Adjoint equation for coupled porous media flow and scalar transport equations

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1 Equations

The original governing equation:

$$\begin{aligned} \vec{v} &= -a\nabla p \\ \nabla \cdot \vec{v} &= s - \gamma p \\ \frac{\partial c}{\partial t} &= -cs - \vec{v} \cdot \nabla c + \nabla \cdot (\mu \nabla c) \end{aligned} \tag{1}$$

The 3rd equation of Eqn (1) *can be re-written in the conservative form:*

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{v}) = -c\gamma p + \nabla \cdot (\mu \nabla c) \tag{2}$$

Boundary condition

$$\begin{aligned} \vec{v} \cdot \hat{n} = 0 \quad \text{or} \quad \nabla p \cdot \hat{n} = 0 \\ \nabla c \cdot \hat{n} = 0 \end{aligned} \tag{3}$$

At the injection wells,

$$c = 0\ . \tag{4}$$

Objective function: $J = \int_0^T \int_\Omega \gamma pc$
Adjoint equations:

$$\begin{aligned} \frac{\partial \sigma}{\partial t} &= \gamma p(1+\sigma) - \vec{v} \cdot \nabla \sigma \underbrace{- \nabla \cdot (\mu \nabla \sigma)}_{-t \text{ stabilizer}} \\ \nabla \cdot \Big(a(\nabla \lambda + \sigma \nabla c) \Big) &+ \gamma (c - \lambda) = 0 \end{aligned} \tag{5}$$

Boundary and Initial conditions:

$$\begin{aligned} \hat{n} \cdot \nabla \sigma &= 0 \\ \hat{n} \cdot \nabla \lambda &= 0 \\ \sigma(T) &= 0 \end{aligned} \tag{6}$$

Sensitivity:

$$\delta J = \int_\Omega \int_T (\sigma c + \lambda) \delta s \tag{7}$$

Introduce time reversal, $t' = T - t$, Adjoint equations:

$$\begin{aligned} \frac{\partial \sigma}{\partial t'} &= -\gamma p(1+\sigma) - \vec{v} \cdot \nabla \sigma + \nabla \cdot (\mu \nabla \sigma) \\ \nabla \cdot \Big(a(\nabla \lambda + \sigma \nabla c) \Big) &+ \gamma (c - \lambda) = 0 \end{aligned} \tag{8}$$

Notice: $\vec{v} = \vec{v}_{t'}(t') \equiv \vec{v}_t(T - t')$
New initial condition:

$$\sigma(0') = 0 \tag{9}$$

Compare the c solver equation and σ equation:

$$\begin{aligned} \frac{\partial c}{\partial t} &= -cs \qquad\qquad - \vec{v} \cdot \nabla c + \nabla \cdot (\mu \nabla c) \\ \frac{\partial \sigma}{\partial t'} &= -\gamma p(1+\sigma) - \vec{v} \cdot \nabla \sigma + \nabla \cdot (\mu \nabla \sigma) \end{aligned} \tag{10}$$

2 Appendix of Equations

The first Lagrangian (linearize the 2nd equation of (1)):

$$0 = \int_\Omega \int_T -a \nabla \delta p \cdot \nabla \lambda + \lambda \delta s - \gamma \lambda \delta p \tag{11}$$

$\mapsto$

$$0 = \int_\Omega \int_T \delta p \nabla \cdot (a \nabla \lambda) + \lambda \delta s - \lambda \gamma \delta p - \int_{\partial\Omega} \int_T a \delta p \nabla \lambda \cdot \hat{n} \tag{12}$$

The second Lagrangian (linearize the 3rd equation of (1)):

$$0 = \int_\Omega \int_T \underbrace{\sigma \frac{\partial \delta c}{\partial t}}_{\text{A}} + \sigma s \delta c + \sigma c \delta s + \underbrace{\sigma \delta \vec{v} \cdot \nabla c}_{\text{B}} + \underbrace{\sigma \vec{v} \cdot \nabla \delta c}_{\text{C}} \underbrace{- \sigma \nabla \cdot (\mu \nabla \delta c)}_{\text{D}} \tag{13}$$

A:

$$\begin{aligned} &\int_\Omega \int_T \sigma \frac{\partial \delta c}{\partial t} \\ &= \int_\Omega (\sigma \delta c)\big|_0^T - \int_\Omega \int_T \delta c \frac{\partial \sigma}{\partial t} \end{aligned} \tag{14}$$

B:

$$\begin{aligned} &\int_\Omega \int_T \sigma \delta \vec{v} \cdot \nabla c \\ &= \int_\Omega \int_T -a \sigma \nabla \delta p \cdot \nabla c \\ &= \int_\Omega \int_T \delta p \nabla \cdot (a \sigma \nabla c) - \int_{\partial\Omega} \int_T a \sigma \delta p \nabla c \cdot \hat{n} \end{aligned} \tag{15}$$

C:

$$\begin{aligned} &\int_\Omega \int_T \sigma \vec{v} \cdot \nabla \delta c \\ &= \int_\Omega \int_T -\delta c \nabla \cdot (\sigma \vec{v}) + \int_{\partial\Omega} \int_T \sigma \vec{v} \delta c \cdot \hat{n} \end{aligned} \tag{16}$$

D:

$$\begin{aligned} &\int_\Omega \int_T -\sigma \nabla \cdot (\mu \nabla \delta c) = \\ &= \int_\Omega \int_T -\delta c \nabla \cdot (\mu \nabla \sigma) + \int_{\partial\Omega} \int_T \big(\mu \delta c \nabla \sigma - \sigma \mu \nabla \delta c\big) \cdot \hat{n} \end{aligned} \tag{17}$$

$\mapsto$ the second Lagrangian:

$$\begin{aligned}0 = &\int_\Omega \int_T \delta c\Big(-\frac{\partial \sigma}{\partial t} + \sigma s - \nabla\cdot(\sigma\vec{v}) - \nabla\cdot(\mu\nabla\sigma)\Big) + \delta p \nabla\cdot\big(a\sigma\nabla c\big) + \sigma c \delta s \\ &+ \int_{\partial\Omega}\int_T \Big(-a\sigma\delta p \nabla c - \sigma\mu\nabla\delta c + \sigma\vec{v}\delta c + \mu\delta c\nabla\sigma\Big)\cdot\hat{n} + \int_\Omega \big(\sigma\delta c\big)\Big|_0^T\end{aligned} \tag{18}$$

Therefore, the final linearized equation is:

$$\begin{aligned}\delta J = \int_\Omega\int_T &\gamma c\delta p + \gamma p \delta c + \delta c\Big(-\frac{\partial\sigma}{\partial t} + \sigma s - \nabla\cdot(\sigma\vec{v}) - \nabla\cdot(\mu\nabla\sigma)\Big) \\ &+\delta p\nabla\cdot\big(a\sigma\nabla c\big) + \sigma c\delta s + \delta p\nabla\cdot\big(a\nabla\lambda\big) + \lambda\delta s - \lambda\gamma\delta p\end{aligned} \tag{19}$$

Boudary condition:

$$0 = \Big(-a\sigma\nabla c\delta p - \sigma\mu\nabla\delta c + \sigma\vec{v}\delta c + \mu\delta c\nabla\sigma - a\delta p\nabla\lambda\Big)\cdot\hat{n} \tag{20}$$

Initial condition:

$$0 = \sigma(T) \tag{21}$$

Finally, we get the adjoint equation:

$$\begin{aligned}0 &= \frac{\partial\sigma}{\partial t} - s\sigma + \nabla\cdot\big(\sigma\vec{v} + \mu\nabla\sigma\big) - \gamma p \\ 0 &= \nabla\cdot\Big(a(\nabla\lambda + \sigma\nabla c)\Big) + \gamma\big(c - \lambda\big) \\ \hat{n}\cdot\nabla\sigma &= 0 \qquad \hat{n}\cdot\nabla\lambda = 0 \qquad \sigma(T) = 0\end{aligned} \tag{22}$$

Equation (5) is a different format of the ajoint equation above.

3 Convection-Diffusion Solver

Discretize on a circle domain and initialize the pressure field.
For a triangle element, we have:

$$\frac{d\bar{c}}{dt} = \underbrace{-\frac{1}{A}\int_{\partial\Omega} c\vec{v}\cdot\hat{n}\,ds}_{R_c} + \underbrace{\frac{1}{A}\int_{\partial\Omega}\mu\nabla c\cdot\hat{n}\,ds}_{R_d} - \underbrace{\bar{c}\gamma\bar{p}}_{R_s} \tag{23}$$

3.1 1st Order Upwind

For triangle T_0, the convection is given by:

$$R_c = \sum_{i=1}^{3}\underbrace{c_{0i}\vec{v}_{0i}\cdot\hat{n}_{0i}}_{F_{0i}}\,L_{0i} \tag{24}$$

T_1, T_2, T_3 are T_0's three neighbor triangles. $\hat{n}_{0i}$ points from T_0 to T_i. If T_0 has only two neighbors, then drop one term from Eqn (29) because $\vec{v}\cdot\hat{n} = 0$ at boundary. Compute F_{0i} by first-order upwind scheme:

$$\begin{aligned}&\text{if } |c_i - c_0| \geq \epsilon \quad \mapsto \quad F_{0i}^{UP} = \frac{1}{2}\big(c_0\vec{v}_0\cdot\hat{n} + c_i\vec{v}_i\cdot\hat{n}\big) - \frac{1}{2}\big(c_i - c_0\big)\Big|\frac{c_i\vec{v}_i\cdot\hat{n} - c_0\vec{v}_0\cdot\hat{n}}{c_i - c_0}\Big| \\ &\text{if } |c_i - c_0| < \epsilon \quad \mapsto \quad F_{0i}^{UP} = \frac{1}{2}c_0\big(\vec{v}_0 + \vec{v}_i\big)\cdot\hat{n}\end{aligned} \tag{25}$$

$\vec{v}_0$ and $\vec{v}_i$ is the average velocity *inside* each triangle. To compute $\vec{v}$, ie. to compute ∇p, we use Gaussian theorem:

$$\int_\Omega \nabla p\,d\Omega = \int_{\partial\Omega} p\hat{n}\,ds \tag{26}$$

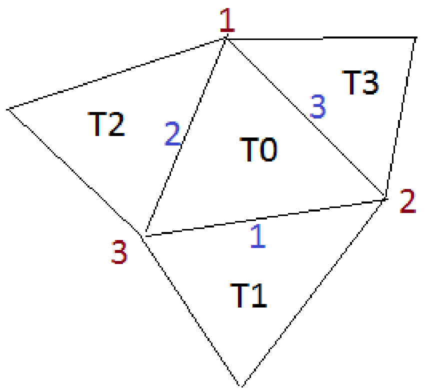

Figure 1: Triangular subscripts

And we get:

$$\nabla p\big|_{T_0} = \frac{1}{2A}\Big((p_2+p_3)L_1\hat{n}_1 + (p_1+p_2)L_3\hat{n}_3 + (p_1+p_3)L_2\hat{n}_2\Big) \tag{27}$$

The diffusion is given by:

$$R_d = \sum_{i=0}^{3} \frac{\mu_i + \mu_0}{2} \frac{c_i - c_0}{|\vec{b}_i - \vec{b}_0|} L_{0i} \tag{28}$$

For the boundary edge just drop the term from the sum because $\nabla c \cdot \hat{n} = 0$. The viscosity μ should be the local viscosity in a given cell. But for simplicity we consider μ to be a constant.

3.2 2nd Order Upwind

Upgrade the convective flux from 1st order to second order, while retain the diffusive flux as described previously.
For triangle T_0, the convection is given by:

$$R_c = \sum_{i=1}^{3} (c\vec{v})_{0i} \cdot \hat{n}_{0i} \, L_{0i} \tag{29}$$

We need to evaluate $c\vec{v}_{0i}$ by piecewise-linear reconstruction. First compute ∇p at each triangle by Eqn(27)

$$\nabla p\big|_{T_0} = \frac{1}{2A}\Big((p_2+p_3)L_1\hat{n}_1 + (p_1+p_2)L_3\hat{n}_3 + (p_1+p_3)L_2\hat{n}_2\Big)$$

Therefore, the flux in triangle T_0 is given by:

$$(c\vec{v})\big|_{T_0} = -a\, c\big|_{T_0} \nabla p\big|_{T_0} \equiv \vec{F}_0 = (F_{0x}, F_{0y}) \tag{30}$$

$\vec{F}_0$ is defined in the centroid of cell T_0. After computing $\vec{F}$ for every triangle, we proceed to reconstruct $\vec{F}$ in order to evaluate its values in the midpoints of cell edges. Take F_x as the example:

3.2.1 compute ∇F_x for each cell

First we compute F_x at the grid vertex by averaging, i.e.,

$$F_{xk'} = \frac{1}{N} \sum_i F_{k_i x} \tag{31}$$

gives F_x at the k_{th} vertex of a given cell. We denote the vertex related quantities with $'$. The sum is over the cells who share this vertex. Note this is an approximated expression in which every cell is weighted equally. Actually the weight should be the angles. Thus it requires good quality of the mesh.
With the vertex F_x at hand, we can compute the gradient of F_x at each cell.

$$\nabla F_x\big|_{T_0} = \frac{1}{2A}\Big((F_{x2'} + F_{x3'})L_1\hat{n}_1 + (F_{x1'} + F_{x2'})L_3\hat{n}_3 + (F_{x1'} + F_{x3'})L_2\hat{n}_2\Big) \tag{32}$$

3.2.2 compute $F_x^{max}\big|_{T_0}$ and $F_x^{min}\big|_{T_0}$ (cell value)

$$\begin{aligned} F_x^{max}\big|_{T_0} &= max\{F_x\big|_{T_0}, F_x\big|_{neighbors}\} \\ F_x^{min}\big|_{T_0} &= min\{F_x\big|_{T_0}, F_x\big|_{neighbors}\} \end{aligned} \tag{33}$$

3.2.3 compute F_x at each cell's vertex

$$F_{x0i'} = F_{0x} + \nabla F_x\big|_{T_0} \cdot \Delta\vec{r}_{0i'} \qquad i' = 1,\, 2,\, 3 \tag{34}$$

3.2.4 compute the limiter $\bar{\Phi}^x_{0i'}$ for each vertice of cell T_0

$$\bar{\Phi}^x_{0i'} = \begin{cases} min\{1, \dfrac{F_x^{max}\big|_{T_0} - F_{0x}}{F_{x0i'} - F_{0x}}\}\ , & \text{if } F_{x0i'} - F_{0x} > \epsilon \\ min\{1, \dfrac{F_x^{min}\big|_{T_0} - F_{0x}}{F_{x0i'} - F_{0x}}\}\ , & \text{if } F_{x0i'} - F_{0x} < -\epsilon \\ 1\ , & \text{else} \end{cases} \tag{35}$$

in which $i' = 1,\, 2,\, 3$

3.2.5 compute the limiter $\Phi_0^{x,y}$ and Φ_0 for cell T_0

$$\Phi_0^x = min\{\bar{\Phi}^x_{01'},\, \bar{\Phi}^x_{02'},\, \bar{\Phi}^x_{03'}\} \tag{36}$$

Notice this is the limiter derived from the x component. Repeat the procedures for the y component and

$$\Phi_0 = min\{\Phi_0^x,\, \Phi_0^y\} \tag{37}$$

3.2.6 compute flux at two sides of an edge's midpoint

Compute F_{0i}^+ and F_{0i}^-, $i = 1,\, 2,\, 3$, which are the values of F_x at boundaries of T_0. $-$ is the interior of T_0 and $+$ is the exterior of T_0.

$$\begin{aligned} F_{x0i}^- &= F_{0x} + \Phi_0 \nabla F_x\big|_{T_0} \cdot \frac{\Delta\vec{r}_{0i}}{2} \\ F_{x0i}^+ &= F_{ix} + \Phi_i \nabla F_x\big|_{T_i} \cdot \frac{\Delta\vec{r}_{i0}}{2} \end{aligned} \tag{38}$$

$\Delta\vec{r}_{0i}$ is the vector from the centroid of T_0 to the centroid of T_i. The y component is computed similarly. Thus we obtain $\vec{F}_{0i}^{\pm}$ for each edge of cell T_0.

3.2.7 upwind scheme

$$\begin{aligned} F_{0i} &= \vec{F}_{0i}^- \cdot \hat{n}_{0i} \qquad \text{if } (\vec{v}_0 + \vec{v}_i) \cdot \hat{n}_{0i} \geq 0 \\ F_{0i} &= \vec{F}_{0i}^+ \cdot \hat{n}_{0i} \qquad \text{if } (\vec{v}_0 + \vec{v}_i) \cdot \hat{n}_{0i} < 0 \end{aligned} \tag{39}$$

And the convection term, i.e. Eqn(29) is given by:

$$R_c = \sum_{i=1}^{3} F_{0i} L_{0i} \tag{40}$$

4 Pressure Solver

The pressure equation is given by:

$$\begin{aligned} -\nabla \cdot (a \nabla u) + \gamma u &= s \qquad a > 0,\, \gamma > 0 \\ \hat{n} \cdot \nabla u &= 0 \end{aligned} \tag{41}$$

We denote the pressure by u following the convention of FEM.
The weak form is given by:

$$a(u, v) = l(v) \tag{42}$$

in which

$$\begin{cases} a(u,v) = \displaystyle\int_\Omega \big(a \nabla u \cdot \nabla v + \gamma u v\big)\, \mathrm{d}A \qquad \text{(SPD)} \\ l(v) = \displaystyle\int_\Omega s v \, \mathrm{d}A \end{cases} \tag{43}$$

4.1 Matrix Evaluation

To evaluate the *stiffness matrix* and the *mass matrix*, we introduce the *local area coordinates* L_1, L_2 , which is related to the global coordinates x, y by the following transformation:

$$\begin{cases} x = x_3 + (x_1 - x_3) L_1 + (x_2 - x_3) L_2 \\ y = y_3 + (y_1 - y_3) L_1 + (y_2 - y_3) L_2 \end{cases} \tag{44}$$

For a triangular element, it's proven that the its 3 nodal piecewise basis are exactly L_1, L_2, L_3, in which

$$L_1 + L_2 + L_3 = 1 \tag{45}$$

The transformation Jacobian is given by:

$$J = \frac{\partial \vec{x}}{\partial \vec{L}} = \begin{pmatrix} x_1 - x_3 & x_2 - x_3 \\ y_1 - y_3 & y_2 - y_3 \end{pmatrix} \tag{46}$$

$$(J^T)^{-1} = \frac{1}{2A_e} \begin{pmatrix} y_2 - y_3 & -y_1 + y_3 \\ -x_2 + x_3 & x_1 - x_3 \end{pmatrix} \tag{47}$$

$$|J| = 2A_e \tag{48}$$

where A_e is the area of the triangle.
The transformed derivatives are given by:

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = (J^T)^{-1} \begin{pmatrix} \frac{\partial}{\partial L_1} \\ \frac{\partial}{\partial L_2} \end{pmatrix} \tag{49}$$

Also,

$$\nabla_L \vec{L} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{pmatrix} \tag{50}$$

We can also prove the following identity:

$$\int_{A_e} L_1^a \, L_2^b \, L_3^c \, \mathrm{d}A = a!\, b!\, c!\, \frac{2A_e}{(a+b+c+2)\,!} \tag{51}$$

The contribution to the bilinear matrix from the cell A_e is given by:

$$a(\phi_{i'}, \phi_{j'})\big|_{A_e} = \int_{A_e} a \left((J^T)^{-1} \nabla_L L_i\right)^T \cdot \left((J^T)^{-1} \nabla_L L_j\right) \, \mathrm{d}A + \int_{A_e} \gamma \, L_i \, L_j \, \mathrm{d}A \tag{52}$$

in which i, j is the local nodal index and i', j' is the global nodal index.

5 Adjoint Solver

For simplicity we assume static pressure.

5.1 reconstruct c

Solve c backward from checkpoints to reconstruct c for a checklength.
The forward c solver is:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (c\vec{v}) + \nabla \cdot (\mu \nabla c) - c\gamma p \tag{53}$$

The backward c solver is:

$$\frac{\partial c}{\partial t'} = -\nabla \cdot \big(c(-\vec{v})\big) + \nabla \cdot \big((-\mu)\nabla c\big) - c\gamma(-p) \tag{54}$$

In practice, we only need to change the signs of p (thus $\vec{v}$) and μ, and use the same c solver. The notation t' does not effect the solver. It only denotes that we need to interpret and store the solution backward in time.
Before the next step, we need to check and ensure the reconstructed c at the end of each checklength matches the corresponding checkpoint. Currently we set $dt = 1 \times 10^{-4}$ and checkpoint at every 100 timesteps. It has been found the error of the worst reconstructed c (at the end of each checklength) and the forward solved c is around 1.5%.

5.2 σ solver

The forward c solver is:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (c\vec{v}) + \nabla \cdot (\mu \nabla c) - c\gamma p \tag{55}$$

The backward σ solver is:

$$\frac{\partial \sigma}{\partial t'} = -\nabla \cdot \big(\sigma(-\vec{v})\big) + \nabla \cdot (\mu \nabla \sigma) - \sigma s - \gamma p \tag{56}$$

The initial σ condition is: $\sigma(t' = 0) = 0$
We write another solver function for σ, though it is very similar to the c solver. Also notice to solve σ, we don't need c, i.e. the c backward solver and the σ solve are independent.

5.3 λ solver

The pressure solver is:

$$-\nabla \cdot (a\nabla p) = -\gamma p + s \tag{57}$$

The λ solver is:

$$-\nabla \cdot (a\nabla \lambda) = -\gamma\lambda + \Big(\nabla \cdot (a\sigma\nabla c) + c\gamma\Big) \tag{58}$$

The only non-trivial work to solve the λ equation is to compute $\Big(\nabla \cdot (a\sigma\nabla c) + c\gamma\Big)$ and replace s in the pressure solver. This corresponds to a modification of the load vector in the FEM solver.
In practice, for each triangle, compute:

$$\lambda \text{ vector}: \qquad \sum_{edge}\Big(\frac{a' + a''}{2}\frac{\sigma_1 + \sigma_2}{2}\frac{c_1 - c_2}{d_{12}} l_{12}\Big) + A_e c\gamma$$

This forms a vector. Then replace the *inWell* vector in the FEM solver by this vector, while setting the number *sCoef* to be 1.

5.4 ajoint sensitivity

We plot $\sigma c + \lambda$ as the transient ajoint sensitivity for the oil production.