{\theta}} \right]$$

$$= \Big(\underbrace{\underline{\underline{I}} - \Delta t\, \underline{\underline{D}} \left[\underline{\underline{GU}}\, \underline{\underline{dKd}} + \underline{\underline{dK}}\, \underline{\underline{G}} \right]}_{\underline{\underline{J}}} \Big) \hat{\underline{\theta}}$$

$$\boxed{\underline{\underline{J}}(\bar{\underline{\theta}}) = \underline{\underline{I}} - \Delta t\, D \left[\underline{\underline{GU}}\, \underline{\underline{dKd}} + \underline{\underline{Kd}}\, \underline{\underline{G}} \right]}$$

to evaluate dKd we need to differentiate $D_H(\theta)\underline{\nabla}$

$$\boxed{\frac{dD_H}{d\theta} = \frac{K_s h_b}{\Delta\theta^2} \frac{1+2\lambda}{\lambda^2} s(\theta)^{1+\frac{1}{\lambda}}} \qquad s = \frac{\theta - \theta_r}{\Delta\theta}, \quad \Delta\theta = \theta_s - \theta_r$$

Implementation pitfalls:

Three versions of unknown vector $\underline{\theta}$

$\underline{r}(\underline{\theta}, \underline{\theta}^n) \qquad \underline{\underline{J}}(\underline{\theta})$

$$\Delta\underline{\theta}^k = -J(\underline{\theta}^k) \backslash r(\underline{\theta}^k, \underline{\theta}^n)$$

$\underline{\theta}^n$ is solution at last time step

u^k is current iterate of N-R

$u^k \rightarrow u = \underline{u}^{n+1}$ as $k \rightarrow \infty$

Note $\underline{u}^k$ is initialized with old solu. $\underline{u}^0 = \underline{u}^n$

Common error is to confuse $\underline{u}^n$ and $\underline{u}^k$

General outline

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for n = 1 : N          % time-stepping loop
    θold = θ           % save old soln    θold = θ^n
    while nres > tol || ndθ > tol || k < kmax
        dθ = -J(θ) \ r(θ, θold)
        θ = θ + dθ
    end
end
```