Notes on Adams-Bashforth and implicit method used in GS2

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February 17, 2001

This short note describes how Dorland implemented the nonlinear terms in the nonlinear gyrokinetic continuum code GS2. Consider a governing equation of the form

$$\frac{\partial f}{\partial t} = -iLf - iN(\Phi, f) \tag{1}$$

where L is some linear integro-differential operator, and N is the nonlinear operator. (I wrote the operators with i's out front, so that for a simple convection or wave problem the eigenvalues of L are real numbers $\omega_k = kv$, which simplifies later numerical stability analysis.)

When Dorland and Liu first put nonlinear terms into GS2, they used a straightforward predictor-corrector method (described later). Dorland then tried alternate algorithms, and eventually settled on a second-order Adams-Bashforth treatment of the nonlinear terms. The resulting algorithm is just

$$\frac{f_{j+1} - f_j}{\Delta t} = -iL\frac{f_{j+1} + f_j}{2} - i\frac{3N_j - N_{j-1}}{2} \tag{2}$$

where $N_j = N(\Phi_j, f_j)$ is the nonlinear term evaluated at the j'th time step, and N_{j-1} is the stored value of the nonlinear term from the previous time step. Note that this is essentially using an estimate of the nonlinear term evaluated at the half time step $N_{j+1/2} \approx N_j + 0.5(N_j - N_{j-1})$, as is needed to be second order accurate.

To write out more of the details of the solution, this is rearranged into the form:

$$f_{j+1} = (1 + i\Delta t L/2)^{-1} \left[(1 - i\Delta t L/2) f_j - i\Delta t(1.5N_j - N_{j-1})\right] \tag{3}$$

Because L is an integro-differential operator, there are some special tricks Kotschenreuther developed to invert the operator $(1 + \Delta t L/2)$ (see Kotschenreuther, Rewoldt, Tang, Comp. Phys. Comm. **88**, 128 (1995)). But however it is done, that inverse only needs to know about the linear operator L and doesn't need to know anything about the nonlinear operator N, which just appears as an inhomogeneous source term involving information from the j and $j-1$ time step and won't alter the implicit inversion algorithm for calculating fields at the $j+1$ time step.

In cases where the time-step $\delta t_{j+1/2} = t_{j+1} - t_j$ is dynamically changing in time, Eq.(2) should be written as

$$\frac{f_{j+1} - f_j}{\Delta t_{j+1/2}} = -iL\frac{f_{j+1} + f_j}{2} - i\left[N_j + \frac{\Delta t_{j+1/2}}{2}\left(\frac{N_j - N_{j-1}}{\Delta t_{j-1/2}}\right)\right] \tag{4}$$

I think this maintains the second-order accuracy with time step, though perhaps it should be double checked (I seem to recall that there are subtleties with variable grids sometimes...).

I could comment further here on some of the numerical properties of an Adams-Bashforth scheme. For example, because it requires information from previous time steps, its initialization is a little subtle. Sometimes people use a predictor-corrector step to give it a second-order-accurate initialization. But often people just use $f_{-1} = f_0$ as the initialization, which is only first-order accurate for the first few time steps. However, the errors quickly damp away to give second-order accuracy after a few time steps. This is because, when viewed as a two-step algorithm to determine (f_{j+2}, f_{j+1}) given (f_j, f_{j-1}), the Adams-Bashforth scheme is found to contain two modes: the desired physical mode with second order accuracy, and a "spurious mode". But this spurious mode is heavily damped and can be ignored as a small temporary transient which dissappears a few time steps after the initialization. The Adams-Bashforth method is used in a number of fluid dynamics codes, and it was used in a 2-D fluid/drift-wave turbulence code Stephen Smith got from Orszag's group.

1 predictor-corrector algorithm

Here we describe an earlier algorithm which Dorland used at first. He later switched to the Adams-Bashforth method described in the previous section. When Dorland and Liu first put nonlinear terms into GS2, they treated the nonlinear terms using a similar kind of predictor-corrector or 2-step Runge-Kutta algorithm as was used in the fully explicit gyrofluid code, but modified some to use GS2's implicit algorithm for linear terms. The resulting algorithm I believe started with a "predictor" step

$$\frac{\hat{f}_{j+1} - f_j}{\Delta t} = -iL\frac{\hat{f}_{j+1} + f_j}{2} - iN[\Phi_j, f_j] \tag{5}$$

to give a "predicted" value of f at the future time $j+1$, $\hat{f}_{j+1}$. By interpolating he then calculated $f_{j+1/2} = (\hat{f}_{j+1} + f_j)/2$, and then did a field solve to find $\Phi_{j+1/2}$. [Actually, there are variations where one interpolates $N_{j+1/2} = (\hat{N}_{j+1} + N_j)/2$, instead of separately interpolating the f and ϕ that go into N, and I don't know for sure which way GS2 did this in the earlier version of the code.] This was then followed by

$$\frac{f_{j+1} - f_j}{\Delta t} = -iL\frac{f_{j+1} + f_j}{2} - iN[\Phi_{j+1/2}, f_{j+1/2}] \tag{6}$$

to give a "corrected" value of f at the future time $j+1$. This is also a second-order accurate algorithm.