Setting up ADR

October 22, 2015

Let us begin with $d=1$ for simplicity. We want to solve

$$\boxed{\frac{Df}{Dt} = D(f)\nabla^2 f + R(f)}$$

Expanding the material derivative,

$$\frac{\partial f}{\partial t} + (\vec{v}\cdot\nabla)f = D(f)\nabla^2 f + R(f)$$

$$\therefore \boxed{\frac{\partial f}{\partial t} = -(\vec{v}\cdot\nabla)f + D(f)\nabla^2 f + R(f)}$$

In 1d,

$$\frac{\partial f}{\partial t} = -V_x \frac{\partial}{\partial x} f + D(f)\frac{\partial^2 f}{\partial x^2} + R(f)$$

To make life more exciting, let's let V_x be a function of x.

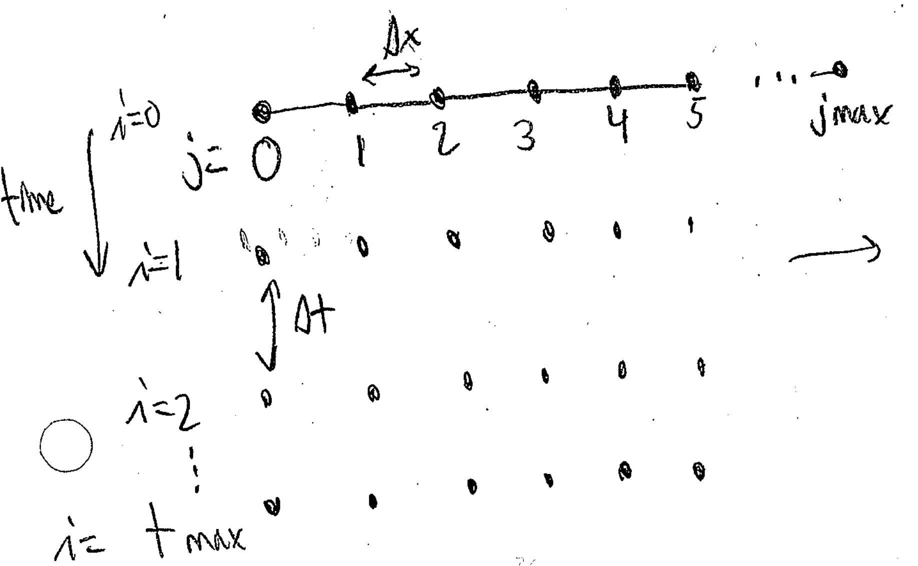
$$\therefore \boxed{\frac{\partial f}{\partial t} = -V_x(x)\frac{\partial}{\partial x} f + D(f)\frac{\partial^2 f}{\partial x^2} + R(f)}$$

Things would be more interesting if there was an interplay between $\vec{v}$ and f. But, let us not do that for simplicity.

Let's play with Fisher waves... Sooo,

$$\boxed{\frac{\partial f}{\partial t} = -V_x(x)\frac{\partial}{\partial x}f + D\frac{\partial^2 f}{\partial x^2} + sf(1-f)}$$

Generally, we set $V_x(x)=0$. for simplicity, since we are in 1d, $V(x)=0$. Now to discretize in an intelligent manner... let's use finite difference. Let's set up our 1d grid... we'll use periodic BC's.



$$\rightarrow \boxed{x = j\cdot\Delta x}$$

$$\rightarrow \boxed{t = i\cdot\Delta t}$$

We will use Crank-Nicolson. This is a semi-implicit technique for stepping time forwards. Right? Our equation is

$$\frac{\partial f}{\partial t} = Lf = \left[-V_x(x)\frac{\partial}{\partial x} + D\frac{\partial^2}{\partial x^2} + s(1-f)\right]f$$

Crank-Nicholson states, treating everything semi-implicitly,

$$\boxed{f_j^{i+1} = f_j^i + \Delta t\left[\frac{1}{2}Lf_j^i + \frac{1}{2}Lf_j^{i+1}\right]}$$

We can rewrite this as

$$f(t+\Delta t) = f(t) + \frac{\Delta t}{2}\left[Lf(t) + L' f(t+\Delta t)\right]$$

or

$$\boxed{f(t+\Delta t) = f(t) + \frac{\Delta t}{2} L \left[f(t) + f(t+\Delta t)\right]}$$

We need to be <u>extremely</u> <u>careful</u> here. We know that

$$\boxed{L = -V_x(x)\frac{\partial}{\partial x} + D\frac{\partial^2}{\partial x^2} + s[1-f(t)]}$$

So that $Lf(t)$ has the correct form. We <u>must</u> be careful, as $L f(t+\Delta t)$ will then create a nonlinear disaster, as we will find $\boxed{s[1-f(t)]f(t+\Delta t)}$ which will be extremely difficult to deal with. Hence, we will only use Crank-Nicholson on the diffusion term. We discretize terms by

1) $$-v(x)\frac{\partial f}{\partial x} = -V_j^i\left[\frac{f_{j+1}^i - f_{j-1}^i}{2\Delta x}\right] = \frac{-V_j^i}{2\Delta x}\left[f_{j+1}^i - f_{j-1}^i\right]$$

$$\therefore \boxed{\left[-v(x)\frac{\partial}{\partial x}\right]_{rc} = \frac{-V_r}{2\Delta x}\left[\delta_{r,c+1} - \delta_{r,c-1}\right] = \underset{\sim}{A}}$$

ii) $D\frac{\partial^2 f}{\partial x^2} = D\left[\frac{f_{j+1} - 2f_j + 2f_{j-1}}{\Delta x^2}\right]$

$$\therefore \boxed{\left[D\frac{\partial^2}{\partial x^2}\right]_{rc} = \frac{D}{\Delta x^2}\left[\delta_{r,c+1} - 2\delta_{r,c} + 2\delta_{r,c-1}\right] = \underset{\approx}{\xi}}$$

iii) $S[1-f]f = S[f - f^2] = Sf - Sf^2$

↳ We break this into two parts.

a) $Sf = (S\underset{\approx}{I})f$

b) $-Sf^2 = \ldots$ outer product?

There is no simple representation here due to nonlinearity. Therefore,

$$\boxed{S[1-f]f = S[1-f_j]f_j = \underset{\sim}{G}(\underset{\sim}{f})}$$

↳ It's a column vector

~~Our equation then becomes, in shorthand,~~

$$\cancel{\underset{\sim}{f}_j^{\,i+1} = f_j^i + \Delta t \sum_z A_{jz} f_z^i + \frac{\Delta t}{2}\left[\sum_z \underset{\sim}{\xi}_{jz} f_z^i + \sum_z \underset{\sim}{\xi}_{jz} f_z^{i+1}\right] + \Delta t\, s\left[1-f_j^i\right] f_j^i}$$

Therefore,

$$\boxed{\underset{\sim}{f}^{\,i+1} = \underset{\sim}{f}^{\,i} + \Delta t\, \underset{\approx}{A}\, \underset{\sim}{f}^{\,i} + \frac{\Delta t}{2}\left[\underset{\approx}{\xi}\, \underset{\sim}{f}^{\,i} + \underset{\approx}{\xi}\, \underset{\sim}{f}^{\,i+1}\right] + \Delta t\, \underset{\approx}{G}(\underset{\sim}{f_i})}$$

We can manipulate this and solve; not too bad.

$$\underset{\sim}{f}^{\,i+1} - \frac{\Delta t}{2}\underset{\approx}{\xi}\, \underset{\sim}{f}^{\,i+1} = \underset{\sim}{f}^{\,i} + \Delta t\, \underset{\approx}{A}\, \underset{\sim}{f}^{\,i} + \frac{\Delta t}{2}\underset{\approx}{\xi}\, \underset{\sim}{f}^{\,i} + \Delta t\, \underset{\approx}{G}(\underset{\sim}{f_i})$$

$$\left(\underset{\approx}{I} - \frac{\Delta t}{2}\underset{\approx}{\xi}\right)\underset{\sim}{f}^{\,i+1} = \left(\underset{\approx}{I} + \Delta t\, \underset{\approx}{A} + \frac{\Delta t}{2}\underset{\approx}{\xi}\right)\underset{\sim}{f}^{\,i} + \Delta t\, \underset{\sim}{G}(\underset{\sim}{f_i})$$

Our solution is thus

$$\boxed{\underset{\sim}{f}^{\,i+1} = \left[\underset{\approx}{I} - \frac{\Delta t}{2}\underset{\approx}{\xi}\right]^{-1}\left\{\left(\underset{\approx}{I} + \Delta t\, \underset{\approx}{A} + \frac{\Delta t}{2}\underset{\approx}{\xi}\right)\underset{\sim}{f}^{\,i} + \Delta t\, \underset{\approx}{G}(\underset{\sim}{f_i})\right\}}$$

We now need to implement this.

Note that if we want to also use Crank-Nickelson on advection, we can just do

$$\underset{\sim}{f}^{n+1} = \left[\underset{\approx}{I} - \frac{\Delta t}{2} \underset{\approx}{\xi} - \frac{\Delta t}{2} \underset{\approx}{A} \right]^{-1} \left\{ \left(\underset{\approx}{I} + \frac{\Delta t}{2} \underset{\approx}{A} + \frac{\Delta t}{2} \underset{\approx}{\xi} \right) \underset{\sim}{f}^{n} + \Delta t \, \underset{\sim}{G}(\underset{\sim}{f}^{n}) \right\}$$

2D-ADR

What changes in 2D? We basically do the same thing. The issue here is how to map our operators to 2D... everything can be done via matrix multiplication as discussed in class. We just have to be clever how we do this, as f_{ij}^{k} is effectively 2d now, but we can be clever and map this into a 1d matrix problem.

Our equation is, in 2d, assuming D is constant but $\vec{v}$ changes, and we are using a logistic-growth reaction term,

$$\boxed{\frac{\partial f(x,y)}{\partial t} = -\left(\vec{v}[x,y] \cdot \nabla\right) f(x,y) + D\nabla^2 f + sf(1-f)}$$

So really, we just have to understand how the advection and diffusion operators change as we increase dimensionality. Let's work through them.

Let $\boxed{\vec{v} = u\hat{x} + v\hat{y}}$

advection

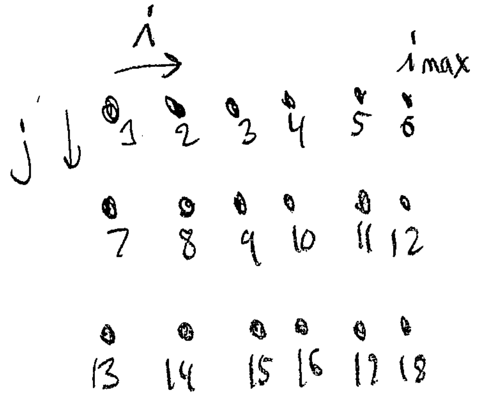
$$-\left[\vec{v}(x,y) \cdot \nabla\right] f(x,y)$$

$$= -\left[v_x(x,y)\frac{\partial}{\partial x} + v_y(x,y)\frac{\partial}{\partial y}\right] f(x,y)$$

$$= v_x(x,y)\frac{\partial}{\partial x} f(x,y) + v_y(x,y)\frac{\partial f(x,y)}{\partial y}$$

$$= u_{ij}\left[\frac{f_{i+1,j} - f_{i-1,j}}{2\Delta x}\right] + v_{ij}\left[\frac{f_{i,j+1} - f_{i,j-1}}{2\Delta y}\right]$$

But the question is, how do we convert this into a matrix multiply as discussed in class? Let's look at a simple example.



If we use an intuitive numerical ordering, logical index

$$\boxed{Q = j \cdot i_{max} + i}$$

More generally, we can get the logical index via a function $\boxed{\bar{Q}(i,j) = Q_{ij}}$ for simplicity

I see. So to get logical index corresponding to $f_{i+1,j}$, we can use $f_{Q(i+1,j)}$. We can make a computer do the lookup for us. Therefore, based on what we have wrote,

$$\underset{\approx}{A} = \left[\vec{V}(x,y)\cdot\nabla\right]$$

Take the element at $Q_{i+1,j}$

$$\boxed{\underset{\approx}{A}_{ij} = u_{Q_{ij}}\left[\frac{Q_{i+1,j} - Q_{i-1,j}}{2\Delta x}\right] + v_{Q_{ij}}\left[\frac{Q_{i,j+1} - Q_{i,j-1}}{2\Delta y}\right]}$$

This is it! Cool. Actually, not quite... in matrix form, how do we take the element at $Q_{i+1,j}$? $Q_{i+1,j}$ returns the logical index... also remember that this matrix is acting on element $f_{Q_{ij}}$. Don't forget that. Ah, the row is then Q_{ij}.

The column to grab is the other Q. Therefore,

$$\underset{\approx}{A}_{ij} = u_{Q_{ij}} \left[\frac{\delta_{Q(i,j),\, Q(i+1,j)} - \delta_{Q(i,j),\, Q(i-1,j)}}{2\Delta x} \right] + v_{Q_{ij}} \left[\frac{\delta_{Q(i,j),\, Q(i,j+1)} - \delta_{Q_{ij},\, Q(i,j-1)}}{2\Delta y} \right]$$

For simplicity, we will express $\boxed{Q_{ij} = Q(i,j) = \{i,j\}}$. Rewriting $\underset{\approx}{A}_{ij}$,

row column

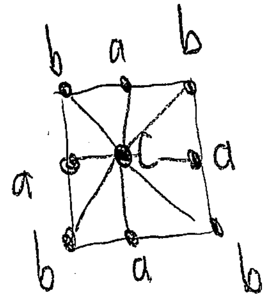
$$\boxed{\begin{aligned} \underset{\approx}{A}_{ij} = {} & u_{\{ij\}} \left[\frac{\delta_{\{i,j\},\{i+1,j\}} - \delta_{\{i,j\},\{i-1,j\}}}{2\Delta x} \right] \\ & + v_{\{ij\}} \left[\frac{\delta_{\{i,j\},\{i,j+1\}} - \delta_{\{i,j\},\{i,j-1\}}}{2\Delta y} \right] \end{aligned}}$$

We just need to do this for the diffusion operator, then we are good.

The diffusion operator is

$$\boxed{\underset{\sim}{\xi} = D\nabla^2 f}$$

There are different ways to handle a Laplacian, as discussed in class. We will take a 2d isotropic stencil,



where $\boxed{a = \frac{4}{36}}$, $\boxed{b = \frac{1}{36}}$, $\boxed{c = \frac{-20}{36}}$

In other words,

$$\boxed{\begin{aligned} \underset{\sim}{\xi} = D\Big[& b\left(f_{i+1,j+1} + f_{i+1,j-1} + f_{i-1,j-1} + f_{i-1,j+1}\right) \\ & + a\left(f_{i,j+1} + f_{i+1,j} + f_{i,j-1} + f_{i-1,j}\right) \\ & + c\, f_{i,j} \Big] \end{aligned}}$$

We will write out the operator on the next page. The diffusion operator then becomes

$$\boxed{\underset{\approx}{\xi}_{ij} = \Big[b\left(\delta_{\{i,j\}\{i+1,j+1\}} + \delta_{\{i,j\}\{i+1,j-1\}} \; \delta_{\{i,j\}\{i-1,j-1\}} + \delta_{\{i,j\}\{i-1,j+1\}}\right) + a\left(\delta_{\{i,j\}\{i,j+1\}} + \delta_{\{i,j\}\{i+1,j\}} + \delta_{\{i,j\}\{i,j-1\}} + \delta_{\{i,j\}\{i-1,j\}}\right) + c\,\delta_{i,j} \Big]}$$

This looks ~ right. But, what about the self/c-term? Won't $\delta_{\{i,j\},\{i,j\}}$ always be one, regardless of i and j? Yeah... am I doing this right? No I don't think so. I think we need both a row and column operator... we'll have to think about this... ah, well, if it's operating on itself, it should be on the diagonal, so δ_{ij}, regardless of the indexing.

Great. I think that's it! We take our new operators and plug them into

$$\boxed{\underset{\sim}{f}^{i+1} = \left[\underset{\approx}{I} - \frac{\Delta t}{2}\underset{\approx}{\xi} - \frac{\Delta t}{2}\underset{\approx}{A}\right]^{-1} \left\{ \left(\underset{\approx}{I} + \frac{\Delta t}{2}\underset{\approx}{A} + \frac{\Delta t}{2}\underset{\approx}{\xi}\right)\underset{\sim}{f}^{i} + \Delta t\, \underset{\sim}{G}(\underset{\sim}{f}^{i}) \right\}}$$

I definitely messed up ξ_{ij}, however, we need Δx and Δy everywhere. Let's rewrite on the next page... otherwise the units don't even work.

Rewriting ξ_{ij} with correct units,

$$\boxed{\begin{aligned}\underset{\sim}{\xi_{ij}} = 0 \Bigg[& \frac{b}{\Delta x \Delta y}\left(\delta\{ij\}\{i+1,j+1\} + \delta\{ij\}\{i+1,j-1\} + \delta\{ij\}\{i-1,j-1\} + \delta\{ij\}\{i-1,j+1\}\right) \\ & + a\left(\frac{\delta\{ij\}\{i,j+1\}}{\Delta y^2} + \frac{\delta\{ij\}\{i+1,j\}}{\Delta x^2} + \frac{\delta\{ij\}\{i,j-1\}}{\Delta y^2} + \frac{\delta\{ij\}\{i-1,j\}}{\Delta x^2}\right) \\ & + C\,\frac{\delta_{i,j}}{\Delta_{grid}^2} \Bigg]\end{aligned}}$$

Where $\boxed{a = \frac{4}{36}}$, $\boxed{b = \frac{1}{36}}$, $\boxed{C = -\frac{20}{36}}$. This looks correct. Wait, what about the units on C? Crap... Is that a mess?

Yes. Blehhhhhhh. Well, thankfully, we know the sum of all terms must be zero... let's use that. Let $\boxed{C = \alpha \tilde{C}}$

$$\therefore \frac{4b}{\Delta x \Delta y} + \frac{2a}{\Delta y^2} + \frac{2a}{\Delta x^2} + C = 0$$

$$\therefore \boxed{C = -\left(\frac{4b}{\Delta x \Delta y} + \frac{2a}{\Delta y^2} + \frac{2a}{\Delta x^2}\right)}$$