Second order schemes for nonlinear transport

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1 Schemes

$$\frac{\partial C}{\partial t} = \frac{1}{g(C)} \nabla \cdot \varphi(C) \tag{1}$$

where

$$g(C) = \omega + \rho_s (1-\omega) \frac{\partial q}{\partial C} \tag{2}$$

and

$$\varphi(C) = -\mathbf{D}\nabla C + \mathbf{u}C. \tag{3}$$

1.1 Extrapolated Euler

Extrapolated Euler uses a backward Euler approximation using a time step of $\frac{\Delta t}{2}$ to obtain a second order approximation to C_h^{n+1}. **Lea: citations?** Add brief explanation using Taylor expansions.. The backward Euler approximation for this problem was analyzed in previous work.

The backward Euler approximation $C^{n+1/2}$ is obtained as the solution to the weak formulation

$$\left(g(C^n)\, \tilde{C}^{n+1/2}, v\right) - (C^n, v) + \frac{\Delta t}{2}\left[\left(\mathbf{D}\nabla\tilde{C}^{n+1/2}, \nabla v\right) - \left(\mathbf{u}\tilde{C}^{n+1/2}, \nabla v\right)\right] \tag{4}$$

where the nonlinearity $g(C)$ is evaluated at $C = C^n$.

The approximation at t_{n+1} is updated using the extrapolation

$$C^{n+1} = 2\tilde{C}^{n+1/2} - C^n. \tag{5}$$

1.2 Trapezoid Method

1.2.1 Method of Lines

The method of lines approach discretizes the governing equation in time first, then applies a temporal integration method. This discretization can also be obtained using the approach of Nochetto and Verdi by using a trapezoid approximation for the temporal integration of the flux term.

In this case, the weak formulation becomes

$$\left(C^{n+1}, v\right) = \left(C^{n}, v\right) + \frac{\Delta t}{2}\left[\left(\frac{1}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right), v\right) + \left(\frac{1}{g\left(C^{n}\right)}\nabla\varphi\left(C^{n}\right), v\right)\right] \tag{6}$$

The flux term can be integrated by parts. As an example, the first term becomes

$$\begin{aligned}\int_\Omega \frac{1}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right) v\, d\Omega &= \int_\Omega \nabla\cdot\varphi\left(C^{n+1}\right)\frac{v}{g\left(C^{n+1}\right)}\, d\Omega \\ &= \int_\Gamma \varphi\left(C^{n+1}\right)\frac{v}{g\left(C^{n+1}\right)}\, d\Gamma \\ &\quad - \int_\Omega \varphi\left(C^{n+1}\right)\cdot\nabla\frac{v}{g\left(C^{n+1}\right)}\, d\Omega\end{aligned}$$

Then

$$\nabla\frac{v}{g\left(C^{n+1}\right)} = \frac{g\left(C^{n+1}\right)\frac{\partial}{\partial x}(v) - v\frac{\partial}{\partial x}g\left(C^{n+1}\right)}{g\left(C^{n+1}\right)^2}$$

where

$$\frac{\partial}{\partial x}g\left(C^{n+1}\right) = \left.\frac{\partial g}{\partial C}\frac{\partial C}{\partial x}\right|_{C=C^{n+1}}$$

1.2.2 Discretize in Time First

An alternative strategy is to discretize first in time, then in space. Applying the trapezoid rule to Eq. (1) gives

$$C^{n+1} = C^{n} + \frac{\Delta t}{2}\left[\frac{1}{g\left(C^{n+1}\right)}\nabla\varphi\left(C^{n+1}\right) + \frac{1}{g\left(C^{n}\right)}\nabla\cdot\varphi\left(C^{n}\right)\right]. \tag{7}$$

At this point, if the weak formulation is found, the representation is the same as in the method of lines scenario. However, at this point one can multiply by $g\left(C^{n}\right)$ to remove the nonlinearity from at least one of the terms.

This may be advantageous as we note that with both the Langmuir and Freundlich isotherms, and based on the shape of isotherm curves in general, $g\left(C^{n}\right) > g\left(C^{n+1}\right)$. Thus, multiplying by $g\left(C^{n}\right)$ will lead to a coefficient larger than one in front of $\varphi\left(C^{n+1}\right)$. This gives

$$g\left(C^{n}\right)\left(C^{n+1} - C^{n}\right) - \frac{\Delta t}{2}\left[\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right) + \nabla\cdot\varphi\left(C^{n}\right)\right] = 0. \tag{8}$$

Multiplying by $v \in V_h$ gives

$$\left(g\left(C^{n}\right)\left(C^{n+1} - C^{n}\right), v\right) - \frac{\Delta t}{2}\left[\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right), v\right) + \left(\nabla\cdot\varphi\left(C^{n}\right), v\right)\right] = 0 \tag{9}$$

The second term in Eq. (9) is evaluated by noting

$$\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right),v\right)=\int_{\Omega}\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}\nabla\cdot\varphi\left(C^{n+1}\right)v\,d\Omega \tag{10}$$

$$=\int_{\Omega}\nabla\cdot\varphi\left(C^{n+1}\right)\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}v\right)\,d\Omega \tag{11}$$

$$=\int_{\Gamma}\left(\frac{g\left(C^{n}\right)v}{g\left(C^{n+1}\right)}\right)\varphi\left(C^{n+1}\right)\cdot\mathbf{n}\,d\Gamma \tag{12}$$

$$-\int_{\Omega}\nabla\left(\frac{g\left(C^{n}\right)v}{g\left(C^{n+1}\right)}\right)\cdot\varphi\left(C^{n+1}\right)\,d\Omega$$

Note that

$$\frac{\partial}{\partial x}\left(\frac{g\left(C^{n}\right)v}{g\left(C^{n+1}\right)}\right)=\frac{g\left(C^{n+1}\right)\frac{\partial}{\partial x}\left(g\left(C^{n}\right)v\right)-g\left(C^{n}\right)v\frac{\partial}{\partial x}\left(g\left(C^{n+1}\right)\right)}{g\left(C^{n+1}\right)^{2}} \tag{13}$$

Then

$$\frac{\partial}{\partial x}\left(g\left(C^{n}\right)v\right)=g\left(C^{n}\right)\frac{\partial}{\partial x}v+v\frac{\partial}{\partial x}g\left(C^{n}\right)$$

where

$$\frac{\partial}{\partial x}g\left(C^{n}\right)=\left.\frac{\partial g}{\partial C}\frac{\partial C}{\partial x}\right|_{C=C^{n}} \tag{14}$$

If $\nabla\cdot\mathbf{u}=0$ is enforced, only the diffusive component of the flux is considered in integration by parts. That is, we have

$$\int_{\Omega}\nabla\cdot\varphi\left(C^{n+1}\right)\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}v\right)\,d\Omega=\int_{\Omega}\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}\left(\mathbf{u}\cdot\nabla C^{n+1}\right)v\,d\Omega \tag{15}$$

$$-\int_{\Gamma}\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}v\right)\mathbf{D}\nabla\left(C^{n+1}\right)\cdot\mathbf{n}\,d\Gamma \tag{16}$$

$$+\int_{\Omega}\nabla\left(\frac{g\left(C^{n}\right)}{g\left(C^{n+1}\right)}v\right)\cdot\varphi\left(C^{n+1}\right)\,d\Omega$$

1.3 Midpoint Method of Lines

The midpoint approximation is generated using

$$\left(C^{n+1},v\right)=\left(C^{n},v\right)+\Delta t\left[\left(\frac{1}{g\left(\frac{C^{n+1}+C^{n}}{2}\right)}\nabla\cdot\varphi\left(\frac{C^{n+1}+C^{n}}{2}\right),v\right)\right] \tag{17}$$

The problem is linearized by using the second order extrapolated Euler approximation, call it $\tilde{C}^{n+1}$ in the evaluation of $g\left(C\right)$.

Integration by parts of the flux term now requires differentiation of the nonlinear function $\frac{v}{g(C)}$. Define $C^{n+1/2} = \dfrac{C^{n+1} + C^n}{2}$. Then

$$\begin{aligned}\int_\Omega \frac{1}{g\left(C^{n+1/2}\right)} \nabla \cdot \varphi \left(C^{n+1/2}\right) v \, d\Omega &= \int_\Omega \nabla \cdot \varphi \left(C^{n+1/2}\right) \frac{v}{g\left(C^{n+1/2}\right)} \, d\Omega \\ &= \int_\Gamma \varphi \left(C^{n+1/2}\right) \frac{v}{g\left(C^{n+1/2}\right)} \, d\Gamma \\ &\quad - \int_\Omega \varphi \left(C^{n+1/2}\right) \cdot \nabla \frac{v}{g\left(C^{n+1/2}\right)} \, d\Omega\end{aligned}$$

Differentiation in the last integral is handled as

$$\nabla \frac{v}{g\left(C^{n+1/2}\right)} = \frac{g\left(C^{n+1/2}\right) \frac{\partial}{\partial x}(v) - v \frac{\partial}{\partial x} g\left(C^{n+1/2}\right)}{g\left(C^{n+1/2}\right)^2}$$

where

$$\frac{\partial}{\partial x} g\left(C^{n+1/2}\right) = \frac{1}{2}\left(\left.\frac{\partial g}{\partial C}\right|_{C^{n+1}} \left.\frac{\partial C}{\partial x}\right|_{C^{n+1}} + \left.\frac{\partial g}{\partial C}\right|_{C^n} \left.\frac{\partial C}{\partial x}\right|_{C^n} \right)$$

Note the evaluation of the integral

$$\int_\Omega \nabla \cdot \varphi \left(\frac{C^{n+1} + C^n}{2}\right) \left(\frac{v}{g\left(\frac{C^{n+1}+C^n}{2}\right)}\right) d\Omega$$

depends on whether $\nabla \cdot \mathbf{u} = 0$ is enforced.

1.4 Alternative Midpoint Method

Alternatively, discretize in time first, then in space. Discretizing in time gives

$$C^{n+1} = C^n + \Delta t \frac{1}{g\left(\frac{C^{n+1}+C^n}{2}\right)} \nabla \cdot \varphi \left(\frac{C^{n+1} + C^n}{2}\right)$$

which can be rearranged as

$$g\left(\frac{C^{n+1} + C^n}{2}\right)\left(C^{n+1} - C^n\right) - \Delta t \nabla \cdot \varphi \left(\frac{C^{n+1} + C^n}{2}\right).$$

Now discretize in space to obtain

$$\left(g\left(\frac{C^{n+1} + C^n}{2}\right)\left(C^{n+1} - C^n\right), v\right) - \Delta t \left(\nabla \cdot \varphi \left(\frac{C^{n+1} + C^n}{2}\right), v\right) \qquad (18)$$

This removes the nonlinearity from the integration by parts of the flux term. The scheme can be linearized using an approximation for C^{n+1} in the nonlinear evaluation $g\left(\dfrac{C^{n+1} + C^n}{2}\right)$.