Notes on Deriving Coefficients for Advection Diffusion Crank Nicolson Solver*

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1 Advection Diffusion Equation

We are interested in solving the Advection Diffusion equation

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) - \nabla \cdot (c\vec{v}) + R \tag{1}$$

with zero-flux boundaries. The three terms on the right hand side correspond to diffusive flux, convective flux, and a source term. The Finite Volume Method (FVM) approach is particularly suitable to this problem since it easily allows to set the zero-flux boundary condition. We also assume that the concentrations are known at cell centers, since this way the faces of the control volume also correspond to the domain boundaries.

1.1 Crank-Nicolson Scheme

We take volume and time integral of both sides,

$$\begin{aligned}
\int_V \int_{t_0}^{t_0+\Delta t} \frac{\partial c}{\partial t} dt dV &= \int_{t_0}^{t_0+\Delta t} \int_V \nabla \cdot (D\nabla c - c\vec{v}) + R dV dt \\
\left(c^{t_0+\Delta t} - c^{t_0}\right) \Delta V &= \int_{t_0}^{t_0+\Delta t} \left[\int_S (D\nabla c - c\vec{v}) \cdot \hat{n} dA + \int_v R dV \right] dt
\end{aligned}$$

Where the right side was rewritten using the divergence theorem. Next, we need to find a way to integrate the time integral on the right hand side. With the finite time discretization, we can approximate it using one of the following three options:

$$\begin{aligned}
\int_{t_0}^{t_0+\Delta t} u dt &\sim u^{t_0} \Delta t && \text{Forward Euler} \\
&\sim u^{t_0+\Delta t} \Delta t && \text{Backward Euler} \\
&\sim 0.5 \left(u^{t_0} + u^{t_0+\Delta t}\right) \Delta t && \text{Crank-Nicolson}
\end{aligned}$$

In addition, in the finite volume approach, we rewrite the surface integral as a summation over the four sides of our 2D control "volume" (the computational cell). Also, we label the current time t_0 with subscript k and the next time step with subscript $k+1$. We obtain

$$\left(c^{k+1} - c^k\right) \Delta V = 0.5 \left[\sum_{i=1}^{4} \left(D\nabla c^k - c^k \vec{v}^k\right) \cdot \hat{n} \Delta A + \sum_{i=1}^{4} \left(D\nabla c^{k+1} - c^{k+1} \vec{v}^{k+1}\right) \cdot \hat{n} \Delta A + \left(R^k + R^{k+1}\right) \Delta V \right] \Delta t$$

The Crank-Nicolson formulation leads to an implicit method, since values at the $k+1$ are required to advance to the $k+1$ step. Our goal is to write the system in a matrix form,

$$\mathbf{A} c^{k+1} = \mathbf{B} c^k + 0.5 \left(R^{k+1} + R^k\right) \tag{2}$$

*See `http://www.particleincell.com/blog/2014/advection-diffusion/`

where R is a source term that is assumed to be known at time $k+1$. Moving all $k+1$ terms to the left side, we have

$$c^{k+1} - \frac{\Delta t}{2\Delta x \Delta y}\left[\sum_{i=1}^{4}\left(D\nabla c^{k+1} - c^{k+1}\vec{v}^{k+1}\right)\cdot\hat{n}\Delta A\right] = c^k + \frac{\Delta t}{2\Delta x\Delta y}\left[\sum_{i=1}^{4}\left(D\nabla c^k - c^k\vec{v}^k\right)\cdot\hat{n}\Delta A\right] + \frac{\Delta t}{2}\left(R^k + R^{k+1}\right)$$

This is

$$\left(\mathbf{I} - \mathbf{M^{k+1}}\right)c^{k+1} = \left(\mathbf{I} + \mathbf{M^k}\right)c^k + 0.5\left(R^{k+1} + R^k\right) \tag{3}$$

1.2 Finite Volume Numerical Discretization

For a Cartesian cell, we simply need to evaluate the surface integral (the sum) over the East, North, West, and South face. We use the standard central difference for the divergence, and approximate convective fluxes as the average of the neighbor cells. The $(D\nabla c - \vec{v}c)\cdot\hat{n}\Delta A$ term then evaluates as follows

East	$\left(\frac{D}{\Delta x}\left(c_{i+1,j} - c_{i,j}\right) - \frac{1}{2}\left(c_{i+1,j}u_{i+1,j} + c_{i,j}u_{i,j}\right)\right)\Delta y$
North	$\left(\frac{D}{\Delta y}\left(c_{i,j+1} - c_{i,j}\right) - \frac{1}{2}\left(c_{i,j+1}v_{i,j+1} + c_{i,j}v_{i,j}\right)\right)\Delta x$
West	$-\left(\frac{D}{\Delta x}\left(c_{i,j} - c_{i-1,j}\right) - \frac{1}{2}\left(c_{i,j}u_{i,j} + c_{i-1,j}u_{i-1,j}\right)\right)\Delta y$
South	$-\left(\frac{D}{\Delta y}\left(c_{i,j} - c_{i,j-1}\right) - \frac{1}{2}\left(c_{i,j}v_{i,j} + c_{i,j-1}v_{i,j-1}\right)\right)\Delta x$

The above terms are multiplied by $\Delta t/(2\Delta x\Delta y)$, and we can simplify the coefficient equations using the following terms $\alpha_x = D\Delta t/(2\Delta^2 x)$, $\alpha_y = D\Delta t/(2\Delta^2 y)$, $\beta_x = \Delta t/(4\Delta x)$, $\beta_y = \Delta t/(4\Delta y)$, and $\gamma = \Delta t/2$. We then have the following coefficients for the $\mathbf{M}$ matrix:

East: $\alpha_x c_{i+1,j} - \alpha_x c_{i,j} - \beta_x c_{i+1,j}u_{i+1,j} - \beta_x c_{i,j}u_{i,j}$
North: $\alpha_y c_{i,j+1} - \alpha_y c_{i,j} - \beta_y c_{i,j+1}v_{i,j+1} - \beta_y c_{i,j}v_{i,j}$
West: $-\alpha_x c_{i,j} + \alpha_x c_{i-1,j} + \beta_x c_{i,j}u_{i,j} + \beta_x c_{i-1,j}u_{i-1,j}$
South: $-\alpha_y c_{i,j} + \alpha_y c_{i,j-1} + \beta_y c_{i,j}v_{i,j} + \beta_y c_{i,j-1}v_{i,j-1}$

By collecting terms, we can write the contributions to the $\mathbf{B}$ matrix:

	Center	East	North	West	South
$c_{i,j}$	1	$-\alpha_x - \beta_x u_{i,j}$	$-\alpha_y - \beta_y v_{i,j}$	$-\alpha_x + \beta_x u_{i,j}$	$-\alpha_y + \beta_y v_{i,j}$
$c_{i+1,j}$		$\alpha_x - \beta_x u_{i+1,j}$			
$c_{i,j+1}$			$\alpha_y - \beta_y v_{i,j+1}$		
$c_{i-1,j}$				$\alpha_x + \beta_x u_{i-1,j}$	
$c_{i,j-1}$					$\alpha_y + \beta_y v_{i,j-1}$

and similarly for the $\mathbf{A}$ matrix (note, velocities here are at time $k+1$):

	Center	East	North	West	South
$c_{i,j}$	1	$\alpha_x + \beta_x u_{i,j}$	$\alpha_y + \beta_y v_{i,j}$	$\alpha_x - \beta_x u_{i,j}$	$\alpha_y - \beta_y v_{i,j}$
$c_{i+1,j}$		$-\alpha_x + \beta_x u_{i+1,j}$			
$c_{i,j+1}$			$-\alpha_y + \beta_y v_{i,j+1}$		
$c_{i-1,j}$				$-\alpha_x - \beta_x u_{i-1,j}$	
$c_{i,j-1}$					$-\alpha_y - \beta_y v_{i,j-1}$

1.3 Boundary Conditions

There are two types of boundary conditions applicable to the advective-convective equation: specified concentration, and specified normal flux. The specified concentration simply prescribes the value of c along the Dirichlet boundary, $c = g(s) \in \Gamma_D$. The specified flux boundary is derived as $(j_{advective} + j_{diffusive})\cdot\hat{n} \equiv (c\vec{v} - D\nabla c)\cdot\hat{n} = h(s) \in \Gamma_R$. Specifically for the zero flux boundary, we have $(c\vec{v} - D\nabla c)\cdot\hat{n} = 0$. Specifying this boundary condition in the finite volume method is easy - we simply don't include the terms for the zero-flux faces.

1.4 Numerical Implementation

The demo code can be seen at `http://www.particleincell.com/blog/2014/advection-diffusion/`. The penta-diagonal matrices are replaced with vectors, such that $(i,j) = a_0$, $(i-1,j) = a_1$, $(i+1,j) = a_2$, $(i,j-1) = a_3$, $(i,j+1) = a_4$. Mapping from (i,j) to u is performed via $u \equiv j\cdot \mathrm{ni} + i$