Lecture 25: Analytical Jacobian

Logistics: - HW 9 due Th 4/18

- HW 7 last chance Th 4/18

Last time: Newtons Method for PDE's $\underline{r}(\underline{u})$

- $\frac{\partial \theta}{\partial t} - \nabla \cdot [D_H(\theta)^{n+1} \nabla \theta^{n+1}] = f_s$

  fully non-linear solution

- Numerical Jacobian

  $\underline{\underline{J}} = \left[\frac{\partial \underline{r}}{\partial \theta_1}, \frac{\partial \underline{r}}{\partial \theta_2}, \frac{\partial \underline{r}}{\partial \theta_3} \cdots \frac{\partial \underline{r}}{\partial \theta_N} \right]$

  $$\boxed{\frac{\partial \underline{r}}{\partial \theta_1} \approx \frac{\underline{r}(\theta_1 + \epsilon) - \underline{r}(\theta_1)}{\epsilon}}$$

- Works well but is slow

Today: Analytical Jacobian derivation

$\Rightarrow$ Directional derivative

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

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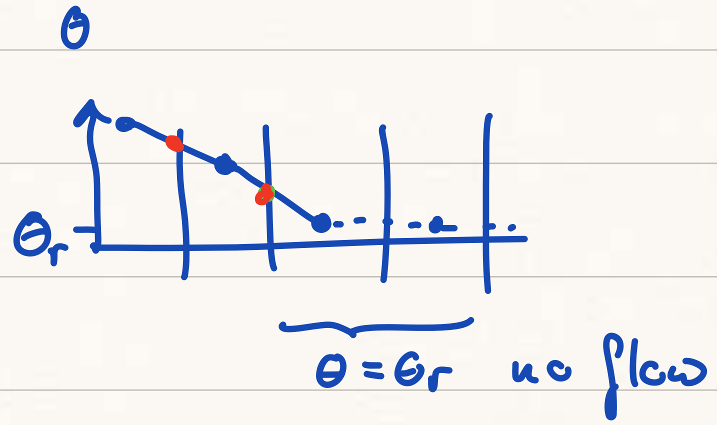
Analytical Jacobian for Richards Equation

PDE: $$\frac{\partial \theta}{\partial t} - \nabla \cdot \big[\underset{\underset{\underline{\underline{Kd}}}{\uparrow}}{D_H(\theta)} \nabla \theta \big] = f_s$$

Discretize with operators & backward Euler

$$\underline{r} = \underset{\underset{\text{find}}{\uparrow}}{\underline{\theta}^{n+1}} - \underset{\underset{\text{known}}{\uparrow}}{\underline{\theta}^{n}} - \Delta t \, \underline{\underline{D}} * \big[\underline{\underline{Kd}}(\underline{\theta}^{n+1}) * \underline{\underline{G}} \big] \underline{\theta}^{n+1} - \Delta t \, \underline{f_s} = 0$$

$$\underline{\underline{Kd}}(\underline{\theta}^{n+1}) = \text{comp\_mean}\big(D_H(\underline{\theta}^{n+1}), \underline{\underline{M}}, \underset{\underset{\text{arithmetic average}}{\uparrow}}{\underline{1}}, \text{Grid}, 1 \big)$$



$$\underline{\underline{Kd}}(\underline{\theta}^{n+1}) = \text{spdiags}\big(\underline{\underline{M}} \, D_H(\underline{\theta}^{n+1}), 0, Nf, Nf \big)$$
$$= \{ \underline{\underline{M}} \, D_H(\underline{\theta}^{n+1}) \}$$

n = superscript for time leve

k = superscript for Newton iteration

$\theta^{n+1} \equiv \theta$

$$\underline{\theta}^{k+1} = \underline{\theta}^{k} + \overbrace{\Delta\theta^{k}}$$
$$= \underline{\bar{\theta}} + \epsilon\, \underline{\hat{\theta}}$$

$\underline{\hat{\theta}}$ = direction unit vector

$$\underline{\underline{L}}_{\underline{\bar{\theta}}}\, \underline{r} = \underline{r}(\underline{\bar{\theta}}) + \nabla \underline{r}(\underline{\bar{\theta}})\, \Delta\underline{\theta}$$

$\nabla \underline{r}(\underline{\theta}) = \underline{\underline{J}}(\theta)$

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

dir. derivative

To derive analytic Jacobian we have to find directional derivative.

$$\underline{r} = \underline{\theta} - \underline{\theta}^{n} - \Delta t\, \underline{\underline{D}} * [\underline{\underline{Kd}}(\underline{\theta}\ ') * \underline{\underline{G}}]\, \underline{\underline{\theta}} - \Delta t\, f_s = 0$$

$$D_{\underline{\hat{\theta}}}\, \underline{r}(\underline{\bar{\theta}}) = \frac{d}{d\epsilon}\, \underline{r}\,(\underbrace{\underline{\bar{\theta}} + \epsilon\, \underline{\hat{\theta}}}_{\theta})\Big|_{\epsilon=0}$$

$$= \frac{d}{d\epsilon}\, \cancel{\underline{\bar{\theta}}} + \epsilon\underline{\hat{\theta}} - \cancel{\underline{\theta}^{n}} - \Delta t\, \underline{\underline{D}} * \left[\underline{\underline{Kd}}(\underline{\bar{\theta}} + \epsilon\underline{\hat{\theta}}) * \underline{\underline{G}}\right](\underline{\bar{\theta}} + \epsilon\underline{\hat{\theta}}) - \cancel{\Delta t f_s}\Big|_{\epsilon=0}$$

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

$$= \underline{\hat{\theta}} - \Delta t\, \underline{\underline{D}} * \Big(\underline{\underline{dKd}}\,(\underline{\bar{\theta}} + \cancel{\epsilon}\underline{\hat{\theta}})\, \underline{\hat{\theta}} * \underline{\underline{G}}(\underline{\bar{\theta}} + \cancel{\epsilon}\underline{\hat{\theta}})$$
$$+ \underline{\underline{Kd}}(\underline{\bar{\theta}} + \cancel{\epsilon}\underline{\hat{\theta}}) * \underline{\underline{G}}\, \underline{\hat{\theta}}\ \Big|_{\epsilon=0}$$

$$\frac{d}{d\epsilon}\,\underline{\underline{Kd}}\,(\underline{\bar{\theta}}+\epsilon\,\underline{\hat{\theta}}) = \frac{d}{d\epsilon}\left\{\underline{\underline{M}}\,\underline{D_H}(\underline{\bar{\theta}}+\epsilon\underline{\hat{\theta}})\right\} = \left\{\underline{\underline{M}}\,\frac{d}{d\epsilon}\,\underline{D_H}\underbrace{(\underline{\bar{\theta}}+\epsilon\underline{\hat{\theta}})}_{\hat{\theta}}\right\}$$

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

$$= \underbrace{\left\{\underline{\underline{M}}\,\frac{dD_H}{d\theta}\left(\underline{\bar{\theta}}+\cancel{\epsilon}^{\,0}\,\underline{\hat{\theta}}\right)\right\}}_{\underline{\underline{dKd}}(\underline{\bar{\theta}})}\underline{\hat{\theta}}$$

$$D_{\underline{\hat{\theta}}}\,\underline{r}(\underline{\bar{\theta}}) = \underline{\underline{I}}\,\underline{\hat{\theta}} - \Delta t\,\underline{\underline{D}} * \Big(\underbrace{\underline{\underline{dKd}}(\underline{\bar{\theta}})}_{\text{known vector}}\underline{\hat{\theta}} * \underbrace{\underline{\underline{G}}\,\underline{\bar{\theta}}}_{\text{known vector}} + \underline{\underline{Kd}}(\underline{\bar{\theta}}) * \underline{\underline{G}}\,\underline{\hat{\theta}}\Big)$$

$$\underline{\underline{G\theta}} = \text{spdiags}(\underline{\underline{G}}\,\underline{\theta}, 0, Nf, Nf)$$

$$\underbrace{\begin{pmatrix}\ddots\end{pmatrix}}_{\underline{\underline{dKd}}}\;\underbrace{\begin{pmatrix}\ddots\end{pmatrix}}_{\underline{\underline{G\theta}}} = \underline{\underline{G\theta}} * dKd$$

$$D_{\underline{\hat{\theta}}}\,\underline{r}(\underline{\bar{\theta}}) = \underbrace{\underline{\underline{I}} - \Delta t\,\underline{\underline{D}} * \left(\underline{\underline{G\theta}} * \underline{\underline{dKd}}(\underline{\bar{\theta}}) + \underline{\underline{Kd}}(\underline{\bar{\theta}}) * \underline{\underline{G}}\right)}_{\underline{\underline{J}}(\underline{\bar{\theta}})}\;\underline{\hat{\theta}}$$

Hence we have

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

$$\underline{\underline{M}} * \underline{\underline{dKd}}(\theta)$$

actually we need to write

$$\mathrm{spdiags}(\underline{D_H}(\underline{\bar{\theta}}), 0, N, N)$$