THE ORIGIN OF NOISE IN SEMI-LAGRANGIAN INTEGRATIONS.

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1. **INTRODUCTION**

Although the semi-Lagrangian semi-implicit (SLSI) discretization of the primitive meteorological equations has resulted in significant savings of CPU, achieving its full potential has been hampered by the intermittent appearance of non-meteorological oscillations; 'noise'. Over the years the sources of this noise have been isolated and solutions have been invented to eliminate or control them.

The most obvious culprit, which is examined in section 2b, is the explicit integration of the non-linear terms. A more subtle phenomenon, looked at in section 2c, is the numerical distortion of the resonance appearing in stationary solutions in response to orographic forcing. Another cause of noise, which we are just beginning to understand, is the extrapolation in time used in evaluating the departure point position in two time level integrations. This is discussed in section 2d. Lastly, a source of noise which is not unique to semi-Lagrangian integrations, the upper boundary condition, is discussed in section 2e.

The SLSI discretization gives us the freedom to use larger time steps than previously for the dynamics. This prompts the question: will the physical parameterization schemes be able to tolerate such large time steps? In order to see where dangers may lurk some simple differential equations, typical of those used in the physics, are discretized and integrated with 'large' time steps in section 3. In sections 3a and 3b it is demonstrated that sudden jumps in the values of fields can lead to instabilities or unphysical oscillations. Also, non-linear terms make large time step integrations even more problematic (section 3c).

Using large time steps raises questions about how to join the physics to the dynamics, and also about how to join the individual physics sub-processes to each other. Lack of balance between them can lead to noisy forecasts. These issues are discussed in sections 4a and 4b. Lastly, a possible source of noise caused by the interaction of steep orography with the physics (or dynamics) is discussed in section 4c.

2. NOISE FROM THE DYNAMICS .

2a. Semi-Lagrangian and semi-implicit discretization.

In this section the two time level semi-Lagrangian and semi-implicit (2TLSLSI) method of discretization is summarized by considering the following generic one-dimensional advection equation:

$$\frac{\partial\psi(x,t)}{\partial t} + u(x,t)\frac{\partial\psi(x,t)}{\partial x} = L\{\psi(x,t)\} + N\{\psi(x,t)\},\tag{2.1}$$

where u is the advecting velocity and L and N represent the linear and non-linear terms, respectively. A popular 2TLSLSI discretization of this equation is

$$\psi_I^{n+1} - \psi_*^n = \left(\frac{\Delta t_+}{2}\right) \left[L^{n+1} + N^{n+1/2} \right]_I + \left(\frac{\Delta t_-}{2}\right) \left[L^n + N^{n+1/2} \right]_*, \tag{2.2}$$

where

$$N^{n+1/2} = (3N^n - N^{n-1})/2, (2.3)$$

and $\Delta t_{\pm} = (1 \pm \epsilon_g) \Delta t$; ϵ_g is called the 'de-centering' parameter. For any field ϕ , $\phi_I^n = \phi(I\Delta x, n\Delta t)$, and $\phi_*^n = \phi(x_*, n\Delta t)$. The position of the departure point, x_* , is estimated by solving the equation

$$\frac{dx}{dt} = u(x,t) \tag{2.4}$$

as

$$x(t+\Delta t) - x(t) = \int_t^{t+\Delta t} u\{x(\tau), \tau\} d\tau.$$
(2.5)

Since u(x,t) is unknown and the integral is along the trajectory of the parcel an approximate method must be devised for finding the departure point, $x(t) = x_*$. (The arrival point, $x(t + \Delta t) = I \Delta x$, is known).

The most popular method can be thought of as approximating the integral in Eq. (2.5) using the 'mid-point rule':

$$x(t) = x(t + \Delta t) - \Delta t u \{ [x(t + \Delta t) + x(t)]/2, t + \Delta t/2 \},$$
(2.6)

and evaluating x(t) iteratively. First, u is extrapolated to time level n + 1/2:

$$u\{x, (n+1/2)\Delta t\} = \frac{3}{2}u\{x, n\Delta t\} - \frac{1}{2}u\{x, (n-1)\Delta t\}.$$
(2.7)

Then the (k+1)st iteration is given by

$$x_*^{(k+1)} = I\Delta x - \Delta t u \{ [I\Delta x + x_*^{(k)}]/2, (n+1/2)\Delta t \} = I\Delta x - \Delta t \hat{u}^{(k)};$$
(2.8)

$$x_*^{(1)} = I\Delta x - \Delta t u_I^{n+1/2}.$$
(2.9)

The integration proceeds as follows. (a) The departure point position associated with each grid point is estimated using Eq. (2.8), and stored. (b) The non-linear terms are computed at time level (n + 1/2) at each grid-point and stored. (c) The linear terms are computed at each grid-point and combined with the non-linear terms and the resultant fields are interpolated to the departure points. (d) Finally, the implicit system,

$$\psi_I^{n+1} - \frac{\Delta t_+}{2} L_I^{n+1} = \left\{ \psi^n + \frac{\Delta t_-}{2} L^n + \frac{\Delta t_-}{2} N^{n+1/2} \right\}_* + \frac{\Delta t_+}{2} N_I^{n+1/2}$$
(2.10)

is solved.

What are the possible sources of instability? (a) The non-linear terms, which are integrated explicitly. (b) In the presence of orography even the linear terms become problematic. (c) The extrapolation in time in Eq. (2.7) is suspect. We return to this in section 2d, whereas in sections 2b and 2c the one-dimensional shallow water equations are used to examine the first two sources of noise.

2b. Instability caused by the non-linear terms.

In this section we try to gain some understanding as to why the non-linear terms are a source of instability, and how we control that instability. To do this, we analyse the following one-dimensional shallow water equations,

$$\frac{\partial u(x,t)}{\partial t} + u(x,t)\frac{\partial u(x,t)}{\partial x} + \frac{\partial \phi(x,t)}{\partial x} = 0 ; \qquad (2.11)$$

$$\frac{\partial \phi(x,t)}{\partial t} + u(x,t)\frac{\partial \phi(x,t)}{\partial x} + \phi(x,t)\frac{\partial u(x,t)}{\partial x} = 0 .$$
(2.12)

Here ϕ is g times the height above a reference level; see Pedlosky (1979), p58. Separating $\phi \partial u / \partial x$ into linear, $\phi_0 \partial u / \partial x$, and non-linear, $\phi' \partial u / \partial x$, components (ϕ_0 , a constant, is $\gg \phi'$) and discretizing as in Eq. (2.2) gives the following:

$$u_I^{n+1} - u_*^n = -\frac{\Delta t_+}{2} (\phi_x)_I^{n+1} - \frac{\Delta t_-}{2} (\phi_x)_*^n, \qquad (2.13)$$

$$\phi_I^{n+1} - \phi_*^n = -\frac{\Delta t_+}{2} \phi_0(u_x)_I^{n+1} - \frac{\Delta t_-}{2} \phi_0(u_x)_*^n -\frac{\Delta t_+}{2} \left\{ \frac{3}{2} (\phi' u_x)^n - \frac{1}{2} (\phi' u_x)^{n-1} \right\}_I - \frac{\Delta t_-}{2} \left\{ \frac{3}{2} (\phi' u_x)^n - \frac{1}{2} (\phi' u_x)^{n-1} \right\}_*$$
(2.14)

To perform a von Neumann stability analysis it is necessary to make two assumptions; that the advecting velocity is constant, $u(x,t) = u_0$, and that $\phi' = \phi_N$ is also a constant. The stability analysis of Eqs. (2.13) - (2.14) is relegated to appendix 1 and results in the cubic equation (A.1.9). It is not difficult to write a programme to solve Eq. (A.1.9) numerically and to look at the stability for different values of ϕ_0, ϕ_N, u_0 , and ϵ_g . This is left as an exercise. Here we try to gain additional insight by looking at analytical results. Consider first of all the solution in the absence of 'de-centering', with no non-linear terms, and with zero advecting velocity; ($\epsilon_g = 0$, $\gamma_N = 0$, and $\Lambda = 1$ in Eq. (A.1.9)). Then the dispersion relation is

$$\lambda^{2}(1+\gamma_{L}) - 2\lambda(1-\gamma_{L}) + (1+\gamma_{L}) = 0, \qquad (2.15)$$

and its solution is

$$\lambda = \frac{1 \pm i\sqrt{\gamma_L}}{1 \mp i\sqrt{\gamma_L}},\tag{2.16}$$

where γ_L is defined in Eq. (A.1.8). Obviously, $|\lambda| = 1$ and the scheme is stable.

What happens when we include the non-linear terms? In the absence of 'de-centering' and with zero advecting velocity ($\epsilon_g = 0$ and $\Lambda = 1$ in Eq. (A.1.9)) the dispersion relation becomes

$$\lambda^{3}(1+\gamma_{L}) + \lambda^{2}(-2+2\gamma_{L}+3\gamma_{N}) + \lambda(1+\gamma_{L}+2\gamma_{N}) - \gamma_{N} = 0, \qquad (2.17)$$

where γ_N is defined in Eq. (A.1.8). This can be solved numerically; see fig. 1 of Gravel, Staniforth and Coté (1993). Let us try to gain some additional insight by doing a perturbation expansion. First divide by $1 + \gamma_L$ and write $\gamma_N/(1 + \gamma_L) = \epsilon$. Then Eq. (2.17) becomes

$$\lambda^3 + \lambda^2 \left\{ -2\left(\frac{1-\gamma_L}{1+\gamma_L}\right) + 3\epsilon \right\} + \lambda(1+2\epsilon) - \epsilon = 0.$$
(2.18)

For small ϵ we can do a perturbation analysis of this equation. The zeroth order solution is given by Eq. (2.16). To $O(\epsilon)$ the solution is given by (see appendix 2)

$$\lambda = \frac{1 \pm i\sqrt{\gamma_L}}{1 \mp i\sqrt{\gamma_L}} + \epsilon \frac{1 \pm 2i\sqrt{\gamma_L}}{\mp i\sqrt{\gamma_L}}; \qquad |\lambda|^2 = 1 + 4\frac{\gamma_N\gamma_L}{(1 + \gamma_L)^2}$$
(2.19)

Since $\gamma_L = \{\sqrt{\phi_0}(\Delta t/\Delta x)\sin(\pi\Delta x/L_x)\}^2$, the limit $\gamma_L >> 1$ can be regarded as the large time step, external gravity mode, short wave-length limit ($\sqrt{\phi_0}\Delta t/\Delta x >> 1$, and $\sin(\pi\Delta x/L_x) \sim O(1)$); (L_x is the wavelength). In this limit we get

$$|\lambda|^2 = 1 + 4\phi_N/\phi_0 \tag{2.20}$$

If we choose ϕ_0 equal to the mean value of ϕ then $|\lambda| > 1$ and the scheme is unstable.

How can we control it? By 'de-centering'. To see why 'de-centering' works consider once more the situation when the non-linear terms and the advecting velocity are zero, but now retaining the 'de-centering' coefficient; ($\gamma_N = 0$ and $\Lambda = 1$ in Eq. (A.1.9)). The solution of the resulting dispersion equation is

$$\lambda = \frac{1 \pm i\sqrt{\gamma_L}(1 - \epsilon_g)}{1 \mp i\sqrt{\gamma_L}(1 + \epsilon_g)}; \quad |\lambda|^2 = \frac{1 + \gamma_L(1 - \epsilon_g)^2}{1 + \gamma_L(1 + \epsilon_g)^2}; \quad (2.21)$$

 $|\lambda|^2 < 1$, for $\epsilon_g > 0$. The derivation of the multi-level equivalent is given by Tanguay et al. (1992) and Bates et al. (1993).

Thus, our expectation is that this damping of the linear terms caused by the de-centering will compensate for the amplification caused by the ϕ_N terms. Including these terms results in the equation for λ is given by Eq. (A.1.9) with $\Lambda = 1$. We can again do a perturbation analysis if we make some reasonable assumptions. First, $O(\epsilon_g \phi_0) = O(\phi_N)$, implying $\epsilon_g \gamma_L = \tau \gamma_N$, where $\tau \sim O(1)$. Making this substitution in Eq. (A.1.9) results in the dispersion equation

$$\lambda^{3} \left\{ 1 + 2\tau\epsilon + \tau\epsilon\epsilon_{g} \right\} + \lambda^{2} \left\{ -2\left(\frac{1-\gamma_{L}}{1+\gamma_{L}}\right) + 3\epsilon + \epsilon\epsilon_{g}(3-2\tau) \right\} + \lambda \left\{ 1 + 2\epsilon(1-\tau) + \epsilon\epsilon_{g}(\tau-4) \right\} - \epsilon + \epsilon\epsilon_{g} = 0, \qquad (2.22)$$

which, making the assumption that $O(\epsilon_g) = O(\epsilon)$, has the following solution to $O(\epsilon)$:

$$\lambda = \frac{1 \pm i\sqrt{\gamma_L}}{1 \mp i\sqrt{\gamma_L}} + \epsilon \left(\frac{1 \pm 2i\sqrt{\gamma_L}}{\mp i\sqrt{\gamma_L}} - 2\tau \frac{1 \pm i\sqrt{\gamma_L}}{1 \mp i\sqrt{\gamma_L}} \right); \quad |\lambda|^2 = 1 + 4 \frac{\gamma_L}{1 + \gamma_L} \left(\frac{\gamma_N}{1 + \gamma_L} - \epsilon_g \right).$$
(2.23)

For $\gamma_L >> 1$ this becomes

$$|\lambda|^{2} = 1 + 4\left(\frac{\phi_{N}}{\phi_{0}} - \epsilon_{g}\right).$$
(2.24)

A typical mean value of the 500hPa geopotential height field is $\phi_0 = 55000m^2/s^2$, and an approximate maximum variation from that mean, $\phi_N = 5500m^2/s^2$. This indicates that $\epsilon_g = 0.1$ will re-establish stability. This agrees with practical experience in multi-level primitive equation models.

There is an alternative method for controlling this instability. To see how it works look at Eq. (2.20) again. Notice that if ϕ_N is negative then $|\lambda|^2 < 1$ and we restore stability. How can we do this? If we choose ϕ_0 to be greater than the maximum geopotential height then ϕ' in Eq. (2.14) will always be negative, as will ϕ_N , by implication. This was stated by Coté and Staniforth (1988), but its full significance was not realised until Simmons and Temperton (1997) pointed out that in a multi-level model the equivalent stabilizing procedure was to choose T^0 , the constant temperature associated with the resting basic state of the atmosphere, to be greater than the maximum atmospheric temperature. (They chose 350K).

Equation (21) of Simmons and Temperton (1997) is the multi-level spectral version of our Eq. (2.18); (put $\gamma_L = \beta^2$, $\epsilon = \mu$). It is interesting to note that Gravel, Staniforth, and Coté (1993), who performed the same analysis for a multi-level grid-point model did not realise the significance of their Eq. (40) in this regard. Because, in the absence of divergence damping it is formally the same as Eq. (A.1.9), they were in a position to conclude that if they chose T^I (their notation) to be greater than the maximum temperature then T^E (their notation) would always be negative, thus restoring stability without recourse to divergence damping or 'de-centering'.

Other methods are used to control this noise. For instance, McDonald and Haugen (1993) time-filter the non-linear terms and also employ divergence damping in their model. The

latter, however, has been somewhat discredited by Gravel, Staniforth, and Coté (1993). Also, because the de-centering described by Eq. (2.2) is $O(\Delta t)$ accurate schemes which are $O(\Delta t^2)$ accurate have been suggested by Rivest et al. (1994) and Simmons and Temperton (1997).

So far we have only considered stability with $u_0 = 0$. To see the effects of non-zero advecting velocities we must solve Eq. (A.1.9) numerically. The main impact of the semi-Lagrangian interpolations is to damp the shorter waves. For example, compare figures 2 and 1 in Gravel, Staniforth, and Coté (1993).

2c. Un-meteorological stationary solutions with orographic forcing.

The linearized primitive equations have a stationary solution in response to orographic forcing. Coiffier, Chapelet, and Marie (1987) demonstrated that this solution is distorted by the semi-Lagrangian discretization and that this distortion becomes worse as the time step is increased. We will examine the phenomenon in this section by looking again at the one-dimensional shallow water equations; now with orography included. Then Eq. (2.11) remains unaltered but (2.12) is changed; see Pedlosky (1979), pp 61-62:

$$\frac{\partial\phi(x,t)}{\partial t} + u(x,t)\frac{\partial\phi(x,t)}{\partial x} + \{(\phi(x,t) - \phi_s(x))\}\frac{\partial u(x,t)}{\partial x} = u(x,t)\frac{\partial\phi_s(x)}{\partial x}.$$
 (2.25)

where $\phi_s(x)$ is g times the height of the bottom topography. Linearizing Eqs. (2.11) and (2.25) and assuming $\phi_s(x) \ll \phi_0$ gives

$$\frac{\partial u(x,t)}{\partial t} + u_0 \frac{\partial u(x,t)}{\partial x} + \frac{\partial \phi(x,t)}{\partial x} = 0.$$
 (2.26)

$$\frac{\partial \phi(x,t)}{\partial t} + u_0 \frac{\partial \phi(x,t)}{\partial x} + \phi_0 \frac{\partial u(x,t)}{\partial x} = u_0 \frac{\partial \phi_s(x)}{\partial x}.$$
(2.27)

This is a system of inhomogeneous linear partial differential equations with constant coefficients. The solution is summarised in Appendix 3. We are particularly interested in the stationary solution :

$$\hat{\phi}_p = \frac{u_0^2}{u_0^2 - \phi_0} \hat{\phi}_s, \tag{2.28}$$

which has a resonance centered at $\sqrt{\phi_0} = \pm u_0$.

What happens to this resonance when we perform a semi-Lagrangian discretization of Eqs. (2.26) and (2.27)? Consider first of all what happens with no de-centering and with the original approach to the orographic term:

$$\frac{u(x,t+\Delta t) - u(x-u_0\Delta t,t)}{\Delta t} + \frac{\phi_x(x,t+\Delta t) + \phi_x(x-u_0\Delta t,t)}{2} = 0,$$
 (2.29)

$$\frac{\Phi(x,t+\Delta t) - \Phi(x-u_0\Delta t,t)}{\Delta t} + \phi_0 \frac{u_x(x,t+\Delta t) + u_x(x-u_0\Delta t,t)}{2} = 0, \qquad (2.30)$$

where $\Phi = \phi - \phi_s$. As is shown in Appendix 3, this leads to the stationary solution being changed to the following:

$$\hat{\phi}_p = \frac{u_0^2 S^2}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s, \qquad (2.31)$$

where S and C are both equal to 1 when $\Delta t = 0$; (see Appendix 3). Comparing Eq. (2.31) with Eq. (2.28) we see that the solution has been distorted by the semi-Lagrangian discretization. This may cause difficulties if we wish to model stationary waves accurately and use large time steps. See Pinty et al. (1995) and Héreil and Laprise (1996).

To get a feeling for why it may cause noise as well consider what happens when C = 0. Then Eq. (2.31) becomes $\hat{\phi}_p = \hat{\phi}_s$. Compare this with the analytical solution in the 'external gravity mode limit', $(u_0^2 \ll \phi_0)$; $\hat{\phi}_p = -(u_0^2/\phi_0)\hat{\phi}_s$. The solution of the discretized equations is much too large and has the wrong sign. Since $C = \cos(\pi \alpha \Delta x/L_x)$ this can happen for two-grid-waves $(L_x = 2\Delta x)$ when the Courant number (α) equals 1.

In order to gain further insight into the methods used to improve this bad behaviour it is useful to display the solution in the limit $u_0^2 \ll \phi_0$, where it seems to have singular behaviour when C = 0:

$$\hat{\phi}_p = -(u_0^2 S^2 / \phi_0 C^2) \hat{\phi}_s.$$
(2.32)

Can we alleviate this numerical anomaly? Ritchie and Tanguay (1996) made the following suggestion. Instead of a Lagrangian differentiation of the orographic term do a Lagrangian averaging along the trajectory. Therefore Eq. (2.30) is replaced by

$$\frac{\phi(x,t+\Delta t) - \phi(x-u_0\Delta t,t)}{\Delta t} + \phi_0 \frac{u_x(x,t+\Delta t) + u_x(x-u_0\Delta t,t)}{2} = u_0 \frac{\phi_{s,x}(x) + \phi_{s,x}(x-u_0\Delta t)}{2},$$
(2.33)

which leads to (see Appendix 3),

$$\hat{\phi}_p = \frac{u_0^2 SC}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s, \qquad (2.34)$$

which gives $\hat{\phi}_p = 0$ when C = 0, which is much closer to the correct answer, $\hat{\phi}_p = -(u_0^2/\phi_0)\hat{\phi}_s$ in the limit $u_0^2 \ll \phi_0$. In this limit Eq. (2.34) becomes

$$\hat{\phi}_p = -(u_0^2 S/\phi_0 C)\hat{\phi}_s.$$
(2.35)

This still tends to infinity as $L_x \to 2\alpha \Delta x$, but not as rapidly as Eq. (2.32).

Averaging the orographic term along the trajectory had the effect of reducing the 'singularity' by multiplying Eq. (2.32) by a term proportional to C/S'. The reason for this becomes obvious if we compare Eqs. (A.3.8) and (A.3.12); Lagrangian *differentiation* leads to an 'S'; Lagrangian *averaging* leads to a 'C'. Can a scheme be devised which has the effect of multiplying Eq. (2.32) by a term proportional to C^2/S' ? Yes, with a 'doubly

spatially averaged' scheme (Laprise, private communication). For instance, replacing the spatially averaged orographic term in Eq. (2.33) with

$$\frac{u_0}{4} \Big\{ \phi_{s,x}(x + u_0 \Delta t/2) + 2\phi_{s,x}(x - u_0 \Delta t/2) + \phi_{s,x}(x - 3u_0 \Delta t/2) \Big\}$$
(2.36)

results in

$$\hat{\phi}_p = \frac{u_0^2 S C^2}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s, \qquad (2.37)$$

which, in the limit $u_0^2 << \phi_0$ becomes

$$\hat{\phi}_p = -(u_0^2 S/\phi_0) \hat{\phi}_s.$$
(2.38)

This has no infinity when $L_x = 2\alpha \Delta x$.

Eq. (2.36) implies three additional interpolations. We can reduce this to two additional interpolations by using

$$\frac{u_0}{8} \left\{ \phi_{s,x}(x+u_0\Delta t) + 3\phi_{s,x}(x) + 3\phi_{s,x}(x-u_0\Delta t) + \phi_{s,x}(x-2u_0\Delta t) \right\}$$
(2.39)

which 'over-kills' the 'external mode large Courant number' 'singularity':

$$\hat{\phi}_p = \frac{u_0^2 S C^3}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s. \tag{2.40}$$

Another way of attacking this problem is to resort to de-centering. It is left as an exercise to show that the de-centered equations:

$$u(x,t+\Delta t) - u(x - u_0 \Delta t, t) + \left\{ \frac{\Delta t_+}{2} \phi_x(x,t+\Delta t) + \frac{\Delta t_-}{2} \phi_x(x - u_0 \Delta t, t) \right\} = 0 \quad (2.41)$$

$$\Phi(x,t+\Delta t) - \Phi(x-u_0\Delta t,t) + \phi_0 \left\{ \frac{\Delta t_+}{2} u_x(x,t+\Delta t) + \frac{\Delta t_-}{2} u_x(x-u_0\Delta t,t) \right\} = 0 \quad (2.42)$$

give rise to the following stationary solution:

$$\hat{\phi}_p = \frac{u_0^2 S^2}{u_0^2 S^2 - \phi_0 (C + iS\epsilon_g k u_0 \Delta t/2)^2} \hat{\phi}_s \tag{2.43}$$

As long as $\epsilon_g \neq 0$ the 'external mode large Courant number' 'singularity' is removed from the stationary solution. It is replaced with a peak whose half-width is is proportional to ϵ_g . The larger ϵ_g the more the peak will spread out. However, since large ϵ_g has negative effects on the overall integration there exists a contradiction between damping the numerical resonance and accurate integration. See Rivest, Staniforth and Robert, (1994) who investigate this dilemma and propose an $O(\Delta t^2)$ de-centering solution.

2d. Extrapolation to find the departure point.

Hortal (1998) has demonstrated that, in some weather regimes, there appear in forecasts of the ECMWF 2TSLSI spectral model non-meteorological oscillations whose origin can be traced to the computation of the departure point position. See also his presentation to this seminar. In this section an attempt is made to gain some insight into the cause of these oscillations inspired by a personal communication from Dale Durran; see also Durran (1998).

How can we perform a stability analysis of the non-linear equation dx/dt = u(x,t)? Let us resort to the standard procedure of assuming that we can gain some useful insight by investigating the oscillation equation,

$$\frac{\partial \chi(x,t)}{\partial t} + u_0 \frac{\partial \chi(x,t)}{\partial x} = i\nu\chi(x,t) , \qquad (2.44)$$

as a 'first order' linear representation of dx/dt = u(x,t).

Consider first of all the method of computing the departure point indicated by Eq. (2.8):

$$\chi\{x, (n+1)\Delta t\} - \chi\{x - u_0\Delta t, n\Delta t\} =$$

$$i\nu\Delta t \left(\frac{3}{2}\chi\{x - u_0\Delta t/2, n\Delta t\} - \frac{1}{2}\chi\{x - u_0\Delta t/2, (n-1)\Delta t\}\right)$$
(2.45)

Substituting the solution $\chi\{x, n\Delta t\} = \hat{\chi}\lambda^n \exp ikx$ and multiplying by $\exp 2iku_0\Delta t$ gives

$$\lambda^2 e^{2iku_0\Delta t} - \lambda e^{iku_0\Delta t} \{1 + 3i(\nu\Delta t/2)e^{iku_0\Delta t/2}\} + i(\nu\Delta t/2)e^{3iku_0\Delta t/2} = 0, \qquad (2.46)$$

whose solution is

$$\lambda e^{iku_0\Delta t} = \frac{1}{2} + \frac{3i\nu\Delta t}{4} e^{iku_0\Delta t/2} \pm \frac{1}{2}\sqrt{\{1 + 3i(\nu\Delta t/2)e^{iku_0\Delta t/2}\}^2 - 2i\nu\Delta t e^{3iku_0\Delta t/2}}$$
(2.47)

Notice that $|\lambda|$ is a function of u_0 . To get some indication of its behaviour consider the solution for $\nu \Delta t \ll 1$:

$$|\lambda|^2 = 1 - 4\nu\Delta t \sin^3(ku_0\Delta t/2) + O(\nu^2) = 1 - 4\nu\Delta t \sin^3(\alpha\pi\Delta x/L_x) + O(\nu^2\Delta t^2).$$
(2.48)

Therefore, although the leading term is $O(\Delta t^4)$, $|\lambda|^2$ becomes effectively $1 + O(\Delta t)$ for two grid waves with Courant number equal to 1. (There is also a numerical mode whose leading term is $O(\nu^2 \Delta t^2)$).

Next consider the 'extrapolation along the trajectory' method of computing the departure point:

$$\chi\{x, (n+1)\Delta t\} - \chi\{x - u_0\Delta t, n\Delta t\} = i\nu\Delta t \left(\frac{3}{2}\chi\{x - u_0\Delta t, n\Delta t\} - \frac{1}{2}\chi\{x - 2u_0\Delta t, (n-1)\Delta t\}\right)$$
(2.49)

Substituting the solution $\chi\{x, n\Delta t\} = \hat{\chi}\lambda^n \exp ikx$ and multiplying by $\exp 2iku_0\Delta t$ gives

$$\lambda^2 e^{2iku_0\Delta t} - \lambda e^{iku_0\Delta t} \{1 + 3i(\nu\Delta t/2)\} + i(\nu\Delta t/2) = 0, \qquad (2.50)$$

whose solution is

$$\lambda e^{iku_0\Delta t} = \frac{1}{2} + \frac{3i\nu\Delta t}{4} \pm \frac{1}{2}\sqrt{\{1 + 3i(\nu\Delta t/2)\}^2 - 2i\nu\Delta t}$$
(2.51)

Notice that $|\lambda|$ is now no longer a function of u_0 . The solution for $\nu \Delta t \ll 1$ is

$$|\lambda|^2 = 1 + (1/2)(\nu \Delta t)^4 + O(\nu^5 \Delta t^5)$$
(2.52)

Therefore, the solution is weakly amplifying, but is independent of how strong the advecting velocity is. (There is also a numerical mode whose leading term is $O(\nu^2 \Delta t^2)$).

It is left as an exercise to show that

$$|\lambda|^{2} = 1 + 2(\nu \Delta t)^{2} \sin^{2}(\alpha \pi \Delta x/L_{x}) + O(\nu^{3} \Delta t^{3}).$$
(2.53)

for the following scheme, corresponding to that suggested by Eqs. (6) and (7) of Hortal (1998),

$$\chi\{x, (n+1)\Delta t\} - \chi\{x - u_0\Delta t, n\Delta t\} =$$
$$i\nu\Delta t \left(\frac{1}{2}\chi\{x, n\Delta t\} + \chi\{x - u_0\Delta t, n\Delta t\} - \frac{1}{2}\chi\{x - u_0\Delta t, (n-1)\Delta t\}\right)$$
(2.54)

Now, in contrast to Eq. (2.48), $|\lambda|^2$ becomes effectively $1 + O(\Delta t^2)$ for two grid waves with Courant number equal to 1. However, the dependence on α remains, in contrast to Eq. (2.52).

Although it must be admitted that it bears a somewhat tenuous connection to the highly non-linear problem being examined, this stability analysis points strongly toward 'extrapolation along the trajectory' being the most attractive method for calculating the departure point position. Therefore, it is disconcerting to note that Temperton and Staniforth (1987), in shallow water experiments, found that with this scheme 'results were consistently worse than those for the simpler method 2' (their method 2 corresponds to our Eq. (2.8)).

2e. The upper boundary condition.

The upper boundary condition used in SLSI schemes is usually a lid condition with the vertical motion set to zero. This has no physical basis and is a source of false reflections which can cause standing waves to form in the model atmosphere. The standard device to handle this problem consists in using diffusion with a coefficient which increases with height. An attractive alternative would be to use a radiation upper boundary condition, which is more physical. Herzog (1995) expanded on the work of Klemp and Durran (1983) and Bougeault (1983) in order to derive a radiation upper boundary condition for

a hybrid vertical coordinate. As he says in his report, 'the application of radiation upper boundary conditions becomes more necessary with increasing grid resolution'. His scheme is unstable for large time steps and thus is not appropriate for a semi-Lagrangian model. A radiation upper boundary condition scheme within a semi-Lagrangian semi-implicit model has not yet been invented.

3. NOISE FROM THE 'PHYSICS'.

Because the semi-Lagrangian semi-implicit scheme has an extremely liberal stability criterion we can, in principle, use very large time steps to integrate the dynamics in primitive equation models. This prompts the question: can we use equally large time steps when updating the physical processes?

Actually, noise originating in the physics is not exclusive to semi-Lagrangian integrations. In Eulerian models, Kållberg and Gollvik (1983) discuss spurious oscillations caused by the vertical diffusion scheme, and their elimination, as does Hammarstrand (1997). Kalnay and Kanamitsu (1988) and Girard and Delage (1990) also describe spurious oscillations originating in the surface schemes and vertical diffusion schemes in Eulerian integrations. As we move to relatively larger time steps and finer grids we can expect these problems to be exacerbated; see Bénard and Yassad (1995). They encountered very strong high frequency oscillations in their vertical diffusion scheme when they used large time steps with high vertical resolution near the surface in a semi-Lagrangian integration.

In order to use bigger time steps in the 'physics' we must make sure that the time discretization schemes we use are accurate, stable, and non-oscillating. In this section some possibly unexpected sources of inaccuracy, instability, and unwanted oscillations, which may arise when large time steps are used in the 'physics', are examined. This is done by employing some widely used strategies to integrate a number of simple differential equations which are typical of the kind used in the physical parameterization schemes.

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Consider the equation

$$\frac{du(t)}{dt} = -K[u(t) - F(t)] + \frac{dF(t)}{dt}; \quad u(0) = 0.$$
(3.1)

K is a positive constant. The solution is given by

$$u(t) = [u(0) - F(0)]exp(-Kt) + F(t)$$
(3.2)

If we choose $K = 100hr^{-1}$ and F(t) = t/10 + 0.5, ('t' is in units of hours), then we see that the solution consists of a slowly varying part, F(t), and a rapidly varying part, exp(-100t); see the line made of long dashes in fig. 1. If we are only interested in the

slowly evolving part of this solution then we would like to be able to use a large time step to get as accurate an integration of Eq. (3.1) as we require. Looking naively at fig. 1, a time step of 0.5hr would seem to be a conservative choice. Let us examine what happens when we use this time step with three simple integration schemes, all of which are used widely in the 'physics'. These are the Euler explicit, the trapezoidal, and the Euler implicit schemes. These correspond to $\gamma = 0, \gamma = 0.5$, and $\gamma = 1$, respectively, in Eq. (3.3):

$$(u^{n+1} - u^n)/\Delta t = -K[\gamma u^{n+1} + (1 - \gamma)u^n] + KF^n + (F')^n$$
(3.3)

With $\Delta t = 0.5$ hr the Euler explicit scheme is unstable. The values of u for the first five time steps are 0, 25, -1195, 58589, -2870871. This growing oscillation continues until we get a floating overflow. We must use a very small time step ($\Delta t = 0.01hr$) to get a stable and oscillation-free integration.



FIGURE 1. Graphs of the solutions to Eq. (3.3) using $\Delta t = 0.5, K = 100.0$ and various values of γ .

This illustrates the phenomenon of *stiffness*; the time step is restricted by stability requirements, rather than accuracy. A good working definition of stiffness is as follows. A system is *stiff* if the solution we seek is slowly varying but other solutions exist which decay rapidly.

A stability analysis of the homogeneous part of Eq. (3.3) can be performed by substituting

 $u(n\Delta t) = \lambda^n \hat{u}$, giving

$$\lambda = \frac{1 + \Delta t K(\gamma - 1)}{1 + \Delta t K \gamma}.$$
(3.4)

For the Euler explicit scheme ($\gamma = 0$) we must have $K\Delta t \leq 2$ for stability.

Notice that the trapezoidal scheme ($\gamma = 0.5$) has $|\lambda| \leq 1$. Thus an integration with $\Delta t = 0.5$ hr will be unconditionally stable. This is in fact true, as can be seen from fig. 1, where the solution is displayed as a continuous line. Unfortunately it oscillates about the correct solution before settling down. Stiffness strikes again!

We can understand what is happening here by noticing that for $\gamma = 0.5$ and $K\Delta t = 50, \lambda = -0.92$. Therefore, the homogeneous solution will oscillate, because $u(\Delta t) = -0.92\hat{u}; u(2\Delta t) = (-0.92)^2\hat{u} = 0.85\hat{u}; u(3\Delta t) = (-0.92)^3\hat{u} = -0.79\hat{u}$, and so on.

Obviously, if we wish to eliminate this oscillation from the homogeneous solution we must choose γ such that $\lambda \geq 0$, that is, $\gamma \geq 1$. With $\gamma = 1$, (the Euler implicit scheme) and $\Delta t = 0.5hr$, then $\lambda = 0.02$ and the transient solution disappears rapidly, as it should. The integration is then stable and non-oscillatory. See the line made with short dashes in fig. 1.

The above simple analysis is actually indicative of some very general results. 1. No explicit scheme will be stable for a stiff system. 2. The choice of implicit schemes which are stable and non-oscillatory is extremely restricted. 3. $O(\Delta t^2)$ accurate schemes will be computationally expensive. 1 and 2 above, when expressed in precise mathematical terms, are known as the 'second Dalquist barrier'; see Dalquist (1963), and section 6.6 of Lambert (1991). The latter also contains an excellent discussion on the nature of stiffness in sections 6.1 and 6.2.

Where can stiffness arise in the 'physics'? One possibility is if a process is 'switched on' or 'switched off' instantaneously. Since this represents a very fast process indeed it is a prime candidate for stiffness.

3b. Boundaries.

Spatial boundaries can also be a source of oscillating solutions when large time steps are used. To illustrate this let us solve solve the diffusion equation,

$$\frac{\partial X(z,t)}{\partial t} = \kappa \frac{\partial^2 X(z,t)}{\partial z^2},\tag{3.5}$$

with the following boundary conditions: X(0,t) = 0; X(Z,t) = 0; and the following initial condition: $X(z,0) = X_0$ for 0 < z < Z. The parameter κ is a positive constant.

This is the classic problem of a bar initially at temperature X_0 whose ends are placed against blocks of ice. Physically, the bar gradually cools, most rapidly near the ends, and

more slowly at the centre. There is an analytical solution; see Churchill (1963). For our purposes we can also regard it as column model of a tongue of warm air between the cold ground and the cold free atmosphere. Let us discretize as follows:

$$\frac{(X^{n+1} - X^n)}{\Delta t} = \kappa \left[\gamma \left(\frac{\partial^2 X}{\partial z^2} \right)^{n+1} + (1 - \gamma) \left(\frac{\partial^2 X}{\partial z^2} \right)^n \right]$$
(3.6)

$$\left(\frac{\partial^2 X}{\partial z^2}\right)_k = \frac{X_{k+1} - 2X_k + X_{k-1}}{\Delta z^2} \tag{3.7}$$

I have chosen $X_0 = 16^\circ$, Z = 1600m, $\kappa = 20m^2 sec^{-1}$, and $\Delta z = 100m$. With these choices $\kappa \Delta t / \Delta z^2$ varies between 0.2 and 7.2 as Δt goes from 100sec to 1 hour. Let us examine what happens if we use the trapezoidal scheme to integrate. Since this has $\gamma = 0.5$ it is $O(\Delta t^2)$ accurate, and would seem to be the optimal choice. For small values of $\kappa \Delta t / \Delta z^2$ we get stable and accurate integrations. See the line joining the small dots in fig. 2. This shows the evolution of the temperature at z = 100m over the first five hours of the integration, using a time step of 100 sec.



FIGURE 2. Graph of the temperature at z = 100m predicted by Eq. (3.6) for various values of Δt and γ . In the labels within the figure $cfl = \kappa \Delta t / \Delta z^2$.

If we are interested only in the longer-term changes in the temperature at 100m we would like to be able to integrate with a large time step. However, with the trapezoidal scheme a nasty oscillation occurs if we do this. See the line joining the triangles in fig. 2. For this integration $\Delta t = 3600 \sec (\kappa \Delta t / \Delta z^2 = 7.2)$. Notice that the integration is settling down as time goes on; the scheme is 'stable but oscillating'.

The Euler implicit scheme ($\gamma = 1$) has no oscillations. See the line joining the squares in fig. 2, which again shows the integration with $\kappa \Delta t / \Delta z^2 = 7.2$. Of course, there is some loss in accuracy initially.

Sudden jumps in space can also lead to oscillating solutions and must be treated carefully.

3c. Non-linear terms.

The results and arguments of Kalnay and Kanamitsu (1988) are used extensively in this section.

In order to illustrate additional problems posed by 'non-linear terms' when updating the 'physics' with large time steps consider the following simple damping equation,

$$\frac{\partial X}{\partial t} = -KX^{P+1}(t) + D(t) \tag{3.8}$$

To give a meteorological flavour to the interpretation of the results let X be the temperature difference between the ground and air, KX^P represents the exchange coefficient, and all slowly varying processes are included in D(t), to which we will assign a diurnal cycle: $D(t) = 1 - sin(2\pi n\Delta t/24)$, (Δt is measured in units of hours in this section); K = 10 and P = 3. With these choices, the solution is slowly varying, see the line joining the dots in fig. 3, and $\Delta t = 0.5$ hr would seem to be sufficient to maintain our required accuracy.

Let us examine first of all a most disconcerting result. A predictor-corrector discretization which treats the linear term implicitly is

$$(\tilde{X} - X^n)/\Delta t = -K(X^n)^P \tilde{X} + D^n$$
(3.9a)

$$(X^{n+1} - X^n) / \Delta t = -K \tilde{X}^P X^{n+1} + D^n$$
(3.9b)

With $\Delta t = 0.5$ hr time step this gives a solution which is stable and non-oscillatory, and completely wrong. See the line joining the '+'s in fig. 3, and compare with the correct solution. (An accurate integration can be restored by reducing the time step to 0.166 hr).

The Euler implicit scheme served us well in sections 2a and 2b. Thus, let us try the following scheme with $\gamma = 1$

$$(X^{n+1} - X^n) / \Delta t = -K(X^n)^P [\gamma X^{n+1} + (1 - \gamma)X^n] + D^n$$
(3.10)

With a $\Delta t = 1.0$ hr time step this produces an unpleasant result. The solution oscillates wildly. See the line joining the squares in fig. 3.

The linear analysis of Kalnay and Kanamitsu shows us that the amplification factor for the scheme of Eq.(3.10) is

$$\lambda = \frac{1 - \beta (P + 1 - \gamma)}{1 + \beta \gamma} \tag{3.11}$$

where $\beta = KX_0^P \Delta t$, X_0 being the equilibrium temperature used to linearise the equation. Thus, the linear stability requirement is violated for large β when P = 3 and $\gamma = 1$, since $\lambda \approx -3$. This analysis also tells us that $\gamma = P + 1$ gives a non-oscillating unconditionally stable scheme since $0 \leq \lambda \leq 1$. Such a solution is plotted as the line joining the 'x's in fig. 3.



FIGURE 3. Graphs of solutions to Eq. (3.8) using the predictor-corrector scheme, Eq. (3.9) and simple implicit schemes (Eq. (3.10) with various values of γ)

Is there a scheme which does not depend on knowing P? Consider the generic equation dX/dt = f(X) discretized as follows:

$$\frac{(X^{n+1} - X^n)}{\Delta t} = f(X^n) + \frac{(X^{n+1} - X^n)}{2} \frac{df}{dX}(X^n).$$
(3.12)

Notice that if we apply this idea to Eq. (3.8) we get Eq. (3.10) with $\gamma = P + 1$, an unconditionally stable and oscillation-free scheme according to Eq. (3.11), as we discussed in the previous paragraph. There are two drawbacks (a) df/dX may not be easily computed, and (b) it is $O(\Delta t)$ accurate.

We have shown that explicit schemes lead to instability and naive application of implicit schemes can lead to oscillating solutions for stiff systems and also for systems such that the boundary values differ markedly from the interior values. For both these problematic systems the Euler implicit scheme gave stable and oscillation-free integrations. However,

it is only $O(\Delta t)$ accurate. It is the $O(\Delta t)$ accurate representative of a class of (*L*-stable) schemes which are appropriate for solving these kinds of problems. There are higher order members of the class of *L*-stable schemes. All seem to be computationally expensive. See, for example, section 6.3 of Lambert (1991).

When non-linear terms appear in the equations then stable schemes which are computationally inexpensive are more difficult to invent. The 'over-implicit' scheme (large γ in Eq. (3.10)) is effective. If that fails the method of Eq. (3.12) seems to be the most reliable. Again, both of these schemes are $O(\Delta t)$ accurate, and higher order accurate versions of them will almost certainly be computationally expensive.

4. THE INTERFACE BETWEEN THE PHYSICS AND DYNAMICS.

4a. Splitting the physics from the dynamics.

The methods by which the physical parameterization schemes ('the physics') is joined to the dynamics can be summarised by considering the generic equation with physics added:

$$\frac{d\psi}{dt} = L(\psi) + N(\psi) + P(\psi), \qquad (4.1)$$

where L and N represent the linear and non-linear terms coming from the dynamics and P represents all of the physics. The natural way to proceed would be to divide the physics into linear and non-linear terms, $P(\psi) = L_P + N_P$, and subsequently solve the new 2TLSLSI system:

$$\psi^{n+1} - \frac{\Delta t}{2} \left\{ L^{n+1} + L_P^{n+1} \right\} = \left[\psi^n + \frac{\Delta t}{2} \left\{ L^n + L_P^n + N^{n+1/2} + N_P^{n+1/2} \right\} \right]_* + \frac{\Delta t}{2} \left\{ N^{n+1/2} + N_P^{n+1/2} \right\}$$
(4.2)

This has not been done because, firstly, in a multi-level primitive equation model the left hand side of Eq. (4.2) represents a system of equations which is expensive to solve. (However, Grabowski and Smolarkiewicz (1996) have taken a step in this direction). Secondly, because some of the terms contributing to $N_P^{n+1/2}$ may lead to instability. Thirdly, because some of the physical parameterization schemes may need dynamical tendencies as independent input.

There are two separate ways in which a particular physics sub-process may require a knowledge of $(\partial \psi/\partial t)_{dyn}$. First, it may require it as an independent input, for instance, moisture convergence for Kuo closure in some convection schemes. Second, as part of a 'fractional stepping' approach to updating the physics. We will leave discussion of the latter to the next section. In what follows we assume that the physics requires, for whichever reason, a reasonable approximation of $(\partial \psi/\partial t)_{dyn}$.

The solution has been to split computation of the physics from the computation of the dynamics, do them separately, and to subsequently join them together. There is no unique way of doing this. Thus many different options have been tried. In order to give a theme to the discussion we will take the point of view that Eq. (4.2) is a 'holy grail', and therefore worthy of pursuit.

The cheapest and simplest approach is to compute the physics *after* the semi-implicit adjustment and *after* the semi-Lagrangian interpolation:

$$\psi^{n_{+}} - \frac{\Delta t}{2} L^{n_{+}} = \left[\psi^{n} + \frac{\Delta t}{2} \left\{ L^{n} + N^{n+1/2} \right\} \right]_{*} + \frac{\Delta t}{2} N^{n+1/2}$$
(4.3*a*)

Having solved this implicit system we can now use $(\partial \psi / \partial t)_{dyn} = (\psi^{n+} - \psi^n) / \Delta t$ in any physics subroutine where it is needed and complete the integration as follows:

$$\psi^{n+1} = \psi^{n+1} + \Delta t P^{n+1} \tag{4.3b}$$

As we discuss in the next section, we could use P^n instead of P^{n+} in Eq. (4.3b), although this is not in the spirit of Marchuk (1974) splitting.

If we accept that Eq. (4.2) as an ideal we should aim for then the approach of Ritchie et al. (1995), who compute the physics *before* the semi-implicit adjustment and *after* the semi-Lagrangian interpolation, takes a step toward that ideal. Theirs is a three time level scheme. The equivalent two time level scheme might proceed as follows.

$$\psi^{n_{+}} = \left[\psi^{n} + \frac{\Delta t}{2} \left\{ L^{n} + N^{n+1/2} \right\} \right]_{*} + \frac{\Delta t}{2} \left\{ L^{n} + N^{n+1/2} \right\}$$
(4.4*a*)

Notice an additional computation has been performed (L^n) . The reason is to provide an approximate value for $(\partial \psi / \partial t)_{dyn}$, ($\approx (\psi^{n_+} - \psi^n) / \Delta t$), needed for the physics, which can now be computed, and the semi-implicit adjustment can subsequently be performed, remembering to subtract out the anomalous linear term:

$$\psi^{n+1} - \frac{\Delta t}{2}L^{n+1} = \psi^{n+1} - \frac{\Delta t}{2}L^n + \Delta tP^n$$
(4.4b)

One way of taking a further step toward Eq. (4.2) is to compute the physics before the semi-implicit adjustment and before the semi-Lagrangian interpolation. Then the question is: what do we use for $(\partial \psi / \partial t)_{dyn}$? One approach, that used at Météo France, is to compute it explicitly at the beginning of each time step, which is expensive. We are then in a position to solve a more balanced looking system:

$$\psi^{n+1} - \frac{\Delta t}{2}L^{n+1} = \left[\psi^n + \frac{\Delta t}{2} \left\{L^n + N^{n+1/2} + P^n\right\}\right]_* + \frac{\Delta t}{2} \left\{N^{n+1/2} + P^n\right\}$$
(4.5)

It should be pointed out that at Météo France they disagree with the 'holy grail' point of view and argue that all of the physics should be included at the departure point, that is, they replace $P_*^n + P^n$ with $2P_*^n$ in Eq. (4.5).

A clever way of almost reaching the same objective which avoids the additional expense of explicitly computing $(\partial \psi / \partial t)_{dyn}$ is that described in Hortal (1998); see also his talk at this seminar. At time level 'n - 1' after computing the contribution from the physical parameterization schemes, P^{n-1} , store these arrays, and, in our notation, replace Eqs. (4.4a) and (4.4b) with

$$\psi^{n+} = \left[\psi^n + \frac{\Delta t}{2} \left\{ L^n + N^{n+1/2} + P^{n-1} \right\} \right]_* + \frac{\Delta t}{2} \left\{ L^n + N^{n+1/2} - P^{n-1} \right\}$$
(4.6*a*)

The 'physics', P^n , can now be computed using $(\partial \psi / \partial t)_{dyn} \approx (\psi^{n+} - \psi^n) / \Delta t$, and subsequently performing the semi-implicit adjustment completes the integration:

$$\psi^{n+1} - \frac{\Delta t}{2}L^{n+1} = \psi^{n+1} + \frac{\Delta t}{2} \Big\{ P^n + P^{n-1} - L^n \Big\}.$$
(4.6b)

Of course, the trade-off is that the extra fields must be stored.

Logically, there is a fourth option, that is, to compute the physics 'after' the semi-implicit adjustment and 'before' the semi-Lagrangian interpolation:

$$\psi^{n_{+}} - \frac{\Delta t}{2} L^{n_{+}} = \psi^{n} + \frac{\Delta t}{2} \Big\{ L^{n} + N^{n+1/2} \Big\}$$
(4.7*a*)

$$\psi^{n+1} = \left[\psi^{n+} + \Delta t P^{n+}\right]_* + \frac{\Delta t}{2} N^{n+1/2}$$
(4.7b)

Doubt about the accuracy of Eqs. (4.3) has arisen as a result of a paper by Caya, Laprise, and Zwack (1998). They demonstrate that for large time steps a localized noise-like feature appears in the upper levels in a forecast using the three time level equivalent of Eqs. (4.3). This feature did not appear in the same forecast using the three time level equivalent of Eqs. (4.4) using the same large time step; (nor in the small-time-step forecast). In contrast, Chen and Bates (1996) found the forecasts using Eq. (4.3) 'showed similar scores' to those using Eq. (4.5).

4b. Splitting within the physics.

Within the physics each different process is computed essentially independently of the others. Thus, the radiation scheme, the vertical diffusion scheme, the condensation scheme, the surface scheme, and so on, are split from each other. Within this context two questions arise. (a) Should the physics be computed using the fields valid at time level 'n', or using fields which have been updated by the dynamics? In the notation of the previous section should we use P^{n_+} instead of P^n in Eqs. (4.4b), (4.5) and (4.6b)? Having decided which of these options to use there arises a separate question. (b) Should a physics sub-process use the fields which have been updated by the previous sub-process, or should it use the starting fields? For example, say we proceed as follows. We call the radiation sub-routine

first. Next, we call the vertical diffusion scheme. In it we have the choice of using the original fields *or* those incremented by the radiation scheme. Should the vertical diffusion update 'know' that the radiation scheme has changed the model atmosphere? We are faced the same dilemma when we call the next physics sub-process.

Beljaars (1991) has used the term 'process splitting' to describe the procedure whereby all of the physics sub-process use the same fields. He also showed that it can be a source of unwanted oscillations in certain circumstances.

He used the term 'fractional stepping' to describe the procedure whereby each physics sub-process uses fields which have been updated by the previous sub-processes. He then argued that where certain processes balance each other in the atmosphere then 'with longer time steps it becomes more and more relevant to keep an accurate balance between processes within a single time step' during the numerical integration. As an example, Janssen et al. (1992) demonstrate the importance of including the Coriolis terms in the vertical diffusion update. If one accepts these arguments, then Eq. (4.2) seems 'as balanced as possible' and therefore worth aiming for.

4c. Orographic noise.

The two-grid-wave group velocity is hopelessly inaccurate for both the semi-Lagrangian and Eulerian discretizations of the advection equation. For example, the one dimensional advection equation,

$$\frac{\partial\psi(x,t)}{\partial t} + u_0 \frac{\partial\psi(x,t)}{\partial x} = 0, \qquad (4.8)$$

using a leapfrog discretization, yields a group velocity which is in the the opposite direction to the advective velocity; $u_g(2\Delta x) = -u_0$. See page 117 of Haltiner and Williams (1980). For the semi-Lagrangian discretization, using a cubic interpolation, the group velocity is given by

$$\frac{u_g}{u_0} = 1 + \frac{\hat{\alpha}}{\alpha} \frac{(1 - \hat{\alpha}^2)(2 - \hat{\alpha})(2\hat{\alpha} - 1)\{3 + \hat{\alpha}(1 - \hat{\alpha})\mathcal{S}\}\mathcal{S}^2/9}{1 - \hat{\alpha}(1 - \hat{\alpha}^2)(2 - \hat{\alpha})\{3 + 2\hat{\alpha}(1 - \hat{\alpha})\mathcal{S}\}\mathcal{S}^2/9}$$
(4.9)

where $S = 2sin^2(k\Delta x/2)$. (Exercise: derive this result using Eqs. (30) and (33) of McDonald (1984)).

The group velocity of the two-grid waves (S = 2) varies between $-1.66u_0$ for $\alpha = 0$ and $-\infty$ for $\alpha = 0.5-$. It varies between $+\infty$ for $\alpha = 0.5+$ and u_0 for $\alpha = 1$. However, since the amplitude of the two-grid wave with $\alpha = 0.5$ is zero these infinite values are not catastrophic. (Because the denominator in Eq. (4.9) is the amplitude squared, the amplitude will always be small when the group velocity is large).

As long as the amplitude of the two-grid wave remains small these inaccuracies need not concern us. By definition we are trying to model much longer wave phenomena. However, big problems occur if their amplitude grows. One can therefore argue that any feature of

the model which can be a source of large amplitude two-grid waves should be removed because the energy associated with it will be advected away totally inaccurately by the advection scheme; this is just noise, by definition.

One possible mechanism for amplifying these waves is the interaction of the physics and/or dynamics with orography which varies significantly from one grid point to the next. Thus it can be argued that the mountains should be smoothed to remove all two-grid features.

McDonald and De Bruijn (1998) showed in a case study that single-grid-point enhancements of rainfall were significantly reduced by removing the two-grid structures from the orography.

The four-grid-wave group velocity is also poorly described; $c_g(4\Delta x) = 0$ for the leapfrog discretization. For the semi-Lagrangian scheme their group velocity ($\mathcal{S} = 1$ in Eq. (4.9)) climbs steadily from $0.33u_0$ (for $\alpha = 0$) to u_0 (for $\alpha = 0.5$), rising to a maximum of $1.116u_0$ (for $\alpha = 0.72$) and falling to u_0 (for $\alpha = 1$). Thus, it is possible to argue that these scales should also be filtered from the orography.

5 FINAL REMARK.

The history of the implementation of 2TLSLSI schemes has been that as the grids have been refined new sources of noise have appeared. Given this, we should anticipate further unpleasant surprises, particularly when we try to integrate SLSI non-hydrostatic models with time steps which are large compared with those allowed by Eulerian schemes.

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6a. APPENDIX 1.

In this section the von Neumann stability analysis of Eqs. (2.13) and (2.14) with $u(x,t) = u_0$ and $\phi' = \phi_N$ is performed.

Substituting as follows for any field

$$\psi_I^n = \hat{\psi} \lambda^n e^{ikI\Delta x},\tag{A.1.1}$$

then, using centered differencing on a c-grid,

$$\left(\frac{\partial\psi}{\partial x}\right)_{I}^{n} = i\frac{\sin(k\Delta x/2)}{\Delta x/2}\psi_{I}^{n} = iK\psi_{I}^{n} \tag{A.1.2}$$

For a Lagrange linear interpolation, (see, for example, Bates and McDonald, 1982)

$$\psi_*^n = (1 - \hat{\alpha})\psi_{I-p}^n + \hat{\alpha}\psi_{I-p-1}^n, \qquad (A.1.3)$$

where $p + \hat{\alpha} = \alpha = u_0 \Delta t / \Delta x$. Substituting ψ_I^n from Eq. (A.1.1) results in

$$\psi_*^n = \{(1 - \hat{\alpha}) + \hat{\alpha}e^{-ik\Delta x}\}e^{-ikp\Delta x}\psi_I^n = \Lambda_1\psi_I^n \qquad (A.1.4)$$

By the same method we get, for a Lagrange cubic interpolation,

$$\psi_*^n = \Lambda_3 \psi_I^n, \tag{A.1.5}$$

where (see, for example, Eq. (16) of McDonald (1987))

$$\Lambda_{3} = \left\{ -\frac{1}{6} \hat{\alpha} (1-\hat{\alpha})(2-\hat{\alpha})e^{+ik\Delta x} + \frac{1}{2}(1-\hat{\alpha})(1+\hat{\alpha})(2-\hat{\alpha}) + \frac{1}{2} \hat{\alpha} (1+\hat{\alpha})(2-\hat{\alpha})e^{-ik\Delta x} - \frac{1}{6} \hat{\alpha} (1-\hat{\alpha})(1+\hat{\alpha})e^{-2ik\Delta x} \right\} e^{-ikp\Delta x}.$$
(A.1.6)

Also,

$$\left(\frac{\partial\psi}{\partial x}\right)_*^n = iK\Lambda\psi_*^n,\tag{A.1.7}$$

where Λ stands for Λ_1 or Λ_3 depending on whether a linear or cubic interpolation is being used to evaluate the field at the departure point.

Using the following definitions of γ_L and γ_N ,

$$\gamma_L = \left(\frac{\Delta t}{2}K\right)^2 \phi_0; \qquad \gamma_N = \left(\frac{\Delta t}{2}K\right)^2 \phi_N, \qquad (A.1.8)$$

then substitution of A.1.1, A.1.2, A.1.5, A.1.7, and A.1.8 into Eqs. 2.13 and 2.14 results in the following dispersion relation:

$$\lambda^{3} \Big\{ 1 + (1 + \epsilon_{g})^{2} \gamma_{L} \Big\} + \lambda^{2} \Big\{ -2\Lambda + 2(1 - \epsilon_{g}^{2})\Lambda\gamma_{L} + \Big[\frac{3}{2}(1 + \epsilon_{g})^{2} + \frac{3}{2}(1 - \epsilon_{g}^{2})\Lambda \Big] \gamma_{N} \Big\} + \\\lambda \Big\{ \Lambda^{2} + (1 - \epsilon_{g})^{2}\Lambda^{2}\gamma_{L} + \Big[-\frac{1}{2}(1 + \epsilon_{g})^{2} + (1 - \epsilon_{g}^{2})\Lambda + \frac{3}{2}(1 - \epsilon_{g})^{2}\Lambda^{2} \Big] \gamma_{N} \Big\} \\ + \Big\{ \Big[-\frac{1}{2}(1 - \epsilon_{g}^{2})\Lambda - \frac{1}{2}(1 - \epsilon_{g})^{2}\Lambda^{2} \Big] \gamma_{N} \Big\} = 0$$
(A.1.9)

6b. APPENDIX 2.

For small ϵ Eq. (2.18) lends itself to a perturbation analysis; see for example, Bender and Orszag (1978). Postulate a solution

$$\lambda = \lambda_0 + \epsilon \lambda_1 + \epsilon \lambda_2 + \dots, \tag{A.2.1}$$

and substitute it in Eq. (2.18):

$$\left\{\lambda_0^3 - 2\lambda_0^2 \left(\frac{1-\gamma_L}{1+\gamma_L}\right) + \lambda_0\right\} + \epsilon \left\{3\lambda_1\lambda_0^2 - 4\lambda_1\lambda_0 \left(\frac{1-\gamma_L}{1+\gamma_L}\right) + 3\lambda_0^2 + 2\lambda_0 + \lambda_1 - 1\right\} + O(\epsilon^2) = 0 \qquad (A.2.2)$$

The zeroth order equation has three solutions; two given by Eq. (2.16), and $\lambda_0 = 0$. The latter corresponds to the computational mode. Here we concentrate on perturbations of the gravity wave solutions. Substituting λ_0 from Eq. (2.16) into the $O(\epsilon)$ equation and using the substitution $2(1 - \gamma_L)/(1 + \gamma_L) = \lambda_0 + 1/\lambda_0$ gives λ_1 in terms of the zeroth order solution:

$$\lambda_1 = \frac{1 - 3\lambda_0}{\lambda_0 - 1} = \frac{1 \pm 2i\sqrt{\gamma_L}}{\mp i\sqrt{\gamma_L}} \tag{A.2.3}$$

It is left as an exercise to derive Eq. (2.23) from Eq. (2.22).

6c. APPENDIX 3.

Equations (2.26)-(2.27) form a system of inhomogeneous linear partial differential equations with constant coefficients. Fourier transformation with respect to 'x' will change it to a system of inhomogeneous *ordinary* differential equations (with respect to time) with constant coefficients, which can be solved by standard methods. (See for example, Ince, ch VI). It is an interesting exercise to do this. Let us take a short-cut by postulating a solution the form

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \left\{ \hat{\psi}_h \exp i(kx - wt) + \hat{\psi}_p \exp ikx \right\}$$
(A.3.1)

where the subscript h refers to the homogeneous part of the solution and the subscript p to the particular integral. For each wave number k the homogeneous system becomes

$$\begin{bmatrix} -\omega + ku_0 & k \\ k\phi_0 & -\omega + ku_0 \end{bmatrix} \begin{bmatrix} \hat{u}_h \\ \hat{\phi}_h \end{bmatrix} \exp i(kx - wt) = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$
(A.3.2)

which only has a non-trivial solution for $\omega = k(u_0 \pm \sqrt{\phi_0})$. These are the two gravity waves. Next substitute the particular solution in the equations and we get for each wave number k:

$$\begin{bmatrix} ku_0 & k\\ k\phi_0 & ku_0 \end{bmatrix} \begin{bmatrix} \hat{u}_p\\ \hat{\phi}_p \end{bmatrix} \exp ikx = \begin{bmatrix} 0\\ ku_0\hat{\phi}_s \end{bmatrix} \exp ikx,$$
(A.3.3)

which, solving for $(\hat{u}_p, \hat{\phi}_p)$, yields

$$\hat{u}_p = -\hat{\phi}_p/u_0; \quad \hat{\phi}_p = \frac{u_0^2}{u_0^2 - \phi_0} \hat{\phi}_s$$
 (A.3.4)

What changes are caused by the semi-Lagrangian discretization? Using Eq. (A.3.1),

$$\psi_h(x,t+\Delta t) - \psi_h(x-u_0\Delta t,t) =$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{\psi}_h \exp i(kx - wt) \left[2i\sin\{(ku_0 - \omega)\Delta t/2\} \exp\{-i(ku_0 + \omega)\Delta t/2\} \right] \quad (A.3.5)$$
$$\psi_h(x, t + \Delta t) + \psi_h(x - u_0\Delta t, t) =$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \hat{\psi}_h \exp i(kx - wt) \left[2 \cos\{(ku_0 - \omega)\Delta t/2\} \exp\{-i(ku_0 + \omega)\Delta t/2\} \right] \quad (A.3.6)$$

The formulae for ψ_p can be obtained by putting $\omega = 0$ in Eqs. (A.3.5)-(A.3.6).

When these are substituted in Eqs. (2.29)-(2.30) then for each wave number k the homogeneous system now gives rise to

$$\begin{bmatrix} (2/\Delta t)sin\{(ku_0 - \omega)\Delta t/2\} & kcos\{(ku_0 - \omega)\Delta t/2\} \\ k\phi_0 cos\{(ku_0 - \omega)\Delta t/2\} & (2/\Delta t)sin\{(ku_0 - \omega)\Delta t/2\} \end{bmatrix} \begin{bmatrix} \hat{u}_h \\ \hat{\phi}_h \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$
(A.3.7)

which only has a non-trivial solution if the determinant of the matrix is zero. Next substitute the particular solution in the equations and we get for each wave number k:

$$\begin{bmatrix} (2/\Delta t)\sin\{ku_0\Delta t/2\} & k\cos\{ku_0\Delta t/2\} \\ k\phi_0\cos\{ku_0\Delta t/2\} & (2/\Delta t)\sin\{ku_0\Delta t/2\} \end{bmatrix} \begin{bmatrix} \hat{u}_p \\ \hat{\phi}_p \end{bmatrix} = \begin{bmatrix} 0 \\ (2/\Delta t)\sin\{ku_0\Delta t/2\}\hat{\phi}_s \end{bmatrix},$$
(A.3.8)

which results in

$$\hat{\phi}_p = \frac{\sin^2\{ku_0\Delta t/2\}}{\sin^2\{ku_0\Delta t/2\} - \phi_0(k\Delta t/2)^2\cos^2\{ku_0\Delta t/2\}}\hat{\phi}_s \tag{A.3.9}$$

In order to make the comparison with Eq. (A.3.4) more transparent define

$$S = \frac{\sin\{ku_0 \Delta t/2\}}{ku_0 \Delta t/2}; \quad C = \cos\{ku_0 \Delta t/2\}$$
(A.3.10)

Then Eq. (A.3.9) becomes

$$\hat{\phi}_p = \frac{u_0^2 S^2}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s \tag{A.3.11}$$

What happens when we replace Eq. (2.30) with the Ritchie-Tanguay (1996) discretization, Eq. (2.33)? Only the right hand side of Eq. (A.3.8) is changed:

$$\begin{bmatrix} (2/\Delta t)\sin\{ku_0\Delta t/2\} & k\cos\{ku_0\Delta t/2\}\\ k\phi_0\cos\{ku_0\Delta t/2\} & (2/\Delta t)\sin\{ku_0\Delta t/2\} \end{bmatrix} \begin{bmatrix} \hat{u}_p\\ \hat{\phi}_p \end{bmatrix} = \begin{bmatrix} 0\\ ku_0\cos\{ku_0\Delta t/2\}\hat{\phi}_s \end{bmatrix},$$
(A.3.12)

leading to

$$\hat{\phi}_p = \frac{u_0^2 SC}{u_0^2 S^2 - \phi_0 C^2} \hat{\phi}_s \tag{A.3.13}$$

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