Solving RAD Equations Edit

How do we solve a reaction-advection-diffusion equation numerically? As an example, we'll deal with a multicomponent biological/physical model

$$\frac{\partial}{\partial t}b_i + u\frac{\partial}{\partial x}b_i = \kappa\nabla^2 b_i + \mathcal{B}_i(b_1, b_2, ..., \mathbf{x}, t)$$

where $\mathcal{B}$ is a nonlinear function expressing the interchanges of biomass or quantity of nutrient between the various components b_i.

Time-stepping Edit

Test version.

First of all, how do we solve a set of ODE's (e.g., if b_i is independent of $\mathbf{x}$)

$$\frac{d}{dt}b_i = \mathcal{B}_i(\mathbf{b}, t)$$

Euler step Edit

testing save stuff

The simplest approach is an Euler step which uses Taylor expansion

$$b_i(t + dt) = b_i(t) + \mathcal{B}_i(\mathbf{b}(t), t)dt + \mathcal{O}(dt^2)$$

The Lotka-Volterra example shows why this approach is not generally useful: it has a bias and, as you can see by experimenting , the convergence is very slow.

The bias can be understood by considering

$$\frac{d}{dt}X = V \quad , \quad \frac{d}{dt}V = -X$$

The Euler step has

$$X^2(t + dt) + V^2(t + dt) = [X^2(t) + V^2(t)](1 + dt^2)$$

so that the energy increases steadily with time whereas the ODE's have

$$\frac{d}{dt}[X^2 + V^2] = 0$$

Leapfrog Edit

So we consider various higher order schemes. The Leapfrog method is based on a second order time derivative

$$b(t + dt) - b(t - dt) = 2\ dt\ \mathcal{B}(\mathbf{b}(t), t) + \mathcal{O}(dt^3)$$

but is subject to an alternating step instability . Try resolving it by adding 95% of the leapfrog and 5% of an Euler step or by doing an Euler step every 20 steps.

Exercise: Convert to a second order Adams-Bashforth scheme

$$b(t + dt) = b(t) + dt\ \mathcal{B}(1.5\mathbf{b}(t) - 0.5\mathbf{b}(t - dt), t + dt/2)$$

by using the saved values of $\mathbf{b}$ differently. You can start with an Euler step.

Runge-Kutta Edit

Runge-Kutta schemes require multiple function evaluations per step. We can think of this as making an estimate of **b** at some point between t and $t + dt$ and then using this to estimate the derivative there. The final step is based on an average of two derivative values:

$$\begin{aligned}\hat{b}_i &= b_i(t) + \alpha dt \mathcal{B}_i(\mathbf{b}(t), t) \\ b_i(t+dt) &= b_i(t) + (1-\beta) dt \mathcal{B}_i(\mathbf{b}(t), t) + \beta dt \mathcal{B}_i(\hat{b}, t + \alpha dt)\end{aligned}$$

which matches the function and the first and second derivatives when $\alpha\beta = 1/2$. We've looked at $\alpha = 1/2$, $2/3$, and 1 corresponding to $\beta = 1$, $3/4$, and $1/2$; the results are pretty similar. The case with $\alpha = 1/2$ is pretty intuitive: the step in b_i is equal to dt times the average derivative in the interval $[t, t + dt]$. We can make a better estimate of the average derivative than using the value at time t by looking at it half way (at $t + dt/2$). The first half step gives an approximation to the value of $b_i(t + dt/2)$ which we use to estimate the derivative $\mathcal{B}_i(\tilde{\mathbf{b}}, t + dt/2)$ and then advance b_i by dt times this estimate of the average derivative. The $\alpha = 1$ case means we're calculating the derivative by averaging the value at t and an estimate of the value at $t + dt$; I usually use this version.

Adams-Bashforth Edit

Adams-Bashforth methods keep a history of the previous $\mathcal{B}_i$ values (unlike the leapfrog method which keeps the b_i) to make a better estimate at the new time step.

$$b_i(t+dt) = b_i(t) + dt\big[\alpha \mathcal{B}_i(\mathbf{b}(t), t) + \beta \mathcal{B}_i(\mathbf{b}(t-dt), t-dt)\big]$$

Taylor-expanding each side using

$$\frac{d}{dt}\frac{d\,b_i}{dt} = \frac{d}{dt} B_i(\mathbf{b}(t), t) = \frac{\partial B_i}{\partial t} + \frac{\partial B_i}{\partial b_j}\frac{\partial b_j}{\partial t}$$

gives

$$\begin{gathered} b_i(t) + dt\frac{d\,b_i}{dt} + \frac{1}{2}dt^2\frac{d^2 b_i}{dt^2} = \\ b_i(t) + dt\mathcal{B}_i + \frac{1}{2}dt^2\left[\frac{\partial \mathcal{B}_i}{\partial t} + \frac{\partial \mathcal{B}_j}{\partial b_j}\frac{\partial b_j}{\partial t}\right] = \\ b_i + dt(\alpha+\beta)\mathcal{B}_i - dt^2\beta\left[\frac{\partial \mathcal{B}_i}{\partial t} + \frac{\partial \mathcal{B}_j}{\partial b_j}\frac{\partial b_j}{\partial t}\right] \end{gathered}$$

Therefore $\alpha + \beta = 1$. $\beta = -\frac{1}{2}$, $\alpha = \frac{3}{2}$. The dt^3 terms will not match up; this is a second order scheme.

Alistair Adcroft (primary numerical analyst for the MITgcm) recommends a version of the Adams-Bashforth based, like the leapfrog method on a history of **b**. The second order scheme is

$$\begin{aligned} b_i(t+dt) &= b_i(t) + \mathcal{B}_i(\hat{\mathbf{b}}(t+dt/2), t+dt/2)dt \\ \hat{\mathbf{b}}(t+dt/2) &= \frac{3}{2}\mathbf{b}(t) - \frac{1}{2}\mathbf{b}(t-dt) \end{aligned}$$

For a different set, try

$$\begin{aligned} \frac{\partial}{\partial t}P &= \mu\frac{PN}{N+k_s} - g\frac{ZP}{P+P_0} - d_pP \\ \frac{\partial}{\partial t}Z &= ag\frac{ZP}{P+P_0} - d_zZ \end{aligned}$$

with $\mu = 0.01$, $N = N_T - P - Z$, $N_T = 5$, $k_s = 0.1$, $P_0 = 0.5$, $g = 0.1$, $a = 1$, $d_p = 0$, $d_z = 0.08$. Comparison is RK4, $dt = 1/8$.

Spatial derivatives Edit

The spatial derivative terms can be approximated by finite differences, finite elements, or spectral schemes. Finite differences are the simplest. We consider the flux form

$$\frac{\partial}{\partial t} b = -\frac{\partial}{\partial x} J \quad , \quad J = ub - \kappa \frac{\partial}{\partial x} b$$

and use a "staggered grid" which has b values in the center of the boxes and J values on the faces. In one dimension, this looks like

$$\begin{array}{c} | - - b(x_{i-1}) - - | - - b(x_i) - - | - - b(x_{i+1}) - - | \\ J(x_{i-1.5}) \qquad J(x_{i-0.5}) \qquad J(x_{i+0.5}) \qquad J(x_{i+1.5}) \end{array}$$

so that

$$\frac{\partial}{\partial t} b(x_i) = -\left[J(x_{i+0.5}) - J(x_{i-0.5}) \leq dx \right]$$

The advantage is that we account for all the material: flux out of one box automatically enters another.

Centered Edit

To evaluate the flux, we again use centered differences for the diffusion term and try a centered difference for the advection term also: we estimate $b(x_{i+0.5}) \simeq \frac{1}{2} b(x_i) + \frac{1}{2} b(x_{i+1})$

$$J(x_{i+0.5}) = u \left[\frac{b(x_i) + b(x_{i+1})}{2} \right] - \kappa \left[\frac{b(x_{i+1}) - b(x_i)}{dx} \right]$$

Upwind Edit

The upwind scheme uses

$$J(x_{i+0.5}) = \begin{cases} ub(x_i) & u > 0 \\ ub(x_{i+1}) & u < 0 \end{cases}$$

i.e., we flux material out of the box which is upwind of the face.

The fourth order scheme uses a cubic polynomial fit to two points to the left and two to the right, while the third order upwind uses two upwind and one downwind point. The estimate of $b(x_{i+0.5})$ is multiplied by the appropriate u.

CFL Edit

All of these schemes are subject to the "CFL" condition. The upwind scheme is simplest to analyze. Consider beginning with b nonzero only at a single point. One time step later

$$b(x_i) = b_0 (1 - \frac{u\,dt}{dx}) \quad , \quad b(x_{i+1}) = b_0 \frac{u\,dt}{dx}$$

Clearly, we have a problem if $u\,dt/dx > 1$. In essence, more tracer is fluxed out of the box in one step than is present there to begin with. So you get b values outside the range of the initial values; this is not physical, and the errors will grow exponentially. Try it in the earlier examples.

Positivity Edit

Keeping b positive is also a problem; it works for upwind differencing but not other forms. In the case of centered differences, we will have

$$\begin{aligned} b(x_{i-1}) &= b_0 \frac{dt}{dx} (-\frac{u}{2} + \frac{\kappa}{dx}) \\ b(x_i) &= b_0 (1 - \frac{2\kappa dt}{dx^2}) \\ b(x_{i+1}) &= b_0 \frac{dt}{dx} (\frac{u}{2} + \frac{\kappa}{dx}) \end{aligned}$$

to maintain positivity, we need $u < 2\kappa/dx$ and $\kappa < dx^2/2dt$.

Flux correction Edit

Flux correction ensures that the fields remain positive, or, more generally, that new values will not exceed the range of values in the original cell and its neighbors.

Two-D Edit

The movie here shows an example.

1) Just to check, we also can load a MITCITE experiment , which should bring up the usual stuff. This is a local case.
2) We can also have remotely run cases such as this: the MITGCM can be used to explore the problem in more detail. The GCM Example xx shows a simulation of the release of a cylinder of heavier water.
3) Regular URL's such as this one for my seminar should work, as should IDV examples.