

## Instability in a class of explicit two-time-level semi-Lagrangian schemes

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### SUMMARY

Recently Gospodinov and collaborators derived a family of second-order two-time-level semi-Lagrangian schemes that contain an undetermined parameter  $\alpha$ . It is shown that, when using one of these schemes to approximate the forcing terms in partial differential equations in a semi-Lagrangian coordinate frame, the choice of  $\alpha$  has a critical influence on the absolute stability of the method. Optimal stability properties are obtained by choosing  $\alpha = 1/4$  which corresponds to the SETTLS scheme proposed by Hortal.

KEYWORDS: Numerical weather prediction    Stability

### 1. INTRODUCTION

Recent attempts to improve the accuracy and stability of nominally two-time-level semi-Lagrangian schemes have been presented by Hortal (2002) and Gospodinov *et al.* (2001). Both authors focused on two particular aspects of such schemes, the methodology for calculating backward trajectories and the evaluation of nonlinear terms in the governing equations themselves. The focus of this note is on the second problem—the integration of partial differential equations of the form

$$\frac{d\psi}{dt} = F(\psi, \mathbf{x}, t), \tag{1}$$

which describes the rate of change of the field variable  $\psi(\mathbf{x}, t)$  moving with the flow in a Lagrangian reference frame subject to the forcing  $F$ .

Define notation such that the superscripts ‘+’, ‘0’ and ‘−’ denote values at time levels  $t + \Delta t$ ,  $t$  and  $t - \Delta t$ , respectively; the subscripts D and A denote evaluation at the departure point  $\mathbf{x}(t)$  and the arrival point  $\mathbf{x}(t + \Delta t)$ , respectively, along a Lagrangian trajectory, and  $\phi_A^+$  denotes the numerical approximation to  $\psi(\mathbf{x}(t + \Delta t), t + \Delta t)$ . Considerations of efficiency and accuracy have led to the approximation of the governing equations (1) in many ‘two-time-level’ semi-Lagrangian methods by expressions of the form

$$\frac{\phi_A^+ - \phi_D^0}{\Delta t} = \frac{1}{2}(L_A^+ + L_D^0) + a_1 N_A^0 + a_2 N_D^0 + a_3 N_A^- + a_4 N_D^-. \tag{2}$$

Here the forcing  $F$  in (1) has been split into a piece  $L$  that is evaluated using a trapezoidal time difference and a piece  $N$  that is evaluated using some explicit time integration formula, and the splitting of  $F$  into  $L$  and  $N$  is designed so that the implicit coupling introduced by the trapezoidal approximation to  $L(\psi)$  yields a simple implicit algebraic system. In the most elementary case,  $L$  and  $N$  represent linear and nonlinear forcings, respectively. The integration of the forcing due to  $N$  in (2) has been a source of instability in some semi-Lagrangian models (Gravel *et al.* 1993).

Recently Gospodinov *et al.* (2001) noted that all  $\mathcal{O}\{(\Delta t)^2\}$  accurate approximations to the nonlinear forcing in (2) that predict  $\psi(\mathbf{x}(t + \Delta t), t + \Delta t)$  from data at time levels  $t$  and  $t - \Delta t$  and spatial locations  $\mathbf{x}(t)$  and  $\mathbf{x}(t + \Delta t)$  may be expressed in the form

$$\frac{\phi_A^+ - \phi_D^0}{\Delta t} = \left(\frac{3}{4} - \alpha\right)N_A^0 + \left(\frac{3}{4} + \alpha\right)N_D^0 - \left(\frac{1}{4} - \alpha\right)N_A^- - \left(\frac{1}{4} + \alpha\right)N_D^-, \tag{3}$$

where  $\alpha$  is an undetermined parameter. In this note we examine how the choice of  $\alpha$  influences the stability of the family of semi-Lagrangian schemes (3).

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2. STABILITY ANALYSIS

One of the most useful ways to characterize the stability of numerical solutions to ordinary differential equations is to examine their *absolute stability*. Absolute stability is defined with respect to the test equation

$$\frac{d\psi}{dt} = (\lambda + i\omega)\psi, \tag{4}$$

where  $\lambda$  and  $\omega$  are real constants and the solution  $\psi(t)$  is complex-valued. *The region of absolute stability is that set of values  $(\lambda\Delta t, \omega\Delta t)$  for which perturbations of the numerical solution at time  $n\Delta t$  will produce a change in subsequent values that does not increase from step to step* (Gear 1971). Although (4) is a very simple equation, its significance arises from the fact that it also describes the local behaviour of numerical solutions to much more general systems of ordinary differential equations. To be specific, consider a general system of nonlinear ordinary differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}). \tag{5}$$

The easiest way to estimate the local stability of a numerical approximation to this equation with respect to variations about an arbitrary state  $\hat{\mathbf{x}}$  is to linearize the problem about  $\hat{\mathbf{x}}$ , in which case the coefficient for the  $i$ th perturbation component of  $\mathbf{x}$  becomes

$$\frac{dx_i}{dt} = f_i(\hat{\mathbf{x}}) + (x_j - \hat{x}_j) \frac{\partial f_i}{\partial x_j}(\hat{\mathbf{x}}). \tag{6}$$

The eigenvalues of the Jacobian  $\partial f_i/\partial x_j$  characterize the fundamental behaviours of the solution to the homogeneous part of (6). The amplitude of each eigenvector composing the homogeneous solution satisfies the simple test problem (4) with  $\lambda + i\omega$  replaced by the eigenvalue corresponding to that eigenvector.

The fundamental stability properties of semi-Lagrangian approximations to (1) can be similarly analysed by examining their absolute stability in the case where  $\psi = \psi(x, t)$ ,  $F = (\lambda + i\omega)\psi$ , and  $dx/dt$  is a constant  $U$ , so that (1) becomes

$$\frac{d\psi}{dt} = \left( \frac{\partial}{\partial t} + U \frac{\partial}{\partial x} \right) \psi = (\lambda + i\omega)\psi. \tag{7}$$

If  $\psi(x, 0) = g(x)$ , the solution to this test problem is

$$\psi(x, t) = g(x - Ut) e^{(\lambda+i\omega)t}, \tag{8}$$

which is non-amplifying for  $\lambda \leq 0$ . The absolute stability of semi-Lagrangian approximations to (7) may be assessed by determining the set of values of  $(U\Delta t/\Delta x, \lambda\Delta t, \omega\Delta t)$  for which both the numerical solution and the true solution decay with time. To simplify the analysis, the errors generated during the interpolation to departure points in the semi-Lagrangian algorithm will be ignored, in which case our results describe the limiting behaviour of a family of semi-Lagrangian schemes that use increasingly accurate interpolation.

We limit our investigation to the behaviour of the explicitly differenced forcing by setting  $L = 0$  and assuming that (7) is approximated by some member of the family of schemes (3). If  $U = 0$ , then  $x(t + \Delta t) = x(t)$ ; all schemes of the form (3) reduce to a second-order Adams–Bashforth time difference, and the region of the  $\lambda\Delta t - \omega\Delta t$  plane throughout which the numerical solution is non-growing (and the scheme is absolutely stable) is that lying inside the thick curve plotted in each of the panels in Fig. 1. Precisely the same region of absolute stability can be obtained, independent of the value of the Courant number  $U\Delta t/\Delta x$ , using the semi-Lagrangian scheme

$$\frac{\phi_A^+ - \phi_D^0}{\Delta t} = \frac{3}{2}G_D^0 - \frac{1}{2}G_{D-}^-, \tag{9}$$

where the subscript D– denotes evaluation at  $\mathbf{x}(t - \Delta t)$  (Durrán 1999, section 6.2). This method uses only data lying exactly along the trajectory terminating at the arrival point  $(\mathbf{x}(t + \Delta t), t + \Delta t)$ . In contrast to (9), all schemes of the form (3) utilize data from points that do not lie along the precise backwards trajectory, and for all of these schemes the region of absolute stability depends on the Courant number.

Hortal (2002) observed that, despite the superior stability of (9) when applied to the test problem (7), the requirement that  $N$  be evaluated at  $\mathbf{x}(t - \Delta t)$  leads to several difficulties in applications to complete weather-prediction models. Hortal therefore proposed a scheme (called SETTLS) that may be expressed in

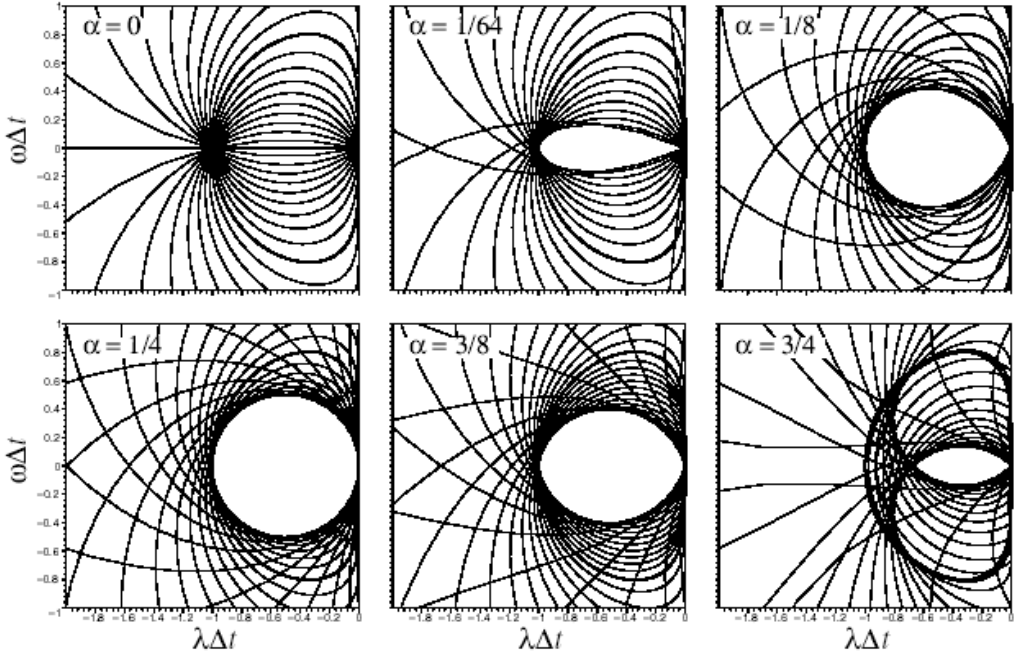


Figure 1. Regions of absolute stability for six values of  $\alpha$ . In each panel the area inside the heavy curve is the region of absolute stability when the Courant number is zero; it is identical for all  $\alpha$ . The individual curves trace out the limits of the absolutely stable region of a  $2\Delta x$  wave for 20 equally spaced values of the Courant number spanning the interval  $(-1, 1]$ . The central white region consisting of the set of points inside all of these curves is the region of the  $\lambda\Delta t-\omega\Delta t$  plane throughout which the method is absolutely stable independent of the Courant number. The absolutely stable region reduces to the single point  $(0, 0)$  when  $\alpha = 0$ . See text for further explanation.

the form (3) by choosing  $\alpha = 1/4$ . Hortal demonstrated that there exists a non-trivial region of the  $\lambda\Delta t-\omega\Delta t$  throughout which the SETTLS scheme yields absolutely stable solutions independent of the value of the Courant number. This region is smaller than that for the scheme (9) but, as will be demonstrated in the following, *it is larger than the absolute stability region obtained using any other choice of  $\alpha$ .*

The absolute stability of the family of semi-Lagrangian approximations (3) to the partial differential equation (7) may be determined by examining the behaviour of a single Fourier mode whose value at point  $(j\Delta x, n\Delta t)$  is  $A^n e^{ikj\Delta x}$ . Substituting this mode into (3) for the case  $N = (\lambda + i\omega)\psi$  and letting  $\theta = Uk\Delta t$ ,  $\gamma = (\lambda + i\omega)\Delta t$ , one obtains the following quadratic equation for the amplification factor  $A$ :

$$A^2 - [\gamma\{\frac{3}{4} - \alpha + e^{-i\theta}(\frac{3}{4} + \alpha)\} + e^{-i\theta}]A + \gamma\{\frac{1}{4} - \alpha + e^{-i\theta}(\frac{1}{4} + \alpha)\} = 0. \tag{10}$$

The amplification factor depends on the strength of the forcing per time step (through  $\gamma$ ) and the Courant number (through  $\theta$ ). Solutions to (10) are periodic in  $\theta$  over the interval  $[-\pi, \pi]$ .

The shortest wavelength resolved on the numerical mesh is  $2\Delta x$ , for which  $k = \pi/\Delta x$  and  $\theta = \pi U\Delta t/\Delta x$ . Thus, the amplification factor determined by (10) for the  $2\Delta x$  wave completes one periodic cycle as  $U\Delta t/\Delta x$  varies over the interval  $[-1, 1]$ . Therefore, except in the relatively inefficient case in which a semi-Lagrangian scheme is utilized with such a small time step that the maximum Courant number is less than unity, a necessary condition for the absolute stability of any of the family of schemes (3) is that the magnitude of the roots of (10) be less than or equal to unity for all  $\theta$ . The individual lines in each panel of Fig. 1 show the numerically computed boundary of the region of absolute stability for each  $\theta$  in the set  $[-9\pi/10, -8\pi/10, \dots, 0, \dots, \pi]$ . The region in which (3) is absolutely stable for all  $\theta$  is the closure of the intersection of the interiors of all these curves.

As indicated in Fig. 1, the region for which (3) yields absolutely stable solutions independent of Courant number (i.e. independent of  $\theta$ ) varies dramatically as a function of  $\alpha$ . This region reduces to the

origin when  $\alpha = 0$ , achieves its maximum size\* when  $\alpha = 1/4$  and gradually shrinks to a negligible size as  $\alpha$  becomes much larger than two. There is no value of  $\alpha$  for which the region of absolute stability includes a finite-length segment of the imaginary axis.

To better understand the significance of the absolute stability regions in Fig. 1, let  $\mu = U \Delta t / \Delta x$  be the Courant number, and let  $(\lambda \Delta t, \omega \Delta t)$  be an arbitrary point outside the region of absolute stability in the left half-plane  $\lambda \Delta t \leq 0$ , then there exists some  $\theta_0 \in (-\pi, \pi]$  for which the numerical solution will undergo spurious amplification. Since  $\theta = \mu k \Delta x$ , this amplification will appear in the Fourier mode of wavelength  $2\pi \mu \Delta x / \theta_0$ . (Again assuming the semi-Lagrangian integration uses Courant numbers larger than unity, the wavelength of the unstable mode will be no shorter than  $2\Delta x$  and will be resolvable on the numerical mesh.)

### 3. CONCLUSIONS

The choice  $\alpha = 0$ , yielding a method referred to as the classical scheme by Gospodinov *et al.* (2001) and the '1997' scheme by Hortal (2002) cannot be recommended for solutions of partial differential equations of the form (7) because the region of absolute stability shrinks to the origin when  $\alpha = 0$ . Although the best results are achieved when  $\alpha = 1/4$ , and this would appear to be the method of choice, the stability of the SETTLS approximation to (7) is still not ideal because, except for the origin, the imaginary axis lies outside its region of absolute stability. Thus, in the purely oscillatory case, for which  $\lambda = 0$  and  $\omega \neq 0$ , the SETTLS scheme generates spurious growth regardless of the size of  $\Delta t$ . Since Gospodinov *et al.* (2001) have demonstrated that all  $\mathcal{O}\{(\Delta t)^2\}$  accurate approximations for the computation of  $\phi_A^+$  involving only data at the arrival and departure points at the two preceding time levels may be written in the form (3), the current stability analysis shows that all such schemes will give unstable approximations when  $N$  is a purely oscillatory forcing, unless the unstable growth is compensated by the numerical approximation to  $L$  or by some other dissipative operator. Note that, in this respect, the stability of SETTLS is exactly opposite that which would be obtained using a three-time-level semi-Lagrangian scheme in which the forcing term  $N$  is integrated using leapfrog time differencing. Again neglecting possible stabilizing influences due to the numerical approximation of  $L$  or other dissipative operators, the leapfrog integration will only give stable results when  $N$  is associated with a purely oscillatory forcing.

Thus it seems advisable to ensure that, when the total semi-Lagrangian forcing  $F$  is split into  $L$  and  $N$  and the forcing  $N$  is integrated using SETTLS, the function  $N$  should not be purely oscillatory in the sense that, when  $N(\psi, \mathbf{x}, t)$  is linearized about arbitrary points in the phase space of the solution, the resulting linear operator should have no purely imaginary eigenvalues. Alternative approaches that can eliminate this type of instability within the context of two-time-level semi-Lagrangian schemes are to avoid the family of methods (3) by either off-centring the time extrapolation in the integration of  $N(\psi, \mathbf{x}, t)$  (Gravel *et al.* 1993), although this decreases the accuracy of the method to first order, or to simply set  $L = F$  and  $N = 0$  in (2) (Coté *et al.* 1998; Cullen 2001), which in most practical applications requires the solution of a more difficult system of nonlinear algebraic equations.

Up to this point, our focus has been on the semi-Lagrangian solution of partial differential equations of the form (1) without considering the method for integrating backward trajectories or the interaction between the trajectory computation and the overall stability of the scheme. Schemes of the form (3) may also be used to compute back trajectories. Indeed, the use of SETTLS for trajectory computations made a major improvement in several forecasts with the model of the European Centre for Medium-Range Weather Forecasts (Hortal 2002).

Semi-Lagrangian trajectory calculations require a backward-in-time integration of the ordinary differential equation (ODE)

$$\frac{d\mathbf{x}}{dt} = \mathbf{V}(\mathbf{x}, t), \quad (11)$$

where  $\mathbf{V}$  is the fluid velocity. Given that each back trajectory is computed only over a time interval  $\Delta t$ , it is probably not important to examine the stability of the solutions to (11) *in isolation*. Furthermore, it is not clear what can be said about the absolute stability of solutions to (11) generated using schemes of the form (3) since, when (3) is applied to an ODE, the method differs from conventional multistep ODE solvers in that the forcing  $\mathbf{V}(\mathbf{x}, t)$  is not only evaluated using approximations to the solution at previous time levels, but also using additional points  $(\mathbf{x}, t)$  that lie off the trajectory. One thing that can be said is that the approximate solutions to ODE generated by (3) are sufficiently stable to converge to the exact solution in the limit  $\Delta t \rightarrow 0$  independent of the value of  $\alpha$ , because (3) satisfies the so-called *root condition* (Isaacson and Keller 1966).

\* The value of  $\alpha$  that yields the maximum region of absolute stability was determined empirically by numerically evaluating the roots of (10) for a series of different  $\alpha$  and is subject to an uncertainty of  $\pm 1/64$ .

The much more important question of the influence of the trajectory calculation on the stability of the overall scheme is a subtle and difficult problem that is beyond the scope of this note. An example of the trouble that can occur is given by Bates *et al.* (1995), who showed that a forward-in-time extrapolation of the velocity field in the back-trajectory calculation may create instability in semi-Lagrangian approximations to Rossby wave solutions to the linearized non-divergent vorticity equation.

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