Solution of transient linear problems

nterested in transient advection diffusion equation

$$\phi \frac{\partial c}{\partial t} + \underbrace{\nabla \left[q c - \underline{\underline{D}}_H \nabla c \right]}_{\underline{\underline{L}}\,\underline{c}} = f_s$$

where $L = \underline{\underline{D}} \left(\underline{\underline{A}}(q) - D_H \underline{\underline{G}} \right)$ from steady problem

$\Rightarrow$ semi-discrete problem $\phi \frac{\partial \underline{c}}{\partial t} + \underline{\underline{L}}\, c = f_s$

Could be solved by ode solver - very large system!

n practica subsurface app ications $\rightarrow$ direct implementation

Theta-method

$$\underline{\underline{M}} \frac{\underline{c}^{n+1} - \underline{c}^n}{\Delta t} + \underline{\underline{L}}\, \underline{c} = \underline{f}_s$$

where $\underline{\underline{M}} = \phi \underline{\underline{I}}$ is "mass matrix"

always diagonal $\Rightarrow$ easy to invert

Choose to evaluate $\underline{\underline{L}}\,\underline{c}$ at 'n' or 'n+1' or in between?

theta method $\underline{\underline{L}}\,\underline{c} = \theta \underline{\underline{L}}\, \underline{c}^n + (1 \theta) \underline{\underline{L}}\, c^{n+1}$ $\qquad \theta \in [0,1]$

substitute and collect terms

$$\underline{\underline{M}} \left(\underline{c}^{n+1} - \underline{c}^n \right) + \Delta t\, \underline{\underline{L}}\, \underline{c} = \Delta t\, \underline{f}_s$$

$$\underline{\underline{M}} \left(\underline{c}^{n+1} - \underline{c}^n \right) + \Delta t\, \theta\, \underline{\underline{L}}\, c^n + \Delta t (1-\theta) \underline{\underline{L}}\, \underline{c}^{n+1} = \Delta t\, \underline{f}_s$$

$$\underbrace{\left(\underline{\underline{M}} + \Delta t (1-\theta) \underline{\underline{L}} \right)}_{\underline{\underline{Im}}} \underline{c}^{n+1} = \underbrace{\left(\underline{\underline{M}} \quad \Delta t\, \theta\, \underline{\underline{L}} \right)}_{\underline{\underline{Ex}}} \underline{c}^n + \Delta t\, \underline{f}_s$$

Timestep $\boxed{\underline{\underline{Im}}\, \underline{c}^{n+1} = \underline{\underline{Ex}}\, \underline{c}^n + \Delta t\, \underline{f}_s}$

Properties of theta-method

For $\Theta = 1$: (Forward) Euler method

$\Rightarrow \underline{\underline{Im}} = \underline{\underline{M}}$ (diagonal)

$c^{n+1} = \underline{\underline{M}}^{-1}(\underline{\underline{Ex}}\, \underline{c}^n + \Delta t\, \underline{f}_s)$

- explicit method
- only matrix vector multiply $\Rightarrow$ cheap
- conditionally stable. $\Delta t < \frac{\Delta x}{v} = \frac{\Phi \Delta x}{q}$ (advection)

  $\Delta t < \frac{\Delta x^2}{2 D_H}$ (diffusion)

- first order accurate in time

For $\Theta = 0$ Backward Euler

$\rightarrow \underline{\underline{Ex}} = \underline{\underline{M}}$

$\underline{\underline{Im}}\, c^{n+1} = \underline{\underline{M}}\, \underline{c}^n + \Delta t\, \underline{f}_s$

- implicit method
- solution of a linear system at every time step
- unconditionally stable
- 1st order in time

For $\Theta = \frac{1}{2}$. Crank-Nicholson / Trapezoidal rule

$\underline{\underline{Im}}\, \underline{c}^{n+1} - \underline{\underline{Ex}}\, c^n + \Delta t\, \underline{f}_s$

implicit

- both solve linear system and matrix vector multiply

unconditionally stable but has an oscillation limit

- 2nd order in time

For advection explicit method ($\Theta = 1$) is least diffusive
$\Rightarrow$ keep advection explicit if possible

Time step limit for diffusion is too strict
$\Rightarrow$ keep diffusion implicit

Two Θ_A separate Θ for diffusion & advection.

$$\underline{\underline{Im}} = \underline{\underline{M}} + \Delta t\,(1-\Theta_A)\,\underline{\underline{D}}\,\underline{\underline{A}}(q) + \Delta t\,(1-\Theta_D)\,\underline{\underline{D}}\,D_H\,\underline{\underline{G}}$$

$$\underline{\underline{Ex}} = \underline{\underline{M}} - \Delta t\,\Theta_A\,\underline{\underline{D}}\,\underline{\underline{A}}(q) + \Delta t\,\Theta_D\,\underline{\underline{D}}\,\underline{\underline{D_H}}\,\underline{\underline{G}}$$

In porous media even advective time step restriction is limiting due to high variability in flow velocity
$\Rightarrow$ Adaptive implicit method. $\underline{\Theta_A}$ Nx by 1 vector

$\Theta_A = 1$ in regions of high flow velocity
$\Theta_A = 0$ in regions of low flow velocity

For problems without diffusion this can speedup solution significantly