Semi-Lagrangian Integration Schemes for Atmospheric Models—A Review

ANDREW STANIFORTH AND JEAN CÔTÉ

Recherche en prévision numérique, Service de l'environnement atmosphérique, Dorval, Québec, Canada

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ABSTRACT

The semi-Lagrangian methodology is described for a hierarchy of applications (passive advection, forced advection, and coupled sets of equations) of increasing complexity, in one, two, and three dimensions. Attention is focused on its accuracy, stability, and efficiency properties. Recent developments in applying semi-Lagrangian methods to 2D and 3D atmospheric flows in both Cartesian and spherical geometries are then reviewed. Finally, the current status of development is summarized, followed by a short discussion of future perspectives.

1. Introduction

Accurate and *timely* forecasts of weather elements are of great importance to both the economy and to public safety. Weather forecasters rely on guidance provided by numerical weather prediction (NWP), a computer-intensive chain of operations beginning with the collection of data from around the world and culminating in the production of weather charts and computer-worded messages. At the heart of the system are the numerical models used to assimilate the data and to forecast future states of the atmosphere. The accuracy of the forecasts depends among other things on model resolution. Increased resolution, given the *real-time* constraints, can only be achieved by judiciously combining the most efficient numerical methods on the most powerful computers with the most appropriate programing techniques.

A long-standing problem in the integration of NWP models is that the maximum permissible time step has been governed by considerations of stability rather than accuracy. For the integration to be stable, the time step has to be so small that the time truncation error is much smaller than the spatial truncation error, and it is therefore necessary to perform many more time steps than would otherwise be the case. The choice of time integration scheme is, therefore, of crucial importance when designing an efficient weather forecast model, and this is also true when designing environmental emergency response models. Early NWP models used an explicit leapfrog scheme, whose time step is limited by the propagation speed of gravitational oscillations. By treating the linear terms responsible for these oscillations in an implicit manner, it is possible to lengthen the time step by about a factor of 6, at little additional cost and without degrading the accuracy of the solution [e.g., Robert (1969); Robert et al. (1972)]. Such a scheme is termed *semi-implicit.* Nevertheless, the maximum stable time step still remains much smaller than seems necessary from considerations of accuracy alone (Robert 1981).

Discretization schemes based on a semi-Lagrangian treatment of advection have elicited considerable interest in the past decade for the efficient integration of weather forecast models, since they offer the promise of allowing larger time steps (with no loss of accuracy) than Eulerian-based advection schemes (whose time-step length is overly limited by considerations of stability). To achieve this end it is essential to associate a semi-Lagrangian treatment of advection with a sufficiently stable treatment of the terms responsible for the propagation of gravitational oscillations. By associating a semi-Lagrangian treatment of advection with a semi-implicit treatment of gravitational oscillations, Robert (1981, 1982) demonstrated a further increase of a factor of 6 in the maximum stable time step, at some additional cost. This idea was demonstrated in the context of a three-time-level shallow-water finite-difference model in Cartesian geometry, and resulted in the time truncation errors that were finally of the same order as the spatial ones.

Since Robert's seminal papers, the semi-Lagrangian methodology for advection-dominated fluid flow problems has been extended in several important ways. The purpose of this paper is to summarize the fundamentals of semi-Lagrangian advection (section 2), to describe its application to coupled sets of equations (section 3), to review recent extensions of the method (section 4) not covered in the discussions of the previous sections, and to draw some conclusions (section 5).

Corresponding author address: Dr. Andrew Staniforth, Recherche en prévision numérique, 2121 Route Trans-Canadienne porte 508, Dorval, Québec H9P 1J3, Canada.

2. Semi-Lagrangian advection

In an Eulerian advection scheme an observer watches the world evolve around him at a fixed geographical point. Such schemes work well on regular Cartesian meshes (facilitating vectorization and parallelization of the resulting code), but often lead to overly restrictive time steps due to considerations of computational stability. In a Lagrangian advection scheme an observer watches the world evolve around him as he travels with a fluid particle. Such schemes can often use much larger time steps than Eulerian ones, but have the disadvantage that an initially regularly spaced set of particles will generally evolve to a highly irregularly spaced set at later times (Welander 1955), and important features of the flow may consequently not be well represented. The idea behind semi-Lagrangian advection schemes is to try to get the best of both worlds: the regular resolution of Eulerian schemes and the enhanced stability of Lagrangian ones. This is achieved by using a different set of particles at each time step, the set of particles being chosen such that they arrive exactly at the points of a regular Cartesian mesh at the end of the time step. This idea gradually evolved from the pioneering work of Fjørtoft (1952, 1955), Wiin-Nielsen (1959), Krishnamurti (1962), Sawyer (1963), Leith (1965) and Purnell (1976). Of the formulations introduced prior to that of Purnell (1976), those of Krishnamurti (1962) and Leith (1965) are perhaps the most similar to those used in present-day semi-Lagrangian advection schemes; however, as formulated they are only valid for Courant numbers ($C = |U|\Delta t/\Delta x$) less than unity.

a. Passive advection in 1D

To present the basic idea behind the semi-Lagrangian method in its simplest context, we apply it to the 1D advection equation

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{dx}{dt}\frac{\partial F}{\partial x} = 0, \qquad (1)$$

where

$$\frac{dx}{dt} = U(x, t), \qquad (2)$$

and $U(x, t)$ is a given function. Equation (1) states that the scalar F is constant along a fluid path (or trajectory or characteristic). In Fig. 1, the *exact* trajectory in the (x–t) plane of the fluid particle that arrives at mesh point x_m at time $t_n + \Delta t$ is denoted by the solid curve AC, and an *approximate* straight-line trajectory by the dashed line $A'C$. Let us assume that we know $F(x, t)$ at all mesh points x_m at times $t_n - \Delta t$ and t_n, and that we wish to obtain values at the same mesh points at time $t_n + \Delta t$. The essence of semi-Lagrangian advection is to approximately integrate (1) along the approximated fluid trajectory $A'C$. Thus,

$$\frac{F(x_m, t_n + \Delta t) - F(x_m - 2\alpha_m, t_n - \Delta t)}{2\Delta t} = 0, \qquad (3)$$

where α_m is the distance BD the particle travels in x in time Δt, when following the approximated space–time trajectory $A'C$. Thus if we know α_m, then the value of F at the arrival point x_m at time $t_n + \Delta t$ is just its value at the upstream point $x_m - 2\alpha_m$ at time $t_n - \Delta t$. However, we have not as yet determined α_m; even if we had, we only know F at mesh points, and generally it still remains to evaluate F somewhere between mesh points.

To determine α_m, note that U evaluated at the point B of Fig. 1 is just the inverse of the slope of the straight line $A'C$, and this gives the following $O(\Delta t^2)$ approximation to (2) (Robert 1981):

$$\alpha_m = \Delta t U(x_m - \alpha_m, t_n). \qquad (4)$$

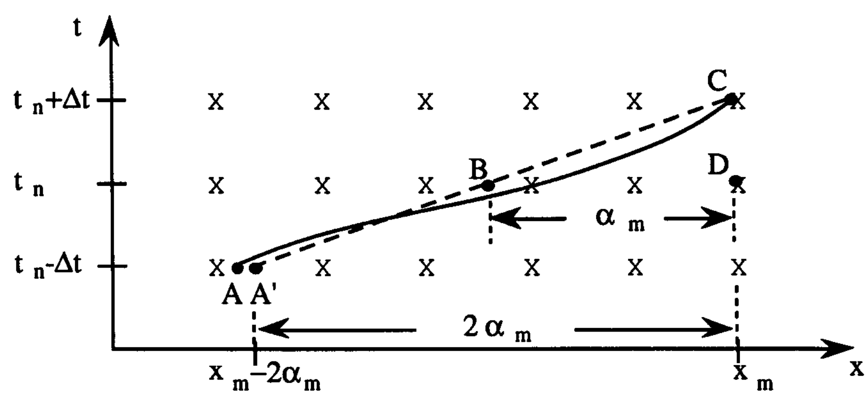

FIG. 1. Schematic for three-time-level advection. Actual (solid curve) and approximated (dashed line) trajectories that arrive at mesh point x_m at time $t_n + \Delta t$. Here α_m is the distance the particle is displaced in x in time Δt.

Equation (4) may be iteratively solved for the displacement α_m, for example by

$$\alpha_m^{(k+1)} = \Delta t U[x_m - \alpha_m^{(k)}, t_n], \quad (5)$$

with some initial guess for $\alpha_m^{(0)}$, provided U can be evaluated between mesh points. To evaluate F and U between mesh points, spatial interpolation is used. The semi-Lagrangian algorithm for passive advection in 1D in summary is thus:

(i) Solve (5) iteratively for the displacements α_m for all mesh points x_m, using some initial guess (usually its value at the previous time step), and an interpolation formula.

(ii) Evaluate F at upstream points $x_m - 2\alpha_m$ at time $t_n - \Delta t$ using an interpolation formula.

(iii) Evaluate F at arrival points x_m at time $t_n + \Delta t$ using (3).

We defer the discussion of interpolation details to section 2d, and first generalize the above three-time-level algorithm to forced advection in several space dimensions (section 2b), and to *two* time levels (section 2c).

b. *Forced advection in multidimensions*

Consider the forced-advection problem

$$\frac{dF}{dt} + G(\mathbf{x}, t) = R(\mathbf{x}, t), \quad (6)$$

where

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \mathbf{V}(\mathbf{x}, t) \cdot \nabla F, \quad (7)$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{V}(\mathbf{x}, t), \quad (8)$$

Here, $\mathbf{x}$ is the position vector (in 1-, 2- or 3D), ∇ is the gradient operator, and G and R are forcing terms. A semi-Lagrangian approximation to (6) and (8) is then:

$$\frac{F^+ - F^-}{2\Delta t} + \frac{1}{2}[G^+ + G^-] = R^0, \quad (9)$$

$$\alpha = \Delta t \mathbf{V}(\mathbf{x} - \alpha, t), \quad (10)$$

where the superscripts "+", "0" and "−", respectively, denote evaluation at the arrival point $(\mathbf{x}, t + \Delta t)$, the midpoint of the trajectory $(\mathbf{x} - \alpha, t)$ and the departure point $(\mathbf{x} - 2\alpha, t - \Delta t)$. Here, $\mathbf{x}$ is now an arbitrary point of a regular (1-, 2- or 3D) mesh.

The above is a centered $O(\Delta t^2)$ approximation to (6) and (8), where G is evaluated as the time average of its values at the end points of the trajectory, and R is evaluated at the midpoint of the trajectory. The trajectories are calculated by iteratively solving (10) for the *vector* displacements α in an analogous manner to the 1D case for passive advection [Eq. (5)]. If G is known (we assume that R is known since it involves evaluation at time t), then the algorithm proceeds in an analogous manner to the 1D passive advection one and is thus,

(i) Solve (10) iteratively for the vector displacements α for all mesh points $\mathbf{x}$, using some initial guess (usually its value at the previous time step), and an interpolation formula.

(ii) Evaluate $F - \Delta t G$ at upstream points $\mathbf{x} - 2\alpha$ at time $t - \Delta t$ using an interpolation formula. Evaluate $2\Delta t R$ at the midpoints $\mathbf{x} - \alpha$ of the trajectories at time t using an interpolation formula.

(iii) Evaluate F at arrival points $\mathbf{x}$ at time $t + \Delta t$ using

$$F(\mathbf{x}, t + \Delta t) = (F - \Delta t G)|_{(\mathbf{x}-2\alpha, t-\Delta t)} + 2\Delta t R|_{(\mathbf{x}-\alpha, t)} - \Delta t G|_{(\mathbf{x}, t+\Delta t)}$$
$$= (F - \Delta t G)^- + 2\Delta t R^0 - \Delta t G^+ \quad (9')$$

If G is not known at time $t + \Delta t$ (for instance if it involves another dependent variable in a set of coupled equations), then this leads to a coupling to other equations (more on this in section 3).

c. *Two-time-level advection schemes (and a pollutant-transport application)*

Present semi-Lagrangian schemes are based on discretization over either two or three time levels, and thus far we have restricted our attention to three-time-level schemes. The principal advantage of two-time-level schemes over three-time-level ones is that they are potentially twice as fast. This is because three-time-level schemes require time steps half the size of two-time-level ones for the same level of time truncation error (Temperton and Staniforth 1987). It is, however, important to maintain second-order accuracy in time in order to reap the full benefits of a two-time-level scheme (since enhanced stability with large time steps is of no benefit if it is achieved at the expense of diminished accuracy). Early two-time-level schemes for NWP models unfortunately suffered from this deficiency (e.g., Bates and McDonald 1982; Bates 1984; McDonald 1986). The crucial issue is how to efficiently determine the trajectories to at least second-order accuracy in time (Staniforth and Pudykiewicz 1985; McDonald 1987).

This problem arises in the context of self-advection of momentum. To see this we reexamine the algorithm of section 2a for 1D advection. Provided U is known at time t_n, *independently of F at the same time,* then it is possible to evaluate the trajectory, and then leapfrog the value of F from time $t_n - \Delta t$ to $t_n + \Delta t$, without knowing any value of F at time t_n. Proceeding in this way, $F(t_n + 3\Delta t)$ is then obtained using values of $F(t_n + \Delta t)$ and $U(t_n + 2\Delta t)$. Thus we have two decoupled independent integrations, one using values of F at even time steps and U at odd time steps, the other using values of F at odd time steps and U at even time steps. Either of these two independent solutions is sufficient, thus halving the computational cost, and we obtain a two-time-level scheme (for the advected quantity F) by merely relabeling time levels $t_n - \Delta t$, t_n and $t_n + \Delta t$, respectively, as t_n, $t_n + \Delta t/2$, and $t_n + \Delta t$ (see Fig. 2). Note that values of U (assumed known) only appear at time level $t_n + \Delta t/2$, and they are *solely* used to estimate the trajectories.

This is the essence of the 2D advection–diffusion algorithm described and analyzed in Pudykiewicz and Staniforth (1984). It led to the development of a three-dimensional pollutant transport model (Pudykiewicz et al. 1985), where a family of chemical species are advected and diffused in the atmosphere using winds and diffusivities: these are either provided by a NWP model (for real-time prediction) or from analyzed data (for postevent simulations). This model is designed to provide real-time guidance in the event of an environmental accident and has been used to successfully simulate the dispersion of nuclear debris from the Chernobyl reactor accident (Pudykiewicz 1989). It has evolved into Canada's Environmental Emergency Response Model (Pudykiewicz 1990).

Returning to the problem of self-advection of momentum, the above argument breaks down in the special case where $F = U$ in (1) or $F = \mathbf{V}$ in (6); i.e., when the transported quantity U or $\mathbf{V}$ is advected by itself, as is the case for the momentum equations of fluid-dynamic problems in general, and NWP models in particular. This problem was addressed simultaneously and independently by Temperton and Staniforth (1987) and McDonald and Bates (1987), opening the way toward stable and accurate two-time-level schemes. The key idea here is to time extrapolate the winds [with an $O(\Delta t^2)$-accurate extrapolator] to time level $t + \Delta t/2$ using the known winds at time levels t and $t - \Delta t$: these winds are then used to obtain sufficiently accurate [$O(\Delta t^2)$] estimates of the trajectories, which in turn are used to advance the dependent variables from time level t to $t + \Delta t$. Thus, the two-time-level algorithm to solve (6)–(8), analogous to the three-time-level one given by (9)–(10), is (see Fig. 2)

$$\frac{F^+ - F^0}{\Delta t} + \frac{1}{2}[G^+ + G^0] = R^{1/2}, \qquad (11)$$

where

$$\alpha = \Delta t \mathbf{V}^*(\mathbf{x} - \alpha/2, t + \Delta t/2), \qquad (12)$$

$$\mathbf{V}^*(\mathbf{x}, t + \Delta t/2) = (3/2)\mathbf{V}(\mathbf{x}, t) - (1/2)\mathbf{V}(\mathbf{x}, t - \Delta t) + O(\Delta t^2); \qquad (13)$$

the superscripts "+", "½", and "0" now, respectively, denote evaluation at the arrival point $(\mathbf{x}, t + \Delta t)$, the midpoint of the trajectory $(\mathbf{x} - \alpha/2, t + \Delta t/2)$, and the departure point $(\mathbf{x} - \alpha, t)$, and α is still the distance the fluid particle is displaced in time Δt.

In the above formulation the evaluation of $R^{(1/2)}$ involves extrapolated quantities and, therefore, could potentially lead to instability. Temperton and Staniforth (1987) did not find this to be a problem when some weak nonlinear metric effects were evaluated in this way in a shallow-water model integrated on a polar-stereographic projection, but it seems preferable to evaluate all nonadvective terms (i.e., G in the above) as time averages along the trajectory whenever possible. [Subsequently Côté (1988) showed how to avoid evaluating the above-mentioned metric terms in terms of extrapolated quantities.] However, Higgins and Bates (1990) report that evaluating the product term (of the geopotential perturbation and divergence) in the continuity equation of a global shallow-water model using time-extrapolated quantities [as in Bates et al. (1990)] leads to the growth of computational noise. An alternative solution is to discretize the continuity equation in logarithmic form as in Côté and Staniforth (1990),

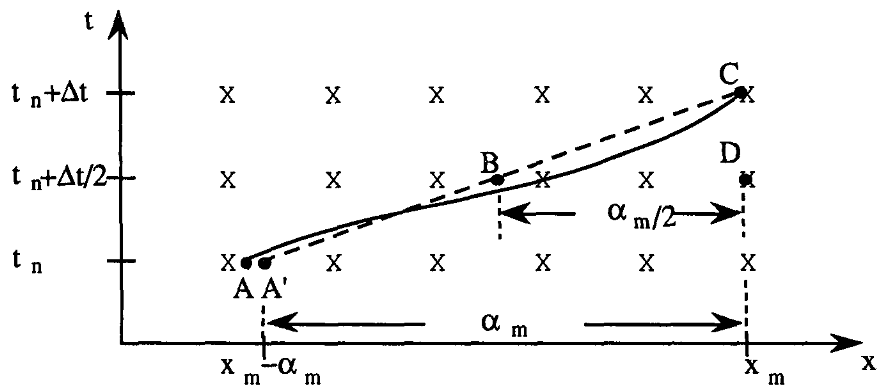

FIG. 2. Schematic for two-time-level advection. Actual (solid curve) and approximated (dashed line) trajectories that arrive at mesh point x_m at time $t_n + \Delta t$. Here α_m is the distance the particle is displaced in x in time Δt.

at the price of making the elliptic boundary-value problem of the semi-implicitly treated terms mildly nonlinear: this has the advantage that it retains $O(\Delta t^2)$ accuracy because it is still a centered approximation. A further possible alternative is discussed in section 4d. Note that when all nonadvective terms are evaluated implicitly as time averages along trajectories, then extrapolated quantities are used *solely* for the purpose of obtaining a sufficiently accurate estimate of the trajectories.

Temperton and Staniforth (1987) examined several alternative ways of extrapolating quantities for the purpose of estimating trajectories. They found that those methods that keep a particle on its exact trajectory for solid-body rotation seem to give better results for the more general problem than those that do not. In particular, they found it advantageous to use a three-term extrapolator (using winds at times t, $t - \Delta t$, and $t - 2\Delta t$ to obtain an extrapolated wind at $t + \Delta t/2$) instead of the two-term extrapolator (13). They also found that time-extrapolating winds along the trajectory (their method 4) is less accurate than time-extrapolating winds at mesh points as in (13).

d. Interpolation

A priori, any interpolation could be used to evaluate F and U (or **V**) between mesh points in the above algorithm. In practice the choice of interpolation formula has an important impact on the accuracy and efficiency of the method. Various polynomial interpolations have been tried including: linear; quadratic Lagrange; cubic Lagrange; cubic spline; and quintic Lagrange.

For step (ii) of the algorithm, it is found (see e.g., Purnell 1976; Bates and McDonald 1982; McDonald 1984; and Pudykiewicz and Staniforth 1984, for analysis) that cubic interpolation is a good compromise between accuracy and computational cost. While quadratic Lagrange interpolation is viable and was used in most of the early studies (e.g., Krishnamurti 1962, 1969; Leith 1965; Mathur 1970, 1974; Bates and McDonald 1982), cubic interpolation has been widely adopted in recent studies (e.g., Robert et al. 1985; McDonald 1986; Bates and McDonald 1987; Ritchie 1988; Côté and Staniforth 1988; Bates et al. 1990). Cubic interpolation gives fourth-order spatial truncation errors with very little damping (it is very scale selective, affecting primarily the smallest scales), whereas linear interpolation (see McDonald 1984 for discussion) has unacceptably large damping (it is also scale selective, but has a much less sharp response). Cubic spline interpolation has the useful property that it conserves mass for divergence-free flows (Bermejo 1990). Purser and Leslie (1988) recommend using at least fourth-order (i.e., cubic) interpolation, and have used quintic interpolation in their recent work (Leslie and Purser 1991). Improving the order of the interpolation formally increases the accuracy, but at additional cost, and the law of diminishing returns ultimately applies.

For step (i), the order of the interpolation is much less important. Theoretically, McDonald (1987) has shown that one should use an interpolation of order one less than for step (ii); e.g., quadratic interpolation of U when using cubic interpolation of F. In practice however, in the context of both passive advection and coupled systems of equations in several spatial dimensions, it is found (Staniforth and Pudykiewicz 1985; Temperton and Staniforth 1987; Bates et al. 1990) that it is sufficient to use linear interpolation for the computation of the displacements, when using cubic interpolation for F, which is very economical. It is also found that there is no advantage in using more than two iterations for solving the displacement equation [step (i)]. McDonald (1987) has shown theoretically that it is not necessary to use the same order of interpolation for each iteration. For example, it is more economical and no less accurate to perform the first iteration using linear interpolation and the second using quadratic, than to use quadratic interpolation for both.

Pudykiewicz et al. (1985) have shown that a sufficient condition for convergence of the iterative solution of step (i) is that Δt be smaller than the reciprocal of the maximum absolute value of the wind shear in any coordinate direction. Thus $\Delta t < [\max(|u_x|, |u_y|, |v_x|, |v_y|)]^{-1}$ for 2D flow, where u and v are the two wind components, and the time step of semi-Lagrangian schemes is not only limited by accuracy considerations (i.e., temporal discretization errors) but also by properties of the flow (i.e., wind shear). They estimated for NWP and long-range transport of pollutants problems that convergence is assured provided Δt is less than 3 h, which is an order of magnitude larger than the maximum time step permitted by Eulerian advection schemes in analogous circumstances.

e. Stability and accuracy (and connection with other advection methods)

Analyses of the stability properties of the semi-Lagrangian advection scheme (e.g., Bates and McDonald 1982; McDonald 1984; Pudykiewicz and Staniforth 1984; Ritchie 1986, 1987) show that the maximum time step is not limited by the maximum wind speed, as is the case for Eulerian advection schemes, and consequently it is possible to stably integrate with Courant numbers ($C = |U|\Delta t/\Delta x$) that far exceed unity. To illustrate this point we reproduce (with permission) the results of Bermejo (1990) for the slotted cylinder test of Zalesak (1979). In Fig. 3a we show the slotted cylinder at initial time, and in Fig. 3b the corresponding result after *six* revolutions of solid-body rotation at uniform angular velocity about the domain center. The experiment was conducted using a cubic-spline interpolator at a Courant number of 4.2, which is consid-

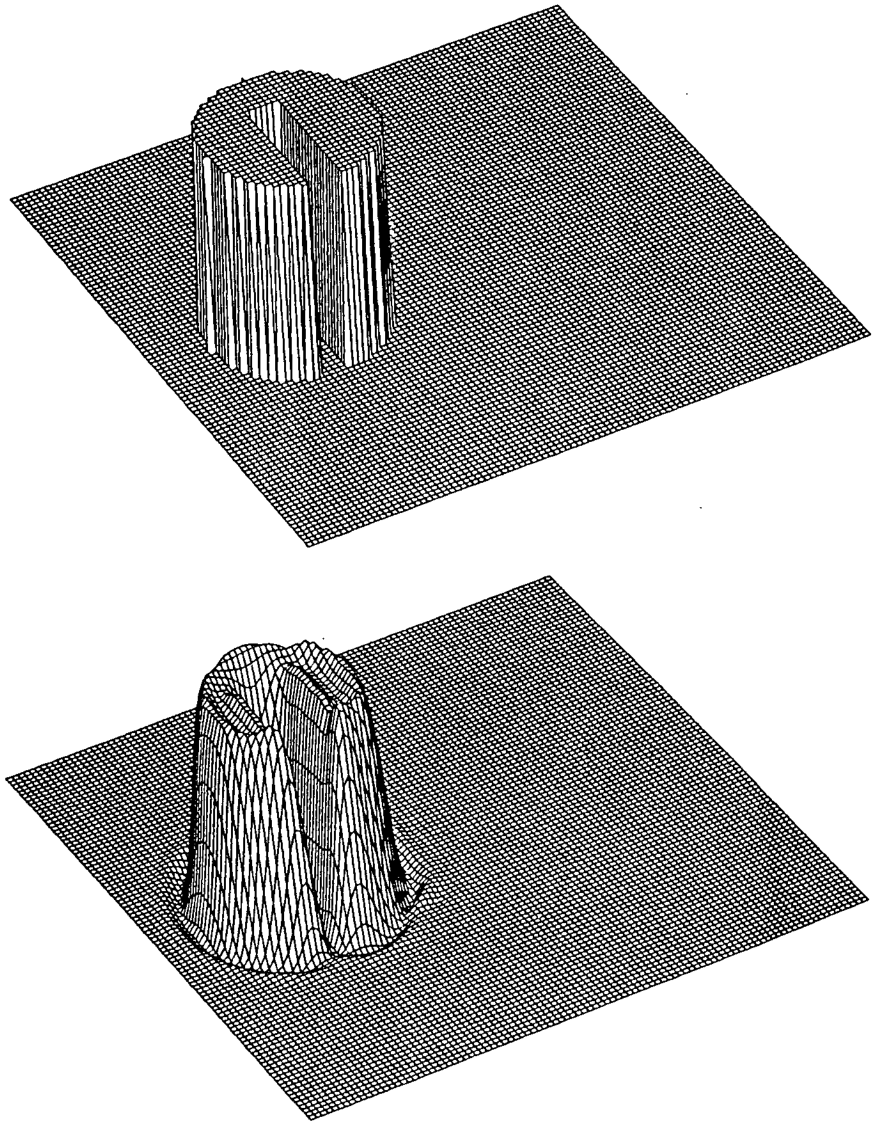

FIG. 3. The "slotted" cylinder, (a) at initial time and (b) after six revolutions.

erably larger than that of an Eulerian advection scheme. This is recognized as being a challenging test, and the result is remarkably good. In particular the results illustrate the scheme's ability to handle sharp discontinuities without disastrous consequences (even though it was not designed specifically to do so) and the absence of noticeable dispersion problems (which are typically present for Eulerian advection schemes).

This behavior in the presence of discontinuities or near discontinuities was also observed in the study of Kuo and Williams (1990) for a scale collapse problem. They concluded that semi-Lagrangian schemes are to be preferred to Eulerian schemes for this kind of problem since they have much smaller dispersion errors (which are localized around the shock) and can be integrated with significantly longer time steps. This is an important finding since, as pointed out by one of the reviewers, there is a mistaken belief that semi-Lagrangian schemes are only good for smooth flows. Their findings clearly show that this is not the case. In a similar vein, Ritchie (1985) argued that the localization of errors to the regions where the gradients are strongest when semi-Lagrangian advection is used is a desirable property that may be advantageously exploited for the treatment of moisture transport in NWP models, since large local gradients frequently occur in moisture fields (e.g., at fronts). He reported that semi-Lagrangian advection led to better results than Eulerian advection in the context of a 48-h forecast.

In general it is found that semi-Lagrangian advection is competitive with Eulerian advection with respect to accuracy, but it has the added advantage that this accuracy can be achieved at less computational cost, since models can be integrated stably with time steps that far exceed the maximum possible time steps of Eulerian schemes. The aforementioned stability analyses show that semi-Lagrangian advection schemes have very good phase speeds with little numerical dispersion, but contrary to some Eulerian schemes (e.g., leapfrog-based schemes) there is some damping due to interpolation as discussed in section 2d. This damping is fortunately very scale selective (at least when using high-order interpolators). McCalpin (1988) has theoretically compared this damping with more traditional forms such as Laplacian and biharmonic dissipation, and derived some criteria to ensure that the damping due to semi-Lagrangian advection is less than that due to the more traditional forms. In practice Ritchie (1988) and Côté and Staniforth (1988) have found that semi-Lagrangian integration schemes have three times less damping than a typical Eulerian global medium-range forecast model run at typical resolution with a typical biharmonic dissipation.

Semi-Lagrangian advection is intimately connected with several other advection methods that have appeared in the literature over the years, including particle-in-cell (e.g., Raviart 1985) and characteristic Galerkin (e.g., Morton 1985; Karpic and Peltier 1990) methods. Indeed for uniform advection in 1D, the simplest semi-Lagrangian advection scheme (using linear interpolation, and not recommended) is equivalent to both classical upwinding and to the simplest characteristic Galerkin method; and semi-Lagrangian advection using cubic-spline interpolation is equivalent to the higher-order characteristic Galerkin methods of Morton (1985) and Karpic and Peltier (1990), and also to a particle-in-cell method described in Eastwood (1987). Further, under more general conditions (including nonuniform advection in 2- and 3D), Bermejo (1990) has shown that semi-Lagrangian advection using cubic-spline interpolation can be viewed as a particle-in-cell finite-element method.

Several well-known Eulerian methods can also be interpreted as being special cases of semi-Lagrangian ones. Thus the Lax–Wendroff, Takacs (1985) third-order, and Tremback et al. (1987) schemes are, respectively, equivalent for 1D uniform advection to semi-Lagrangian schemes with quadratic-Lagrange, cubic-Lagrange and nth-order Lagrange interpolation. Note, however, that these Eulerian methods are restricted to Courant numbers less than unity and are consequently less general than their semi-Lagrangian counterparts.

Although the semi-Lagrangian method is equivalent for uniform 1D advection to several other methods, what distinguishes it from other methods is that it generalizes differently to nonuniform advection in multidimensions. The principal difference is the use of (10), introduced in Robert (1981), for the trajectory calculations. Of particular importance is that *the approximation of the trajectory equation (8) is $O(\Delta t^2)$ accurate.* It is possible to use a simpler, and cheaper, $O(\Delta t)$ accurate method to approximate the displacement equation (8) (as in e.g., Mathur 1970; and Bates and McDonald 1982) but this can dramatically deteriorate the accuracy of the scheme, as shown by Staniforth and Pudykiewicz (1985) and Temperton and Staniforth (1987), and analyzed by McDonald (1987). Consequently most, if not all, recent semi-Lagrangian schemes use an $O(\Delta t^2)$ method for discretizing the trajectory equation.

3. Application to coupled sets of equations

To illustrate how semi-Lagrangian advection can be advantageously used to solve coupled systems of equations, we describe its application to the discretization of the shallow-water equations:

$$\frac{dU}{dt} + \phi_x - fV = 0, \qquad (14)$$

$$\frac{dV}{dt} + \phi_y + fU = 0, \qquad (15)$$

$$\frac{d\ln\phi}{dt} + U_x + V_y = 0, \qquad (16)$$

where U and V are the wind components, ϕ ($=gz$) is the geopotential height (i.e., height multiplied by g) of the free surface of the fluid above a flat bottom, and f is the Coriolis parameter.

These equations are often used in NWP to test new numerical methods, since they are a 2D prototype of the 3D equations that govern atmospheric motions [they can be derived from them under certain simplifying assumptions (Pedlosky 1987)]. They share several important properties with their progenitor. A linearization of the equations reveals that there are two basic kinds of associated motion, slow-moving Rossby modes (most of which affect the large-scale weather motions, and which move to leading order at the local wind speed) and small-amplitude fast-moving gravitational oscillations (which are inadequately represented at initial time due to the paucity of the observational network). From a numerical standpoint this has the important implication that the time step of an explicit Eulerian scheme (e.g., leapfrog) is limited by the speed of the fastest-moving gravity mode. Since for atmospheric motions this speed is six times faster than those associated with the Rossby modes that govern the weather, this leads to time steps that are six times shorter than those associated with an explicit treatment of advection. A time-implicit treatment of the pressure-gradient term of the vector momentum equation [second terms of (14) and (15)] and horizontal divergence of the continuity equation [second and third terms of (16)], introduced in Robert (1969) and termed the *semi-implicit* scheme, allows stable integrations with no loss of accuracy using time steps that are six times longer than that of the leapfrog scheme. The price to be paid for this increase in time-step length is the need to solve an elliptic boundary-value problem once per time step; nevertheless this improves efficiency by approximately a factor of 5. Analysis shows that the maximum possible time-step length is then limited by the Eulerian treatment of advection.

Early applications of semi-Lagrangian advection to coupled sets of equations (e.g., Krishnamurti 1962, 1969; Leith 1965; Mathur 1970, 1974; Mahrer and Pielke 1978) didn't take advantage of the enhanced stability properties of the method, since the models were formulated in such a way that they were not, in the terminology of Bates and McDonald (1982), "multiply upstream" and so the Courant number (associated with the treatment of advection) was always less than unity. Nevertheless these studies did demonstrate that semi-Lagrangian advection is an acceptably accurate method for advection. Robert (1981) reasoned that since semi-Lagrangian advection is stable for Courant numbers significantly larger than unity, it should be possible to associate a semi-Lagrangian treatment of vorticity advection with a semi-implicit treatment of the terms responsible for gravitational oscillations, and thereby obtain stable integrations with time steps four to six times longer than that of a corresponding semi-implicit model employing an Eulerian treatment of advection. Using such a strategy he was able to obtain a computationally stable solution with a 2-h time step (approximately four times longer than that of a corresponding semi-implicit Eulerian model), although there was some evidence of a small noise problem at the western inflow boundary. It was also noted that there was an inconsistency in the formulation inasmuch as the advection terms in the divergence and continuity equations were not evaluated using the semi-Lagrangian technique, and the question of accuracy (as opposed to stability) was deferred to a later study.

It turned out [Robert (1982)] that the Robert (1981) integrations included a divergence diffusion term and a time filter, and that when these were removed an instability was observed. This was attributed to two factors: the explicit treatment of the Coriolis terms, and the application of the semi-Lagrangian technique to only the vorticity equation. To remedy these two deficiencies, Robert (1982) introduced a revised formulation using the primitive (instead of the differentiated vorticity/divergence) form of the equations together with a semi-Lagrangian treatment of all advected quantities and an implicit treatment of the Coriolis terms. This was done in the context of a three-time-level scheme where the metric terms of the momentum equation were treated explicitly at the midpoint of the trajectories [cf., R in (9)] and all other nonadvective terms as time averages of values at the end points of the trajectories [cf., G in (9)]. A stability analysis was given to demonstrate that this scheme should be stable with time steps that exceed those of the gravitational, advective, and inertial limits, and this was verified in sample integrations.

To illustrate the application of the semi-Lagrangian method we discretize the shallow-water equations using a two-time-level semi-implicit semi-Lagrangian scheme, which permits a further doubling of efficiency with respect to the Robert (1982) algorithm at no extra cost. For simplicity we describe the scheme in plane geometry, and it is then formally equivalent to that of Temperton and Staniforth (1987) with the map-scale factor set to unity. In spherical geometry the discretization is a little more complicated due to the appearance of metric terms in the momentum equations. These can be trivially absorbed into the formulation given below, using either the approach of Ritchie (1988) or that of Côté (1988) and Bates et al. (1990) [see section 4c for a further discussion of this point]. Thus,

$$\frac{U^+ - U^0}{\Delta t} + \frac{\phi_x{}^+ + \phi_x{}^0}{2} - \frac{1}{2}[(fV)^+ + (fV)^0] = 0, \quad (17)$$

$$\frac{V^+ - V^0}{\Delta t} + \frac{\phi_y{}^+ + \phi_y{}^0}{2} + \frac{1}{2}[(fU)^+ + (fU)^0] = 0, \quad (18)$$

$$\frac{\ln\phi^+ - \ln\phi^0}{\Delta t} + \frac{1}{2}[(U_x + V_y)^+ + (U_x + V_y)^0] = 0, \quad (19)$$

where (14)–(16) have been discretized using (11) with R set to zero. Here advection terms are treated as time differences along the trajectories and all other terms are treated as time averages along the trajectories, leading to an $O(\Delta t^2)$-accurate scheme. Where traditional (three-time-level) semi-implicit time discretizations have an explicit time treatment of the Coriolis terms, the above discretization employs a time-implicit treatment [as in Robert (1982)] in order to achieve an $O(\Delta t^2)$-accurate scheme: note that explicitly evaluating these terms at time t would not only reduce the accuracy to $O(\Delta t)$ but would also lead to instability. The trajectories are computed using the discretized Eqs. (12)–(13) introduced by Temperton and Staniforth (1987) and McDonald and Bates (1987).

For the 1D shallow-water equations it can be shown that there are three characteristic velocities in the coupled set, one being the local wind speed that is associated with the slow Rossby modes that govern weather motions, the other two being associated with the propagation of gravitational oscillations. Thus the coupling of a semi-Lagrangian treatment of advection with a semi-implicit treatment of gravitational oscillations corresponds to integrating along the most important characteristic direction of the problem (i.e., that associated with the local wind speed); this is somewhat similar in spirit to a suggestion given on page 860 of Morton (1985).

Equations (17) and (18) can be manipulated to give

$$U^+ = -\frac{\Delta t}{2}[a\phi_x{}^+ + b\phi_y{}^+] + \text{known}, \qquad (20)$$

$$V^+ = -\frac{\Delta t}{2}[a\phi_y{}^+ - b\phi_x{}^+] + \text{known}, \qquad (21)$$

where $a = [1 + (f\Delta t/2)^2]^{-1}$ and $b = (f\Delta t/2)a$. Taking the divergence of (20)–(21) and eliminating this in (19) then leads to the elliptic boundary-value problem:

$$\left[(a\phi_x)_x + (a\phi_y)_y + (b\phi_y)_x - (b\phi_x)_y - 4\frac{\ln\phi}{\Delta t^2}\right]\Bigg|_{(\mathbf{x},t+\Delta t)} = \text{known}. \qquad (22)$$

We now summarize the above as the following algorithm:

(i) Extrapolate $\mathbf{V}$ using (13) and solve (12) iteratively for the displacements α_m for all mesh points $\mathbf{x}_m$, using values at the previous time step as initial guess, and an interpolation formula. Note that it is only necessary to perform this computation once per time step, since the same trajectory is used for all three advected quantities.

(ii) Compute upstream (superscript 0) quantities in (17)–(19) by first computing derivative terms (e.g., U_x) and *then* evaluating quantities upstream (these two operations are *not* commutative). Here it is more efficient to collect together all terms to be evaluated upstream in a given equation before interpolating (the distributive law applies).

(iii) Solve the elliptic boundary-value problem (22) for $\phi(\mathbf{x}, t + \Delta t)$.

(iv) Back substitute $\phi(\mathbf{x}, t + \Delta t)$ into (20)–(21) to obtain $U(\mathbf{x}, t + \Delta t)$ and $V(\mathbf{x}, t + \Delta t)$.

The above elliptic boundary-value problem is weakly nonlinear and is solved iteratively using ϕ at the previous time step as a first guess. It is only marginally more expensive to solve than the Helmholtz problem associated with traditional three-time-level semi-implicit Eulerian discretizations. The multigrid method is particularly attractive for solving such elliptic boundary-value problems because of its relatively low arithmetic operation count. Such a solver is described in Barros et al. (1990) and was successfully employed in the global model of Bates et al. (1990) using a discretization scheme very similar to that described above.

Semi-Lagrangian advection has also been successfully coupled with the split-explicit method (Bates and McDonald 1982) and the alternating-direction-implicit method (Bates 1984; Bates and McDonald 1987). Both of these approaches have the virtue of being simpler than the semi-implicit semi-Lagrangian one (there is no elliptic boundary-value problem), but unfortunately they do not perform as well. The split-explicit-based model is less efficient (Bates 1984) than the alternating-direction-implicit-based one, which in turn performs less well (Bates and McDonald 1987) than the semi-implicit semi-Lagrangian model of McDonald (1986). This latter scheme was adopted in the study of McDonald and Bates (1989), and it was subsequently found (Bates et al. 1990) that its performance with large time steps was not as good as had been hoped. This was attributed (McDonald 1989; Bates et al. 1990) to a time-splitting error introduced in the momentum equation associated with the Coriolis terms. To date it appears that the best schemes arise from associating semi-Lagrangian advection with a semi-implicit scheme, and that time splitting is best avoided since it introduces unacceptably large truncation errors for large time steps.

4. Further advances

When Robert (1981) proposed associating a semi-Lagrangian treatment of advection with a semi-implicit treatment of gravitational oscillations, it was thought that this approach was restricted to three-time-level schemes in Cartesian geometry using a finite-difference discretization. This has happily proved not to be the case, and in this section we discuss some important extensions of the approach. Although important, the extension to two-time-level schemes has already been discussed in some detail, and will, therefore, only be briefly discussed in this section in the context of other extensions.

a. Finite-element discretizations and variable resolution

Pudykiewicz and Staniforth (1984) coupled semi-Lagrangian advection with a uniform-resolution finite-element discretization of the diffusion terms in the solution of the 2D advection–diffusion equation, and this was extended to the 3D case in Pudykiewicz et al. (1985). Staniforth and Temperton (1986) extended the methodology in the context of a coupled system of equations (the shallow-water equations) in two ways. First they showed that in this context the semi-Lagrangian method can be coupled to a spatial discretization scheme other than a finite-difference one—viz., a finite-element discretization—and second that it can also be applied on a variable-resolution Cartesian mesh. A set of comparative tests demonstrated that with a time step six times longer it is as accurate as its analogous semi-implicit Eulerian version (Staniforth and Mitchell 1978) when run with its maximum possible time step (which in turn uses a time step six times longer than an Eulerian leapfrog scheme).

A further doubling of efficiency was then demonstrated in Temperton and Staniforth (1987) by replacing the three-time-level scheme of the Staniforth and Temperton (1986) model with a two-time-level one. Both these models use a differentiated (vorticity–divergence) form of the governing equations. This has the advantage of easily allowing variable resolution, but has the disadvantage of incurring additional interpolations and the need to solve two Poisson problems, resulting in an approximately 20% overhead when compared to the ideal. This overhead can be eliminated by the use of the pseudostaggered scheme proposed in Côté et al. (1990) with no loss of accuracy.

b. Noninterpolating schemes

The interpolation in a semi-Lagrangian scheme, as mentioned previously, leads to some damping of the smallest scales. While this damping is very scale selective, it may be argued that it would unacceptably degrade accuracy for very long simulations (e.g., many decades in the context of a climate model). To address this problem Ritchie (1986) proposed a noninterpolating version of semi-Lagrangian advection. The basic idea here is to decompose the trajectory vector into the sum of two vectors, one of which goes to the nearest mesh point, the other being the residual. Advection along the first trajectory is done via a semi-Lagrangian technique that displaces a field from one mesh point to another (and, therefore, requires no interpolation), while the advection along the second vector is done via an undamped three-time-level Eulerian approach such that the residual Courant number is always less than one. Thus the attractive stability properties of interpolating semi-Lagrangian advection are maintained but without the consequent damping. The noninterpolating scheme is also more efficient than a three-time level interpolating one, since there are only half the number of interpolations per time step (i.e., there are no longer any interpolations associated with the middle time level). Ritchie (1986) demonstrated the noninterpolating scheme for a gridpoint shallow-water model on a polar-stereographic projection, and found it to be more efficient and slightly more accurate than an interpolating scheme run at the same resolution.

The noninterpolating methodology is not restricted to gridpoint discretizations and has also been successfully applied to spectral discretizations (Ritchie 1988, 1990). This offers the possibility of retrofitting a noninterpolating semi-Lagrangian scheme into existing spectral models; there is, however, a minor technical complication inasmuch as present spectral models generally use the differentiated vorticity–divergence form of the equations whereas noninterpolating (and interpolating for that matter) semi-Lagrangian spectral models employ the primitive form, and this necessitates some changes to the spectral part of the formulation.

There are, however, a couple of disadvantages of the noninterpolating approach for problems where the small damping of the interpolating scheme is acceptable; this is generally the case for NWP applications, but probably not so for climate models (since they are generally run at much lower resolution and the damping is consequently more severe). First, the noninterpolating method has the dispersive properties of its Eulerian component, which are not generally as good as those of interpolating semi-Lagrangian advection schemes. Second, being based on a three-time-level scheme it is potentially twice as expensive as a two-time-level interpolating scheme.

The scheme proposed in Rančić and Sindjić (1989) is advertised as being a noninterpolating one, but this is not in fact the case (Dietachmayer 1990; Bates 1990). Two schemes are derived for uniform advection in 1D based on the Lax–Wendroff and Takacs (1985) schemes. A close examination of these schemes reveals that the Lax–Wendroff-based scheme is identical to a semi-Lagrangian one with quadratic Lagrange interpolation, whereas the Takacs-based scheme is identical to a semi-Lagrangian one using cubic Lagrange interpolation. A simple and interesting idea, somewhat buried in the detail of the Rančić and Sindjić (1989) paper, is to show how to make a two-time-level Eulerian advection scheme stable for Courant numbers greater than one. The idea, however, unfortunately seems to be limited to the 1D case, since it is predicated on the assumption that a particle passes over a mesh point at some time during the time interval of the time step, which assumption does not hold for multiply-upstream particles in 2D. It is of course possible to split the 2D advection problem into two passes of the 1D algorithm, but this then has the disadvantage that it usually introduces significant splitting errors for large time steps (see e.g., Williamson and Rasch 1989).

An alternative way of viewing the noninterpolating formalism of Ritchie (1986) is presented in Smolarkiewicz and Rasch (1990). They showed that it is possible to convert any advection algorithm into a semi-Lagrangian framework, thus permitting the use of much larger time steps with the scheme for little additional cost. This interesting realization is of potential benefit for models whose maximum time step is limited by an Eulerian treatment of advection. To demonstrate this idea they successfully extended the stability limit of the Tremback et al. (1987) family of algorithms. In so doing they obtained a family of schemes that is equivalent to using a time-split semi-Lagrangian scheme with Lagrange interpolation. They also successfully extended the stability limit of a family of positive-definite monotone advection algorithms. However, after comparing results with those of semi-Lagrangian algorithms, they concluded that for problems where small undershoots and slight lack of conservation are acceptable, this family of positive-definite monotone algorithms cannot compete.

c. Spherical geometry

The convergence of the meridians at the poles of an Eulerian finite-difference model in spherical geometry leads to unacceptably small time steps being required in order to maintain computational stability. The usual approach to this problem is to somehow filter the dependent variables in the vicinity of the poles. While this procedure does relax the stability constraint, it unfortunately deteriorates accuracy (e.g., Purser 1988). Ritchie (1987) demonstrated that it is possible to passively advect a scalar over the pole using semi-Lagrangian advection with time steps far exceeding the limiting time step of Eulerian advection schemes. This paved the way to applications in global spherical geometry. The first such application was to couple semi-Lagrangian advection with a spectral representation (i.e., expansion in terms of spherical harmonics) of the dependent variables to solve the shallow-water equations over the sphere (Ritchie 1988). A new problem arose here associated with the stable advection of a vector quantity (momentum). The solution proposed in Ritchie (1988) is to introduce a tangent plane to avoid a weak instability due to a metric term. The diagnosis of this problem, which led to the tangent plane algorithm, is described in Desharnais and Robert (1990).

An alternative solution, proposed by Côté (1988), is to use a Lagrange multiplier method. In this approach the horizontal momentum equations of the shallow-water equations on the sphere are written in 3D vector form using the undetermined Lagrange multiplier method. These equations are time discretized directly, and the Lagrange multiplier is then determined from the discretized equations to ensure that motion is constrained to follow the surface of the sphere. This is in contrast with the usual approach where the Lagrange multiplier is first determined from the continuous equations, followed by a discretization of the resulting equations. The procedure is applicable to any coordinate system and can also be extended to multilevel models.

Both methods give good results that are almost indistinguishable in practice. More recently Bates et al. (1990) have described an approach based on the discretization of the vector form of the momentum equation. Although they state that their vector discretization is somewhat different from the Lagrange multiplier method of Côté (1988), it can be shown that the resulting algorithms are identical. It also turns out that the tangent-plane algorithm of Ritchie (1988) is identical to the Lagrange-multiplier one in the context of a two-time-level scheme.

Ritchie (1988) successfully integrated his shallow-water model with a time step six times longer than the limiting time step of the corresponding Eulerian semi-implicit spectral model (which in turn uses a time step six times longer than that of an Eulerian leapfrog model). Côté and Staniforth (1988) then further doubled the efficiency of the Ritchie (1988) model by replacing its three-time-level scheme by a two-time-level one analogous to that of Temperton and Staniforth (1987) for Cartesian geometry.

The spectral method (i.e., expansion of the dependent variables in terms of spherical harmonics) has been the method of choice during the past decade for the horizontal discretization of global NWP models. However, the spectral method ultimately becomes very expensive at high enough resolution, due to the $O(N^3)$ cost of computing the Legendre transforms, where N is the number of degrees of freedom around a latitude circle. Finite-difference and finite-element methods on the other hand have a potential $O(N^2)$ cost. This, and the success of the semi-Lagrangian method in addressing the pole problem, suggests that it would be highly advantageous to use a semi-Lagrangian treatment of advection in a finite-difference or finite-element global model for medium-range forecasting.

A first tentative step in this direction was taken by McDonald and Bates (1989), who introduced semi-Lagrangian advection into a two-time-level global semi-implicit shallow-water model using the time discretization of McDonald (1986). Although their scheme was stable with time steps that exceeded the limiting time step of an Eulerian treatment of advection, the enhanced stability was unfortunately achieved at the expense of accuracy. The degradation of accuracy is attributable to a time-splitting error introduced in the momentum equation associated with the Coriolis terms. The solution to this problem is to avoid time splitting altogether and then the algorithm (Bates et al. 1990) is very similar to that employed in Ritchie (1988) and Côté and Staniforth (1988), and results in significant improvements in accuracy for large time steps. Nevertheless, Bates et al. (1990) found it necessary to use divergence damping (with what appears to be a rather large coefficient) in order to integrate to five days, suggesting that some accuracy and/or stability problems still remain.

Côté and Staniforth (1990) replaced the spectral discretization in the Côté and Staniforth (1988) model by a pseudostaggered finite-element one [analogous to that described in Côté et al. (1990)], to obtain a two-time-level semi-implicit semi-Lagrangian global model of the shallow-water primitive equations. Its performance at comparable resolution matched that of their corresponding 1988 model based on a spectral discretization, and this performance was achieved without recourse to any divergence damping.

By evaluating the product term (of the geopotential perturbation and divergence) in the continuity equation using quantities at time t rather than at time $t + \Delta t/2$, but still evaluating it at the trajectory midpoint, Higgins and Bates (1990) show that it is possible to integrate the Bates et al. (1990) model with no divergence damping, although this formally reduces the accuracy of the treatment of this term to $O(\Delta t)$ (but it is not a very important term in a shallow-water model). This result strongly suggests that the source of weak instability observed in the Bates et al. (1990) results (without divergence damping) is somehow due to this term, but it still remains to explain why. We believe the explanation may be found in a stability analysis given in Côté and Staniforth (1988) for a somewhat similar time discretization, which analysis is valid for the Bates et al. (1990) formulation.

Côté and Staniforth (1988) showed that such a time discretization is only stable provided $\phi^* > \phi_{max}$, where ϕ^* is the reference geopotential of the semi-implicit scheme and ϕ_{max} is the maximum-possible value of the geopotential. Thus where this condition is violated, such a time discretization is likely to be unstable, and this is most likely to occur in the tropics where the geopotential is generally largest. We believe that the ϕ^* of the Bates et al. (1990) integrations (without divergence damping) is probably an average value of the geopotential (rather than its maximum value) and thus violates this stability criterion. An examination of the divergence-damping-free result (given in Higgins and Bates 1990) of the Bates et al. (1990) formulation reveals that the forecast is unstable in the tropics, but stable in the extratropics, consistent with the above argument. We, therefore, speculate that the Bates et al. (1990) formulation could be stabilized by merely increasing the value of the reference geopotential, and that this solution would be preferable to the one proposed by Higgins and Bates (1990) since it is $O(\Delta t^2)$ [rather than $O(\Delta t)$] accurate.

d. Conservation, shape preservation, and monotonicity

An important issue for the discretization of global models, and to a lesser extent for regional ones, is the extent to which various properties are conserved. Following the pioneering work of Arakawa (1966), many finite-difference schemes have been derived to maintain different integral and local properties of the underlying continuous equations (e.g., conservation of energy and enstrophy of the rotational part of the flow; conservation of energy and transformation between kinetic and available potential energy; and prevention of spurious generation of vorticity by pressure-gradient terms). For spectral and finite-element models, some of these properties are immediate by virtue of a Galerkin framework [e.g., Bourke (1988); Yakimiw and Girard (1987)]. However, many of the properties that are supposedly conserved by conservative schemes only do so under the assumption that there is a continuous time discretization (which is not in general the case), and such schemes can and do go unstable, particularly in the absence of any time filter (which damps the solution). Nevertheless, such schemes have proven to be quite successful for integrating models, and it is natural to ask the question (as one of the referees did) of how semi-Lagrangian schemes behave in this regard. While there doesn't appear to be a definitive answer to this question at this time, we summarize what is presently known.

From the theoretical standpoint, Bermejo (1990) has shown that semi-Lagrangian schemes using cubic-spline interpolation conserve mass for divergence-free flows, and this is the only exact conservation property of semi-Lagrangian schemes of which we are aware. From the practical standpoint, several studies have measured how well certain quantities are conserved. Ritchie (1988), and to a lesser extent Côté and Staniforth (1988), have examined the conservation of energy in the context of 20-day integrations of three- and two-time-level shallow-water semi-Lagrangian global models. As an indication of the energy conservation that is considered acceptable in typical medium-range forecast models, an Eulerian spectral control model was run at T106 resolution with a ∇^4 diffusion having the same coefficient as that used operationally at this resolution by the European Centre for Medium Range Weather Forecasts. It was found that this control model lost 3% of its total energy after 20 days, whereas the two semi-Lagrangian models at T126 resolution only lost 1%. At lower (T63) resolution, the three-time-level interpolating semi-Lagrangian model lost 5%, while the noninterpolating version again only lost 1%.

These results suggest that (i) interpolating semi-Lagrangian schemes conserve energy acceptably well at resolutions typical of state-of-the-art medium-range forecast models, but don't necessarily do so at resolutions typical of general circulation models, and (ii) noninterpolating semi-Lagrangian schemes conserve energy acceptably well at both resolutions. Ritchie (1988) also compared the enstrophy spectra of various T126 integrations with that of a control T213 integration, and the results suggest that interpolating and noninterpolating semi-Lagrangian models perform as well or better than Eulerian models in this regard. However, these results and conclusions remain to be confirmed for baroclinic models.

Although most authors have adopted polynomial schemes for the interpolatory steps of semi-Lagrangian schemes, other interpolators are also possible. Williamson and Rasch (1989) and Rasch and Williamson (1990a) have examined several different possible interpolators, designed to better preserve the shape of advected fields and to maintain monotonicity. They performed experiments in both Cartesian and spherical geometry, and concluded that the approach is viable. The principal difficulty with the shape-preserving and monotonic approaches appears to be to decide how to precisely determine the required attributes of the interpolator, and how to tailor it to respect them, since there is no universal best choice.

Williamson and Rasch (1989), Williamson (1990), and Rasch and Williamson (1990a, 1990b, 1991) have pursued this approach and thoroughly compared spectral and semi-Lagrangian schemes for the transport of water vapor in otherwise Eulerian, hydrostatic primitive-equation models, in the context of both medium-range forecasting and general circulation modeling. The transport of water vapor is a stringent test of an advection scheme, since the moisture spectrum has much more variance at small scales than do wind and mass spectra. Several important points have emerged from their studies.

Although spectral advection conserves mass well, it does so by producing serious undershoots (negative water vapor) and overshoots (supersaturation), both of which cause serious problems for the parameterization of moist processes, necessitating remedial measures that adversely affect conservation. Semi-Lagrangian advection, particularly monotonic positive-definite versions, conserves mass a little worse for passive advection, but has fewer undershoot/overshoot problems and consequently interacts better with moist parameterizations in forced problems (having moisture sources and sinks). In particular (Williamson 1990) semi-Lagrangian advection leads to much smaller regions of spurious light precipitation for medium-range forecasting.

A particularly troubling result (Rasch and Williamson 1991) is that spectral and semi-Lagrangian advection schemes lead to different climatologies in general circulation models, with semi-Lagrangian advection leading to a generally colder troposphere and warmer stratosphere. These differences are attributed primarily to differences in the numerical treatment of vertical advection, which subsequently lead to different cloud climatologies. Rasch and Williamson (1991) argue that semi-Lagrangian vertical advection is formally fourth-order accurate, whereas Eulerian vertical advection is only first-order accurate, and it should a priori be expected to be more accurate at fixed vertical resolution. They caution the reader, however, that it is difficult to separate cause and effect in such comparisons, and underline the importance of continuing to improve numerical methods for climate models since they still represent an important source of error. These authors have indicated a preference for semi-Lagrangian advection of moisture to spectral advection for climate modeling, and plan to use it in the next version of the NCAR Community Climate Model. This sensitivity of the climatology to the choice of advection scheme is also of importance in NWP applications, but the problems are probably less severe due to the generally higher resolution of NWP models.

e. 3D NWP applications

Thus far we have mostly discussed the use of semi-Lagrangian advection for extending the limiting time step of 2D applications for NWP. To be useful the method must also be applicable in 3D. A first step in this direction was taken in Bates and McDonald (1982), where a semi-Lagrangian treatment of horizontal advection in a 3D (baroclinic primitive equations) model was coupled with a split-explicit time scheme in the Irish Meteorological Service's operational model of the time. This was the first scheme to demonstrate the enhanced stability of semi-Lagrangian advection in a 3D model, and the first to be used operationally. However, it is only $O(\Delta t)$ accurate and although stable with long time steps, the increase in time step is consequently very much limited by accuracy considerations.

The 3D model formulated in McDonald (1986) and improved in McDonald and Bates (1987) [by modifying the trajectory calculations to make them $O(\Delta t^2)$ accurate, which improves accuracy and allows longer time steps] is four times more efficient than the Bates and McDonald (1982) model for the same accuracy and replaced it operationally. Nevertheless, the resulting scheme still has some $O(\Delta t)$ truncation errors and the time step is, therefore, smaller than it would be for an $O(\Delta t^2)$ scheme [see discussion in the preceding subsection of the McDonald (1986) scheme in the context of a global model]. Bates and McDonald (1987) have also coupled a semi-Lagrangian treatment of horizontal advection in a 3D model with the alternating-direction method, but found in comparative experiments that it does not perform as well as the McDonald and Bates (1987) scheme.

Robert et al. (1985) introduced a three-time-level *$O(\Delta t^2)$-accurate* 3D limited-area gridpoint model with a semi-Lagrangian treatment of horizontal advection, and were able to successfully integrate with longer time steps than had hitherto been possible; however, the model had no mountains and a very simple parameterization of physical processes. This semi-Lagrangian semi-implicit model does, however, demonstrate the practical importance of achieving a truly $O(\Delta t^2)$-accurate scheme. Although it employs a three-time-level scheme, it is only marginally more costly per time step than the nominally two-time-level scheme of McDonald and Bates (1987) (which has several substeps) but can be integrated with longer time steps. In principle it should be possible to further double the efficiency of the Robert et al. (1985) algorithm by using a two-time-level scheme. While such an improvement has been achieved in 2D (e.g., Côté and Staniforth 1988; Bates et al. 1990) the extension to 3D applications remains to be demonstrated.

A somewhat similar model to the Robert et al. (1985) one, but with mountains included, is described in Kaas (1987). It was reported that when strong winds blow over steep mountains, instabilities may appear if the linear part $[\nabla(\phi + RT_0 \ln p_s)]$ of the horizontal pressure-gradient term in sigma coordinates [see Mesinger and Janjić (1985) for a related discussion of this problem in the context of Eulerian models] is evaluated as the average of values at the endpoints $[(\mathbf{x}, t + \Delta t), (\mathbf{x} - 2\alpha, t - \Delta t)]$ of the trajectory, but the nonlinear part $[R(T - T_0)\nabla \ln p_s]$ is evaluated at the midpoint $(\mathbf{x} - \alpha, t)$. This behavior was attributed to a lack of balance (in the discrete approximation) between two large terms of opposite sign, due to their being evaluated at different geographical points. The reported solution to this problem is to evaluate the nonlinear part as the average of its values at the geographical points associated with arrival $(\mathbf{x})$ and departure $(\mathbf{x} - 2\alpha)$, both values being taken at the intermediate time level t. This stratagem has also recently been incorporated in the models of Robert et al. (1985), Tanguay et al. (1989), and Ritchie (1991).

While this approach appreciably mitigates the problem, it is not at all clear that it resolves it completely. Coiffier et al. (1987) have studied it in the context of a 2D linearized baroclinic model, and show that the use of semi-Lagrangian advection with *large* time steps leads to an incorrect steady-state solution when the model is orographically forced. Their analysis to explain this behavior also applies to the formulation proposed by Kaas (1987). It suggests that the seriousness of the problem is a function of time step, wind speed, and detail (the larger the time step and wind speed, and the more detailed the orography, the worse is the problem), and of whether the time scheme is a two- or three-time-level one (two-time-level schemes are better since the problem first occurs with time steps twice as long as those of three-time-level schemes). Although this problem has not prevented semi-Lagrangian models from being integrated with larger time steps than Eulerian ones while obtaining results of equivalent accuracy, it does warrant further investigation.

The time steps of the 3D above-mentioned models are limited by the stability of an explicit Eulerian treatment of vertical advection: or put another way, vertical resolution is limited when using a large time step (see Ritchie 1991 for an example). This is an important limitation. An ever-increasing emphasis in model development is being put on the parameterization of physical processes in general, and that of the moist turbulent planetary boundary layer in particular, and results in ever-increasing demands on vertical resolution. To remove this limitation, Tanguay et al. (1989) proposed a three-time-level model that uses semi-Lagrangian advection in all three space dimensions: this finite-element regional model uses a time step that is three-times longer than that of the corresponding Eulerian version (Staniforth and Daley 1979). It is currently used by the Canadian Meteorological Center to operationally produce weather forecasts to 48 h twice daily.

Ritchie (1991) has recently introduced semi-Lagrangian advection into a three-time-level 3D global spectral model in two different ways. The first uses an interpolating semi-Lagrangian scheme in all three dimensions, as in Tanguay et al. (1989), whereas the second uses an interpolating semi-Lagrangian scheme for horizontal (2D) advection and a noninterpolating scheme for vertical advection. These schemes are currently being introduced into the European Centre for Medium Range Weather Forecasts' spectral model. He reports that the latter scheme is more accurate than the former for the experiments he conducted, due to the former unduly smoothing fields in the vertical around the tropopause. The seriousness of this smoothing is a function of the resolution employed and of the order of the interpolator. The trend to higher vertical resolution should diminish the importance of this source of error in the future. In the meantime it suggests that higher-order vertical (i.e., quintic instead of cubic) interpolation is possibly warranted as proposed in Leslie and Purser (1991).

f. Higher resolution and nonhydrostatic systems

As computers become ever more powerful, it becomes possible to run models at higher and higher resolution. A time is approaching (Daley 1988) when it will be possible to run current hydrostatic baroclinic primitive-equation weather forecast models at resolutions for which the hydrostatic assumption can no longer be assumed to hold. This motivates the need to efficiently integrate nonhydrostatic systems of equations for real-time forecasting applications over large domains. Such systems admit acoustic modes, which travel much faster than either Rossby or gravity modes. Consequently if care is not exercised, the limiting time step will be even more restrictive than that associated with an explicit primitive-equations model. This is because an explicit time treatment of the terms associated with the propagation of acoustic energy leads to a limiting time step that is much smaller than that associated with an explicit treatment of gravity-wave terms, completely eliminating the efficiency advantage of a semi-implicit semi-Lagrangian treatment of the gravity–Rossby mode terms.

Since the acoustic modes carry very little energy, it is permissible to slow them down by the use of a time-implicit treatment of the terms responsible for their existence, by analogy with the retarding of the gravity modes by the semi-implicit scheme. This is the approach taken by Tanguay et al. (1990), who generalize the semi-implicit semi-Lagrangian methodology for the hydrostatic primitive equations to the nonhydrostatic case. They show that it is possible to integrate the fully compressible nonhydrostatic equations (that are presumably more correct) for little additional cost, opening the way to highly efficient nonhydrostatic models. Note that this is a proof-of-concept study, since the model employed has several important deficiencies with respect to operational hydrostatic forecast models;

it has no mountains, an extremely simple parameterization of physical processes, and very low vertical resolution (particularly in the planetary boundary layer) such that the time step is not unduly limited by the Eulerian treatment of vertical advection (it is only the horizontal advection that is treated in a semi-Lagrangian manner). Nevertheless, it represents a very important first step towards highly efficient nonhydrostatic forecast models.

Increasing the resolution not only has important implications for the appropriate choice of governing equations, but also for the relative order of the temporal and spatial truncation errors. To date it has been found advantageous to couple semi-Lagrangian advection with a semi-implicit time scheme. This allows integration with larger time steps than would otherwise be possible, chosen such that the temporal and spatial truncation errors are of the same magnitude. We are thus presently in the position where the $O(\Delta t^2)$ temporal truncation errors are approximately equal in magnitude to the $O(\Delta x^4)$ spatial ones (assuming cubic interpolation in the semi-Lagrangian discretization of advection). For sake of argument, assume that this Δt is four times larger than the limiting time step of a corresponding semi-implicit model with an $O(\Delta x^4)$-accurate Eulerian advection scheme. We now ask the important question, what will be the size of the time step (chosen such that the temporal and spatial truncation errors are of the same magnitude) of the semi-implicit semi-Lagrangian model for successive doublings of the spatial resolution, and how will this time step compare to that of the corresponding semi-implicit Eulerian model?

For the first doubling of resolution, the spatial truncation errors will be decreased by a factor of 16 ($=2^4$). To ensure that the temporal truncation errors will be of the same magnitude as the spatial ones it is, therefore, necessary to reduce them also by a factor of 16 ($=4^2$), which implies *reducing* Δt *by a factor of 4*. Comparing this time step now with that of the corresponding Eulerian model for the same doubling of resolution (where the time step is halved to respect the CFL stability criterion), we see that it is only twice as large (whereas before the doubling of resolution it was four times larger) and the relative advantage of the semi-Lagrangian time step is thus halved.

Repeating the argument for a second doubling we see that the time step of the semi-Lagrangian model now equals that of the Eulerian one, and there is no longer any advantage of time-step length for the semi-Lagrangian model. This is because the time step of the semi-Lagrangian model is limited by accuracy considerations (it cannot be any larger otherwise the temporal truncation errors would dominate), and it so happens that the time-step of the Eulerian model is now limited by both stability and accuracy considerations. For any further increase in resolution beyond this critical resolution, the time steps of the two models will be identical since they will be determined solely by accuracy considerations. So we conclude that for this example there is no time step advantage for the semi-Lagrangian model at a quadrupling or more of resolution.

Since the semi-Lagrangian model is somewhat more expensive per time step it is, therefore, debatable as to whether it would be advantageous in the above example to use a semi-Lagrangian treatment of advection at such resolutions rather than an Eulerian one [although one might argue that semi-Lagrangian advection might still be advantageous (particularly for moisture transport) since there are fewer dispersion problems; see e.g., Ritchie (1985) and Rasch and Williamson (1990a)]. The important implication of the above argument is that when the resolution of the Eulerian model is sufficiently high that the time step is governed by its $O(\Delta t^2)$ temporal truncation error (rather than by its CFL stability criterion), it will become important to increase the order of the time discretization of the corresponding semi-Lagrangian model. How this might be done is discussed in McDonald (1987).

With that said, there is perhaps a weakness in the above argument. We have assumed that the dominant source of spatial truncation error is $O(\Delta x^4)$, and for a realistic NWP model this means that we are implicitly assuming that the spatial truncation errors associated with the physical parameterization also behave as $O(\Delta x^4)$. In reality it is highly unlikely that a doubling of resolution reduces these errors by a factor of 16, and it is far more likely that they behave as $O(\Delta x^2)$, in which case this would be the leading source of horizontal truncation error and the efficiency advantage of the semi-Lagrangian model would be maintained for all resolutions.

A further important consideration is that the temporal discretization associated with the incorporation of physical processes in the models be of higher order than the present $O(\Delta t)$ ones in order to benefit from the enhanced stability of semi-Lagrangian schemes. This is intimately connected to the intrinsic time scales of the physical processes being parameterized (e.g., cloud dynamics), and to what extent the chosen parameterizations are valid when using large time steps. It is also an issue for Eulerian models, but is more serious for semi-Lagrangian models because of their generally longer time steps. Present physical parameterizations appear to be rather sensitive to time-step length, and this problem requires further work.

5. Conclusions

During the past decade much progress has been achieved in using semi-Lagrangian advection to improve the efficiency of numerical models of the atmosphere. In this paper we have reviewed the semi-Lagrangian literature for atmospheric models, and have drawn the following conclusions:

1) The semi-Lagrangian methodology has been extended from finite-difference applications in Cartesian geometry to finite-difference, finite-element, and spectral applications in both Cartesian and spherical geometry.

2) The extension to finite-difference and finite-element discretizations for global applications is particularly noteworthy, since such discretizations are asymptotically much cheaper at high resolution than the present method of choice, the spectral method.

3) At the present state of development the efficiency gains are more spectacular in 2D than in 3D.

4) Two-time-level schemes are inherently twice as efficient as three-time-level schemes. This has been clearly shown in 2D, but the full benefits of two-time-level schemes in 3D remain to be demonstrated.

5) Best results are obtained when coupling semi-Lagrangian advection to a semi-implicit treatment of gravitational oscillations, rather than to splitting methods such as split-explicit and alternating-direction-implicit. It is crucial to avoid introducing $O(\Delta t)$ truncation errors in either the trajectory computations or the discretization of the governing equations, in order to fully reap the benefit (i.e., long time steps) of enhanced stability.

6) It is important to use the semi-Lagrangian method for vertical as well as for horizontal advection, in order to avoid unduly limiting vertical resolution.

7) Noninterpolating semi-Lagrangian schemes are attractive for climate applications, due to their lack of damping, a particularly important property for low-resolution simulations.

8) The semi-Lagrangian framework facilitates the incorporation of shape-preserving and monotonic schemes for moisture advection, because of the relatively small dispersion errors in the presence of discontinuities or near discontinuities. It also more easily permits higher-order discretizations of vertical advection.

9) Semi-Lagrangian schemes do not in general formally conserve quantities, but the somewhat limited evidence to date suggests that they perform acceptably well in this regard.

Although much progress has been achieved, there remain several areas that warrant further investigation. The most pressing of these, in our opinion, is the incorporation of orographic (and other) forcing into semi-Lagrangian models in such a way as to obtain the correct response to the stationary component. There is evidence to suggest that present schemes are deficient in this regard for Courant numbers greater than unity. Further research on physical parameterization is also needed, to ensure that they adequately parameterize the essential features of the underlying physical processes when using large time steps. Current parameterizations appear to be overly sensitive in this regard.

As the spatial resolution is increased in a typical semi-Lagrangian model having, respectively, fourth-order spatial and second-order temporal truncation errors, it will become important to increase the order of the time discretization, otherwise there will ultimately be no time-step advantage with respect to an analogous Eulerian model. Research on higher-order time discretizations is, therefore, desirable. A further consequence of increasing spatial resolution is that the hydrostatic approximation becomes increasingly less valid, thus motivating the efficient integration of nonhydrostatic systems of equations. An important first step in this direction has already been achieved, but further research is needed to address several important deficiencies of such a nonhydrostatic model with respect to operational hydrostatic forecast models. In particular, it remains to demonstrate the viability of the method in the presence of realistic parameterizations of physical processes and a semi-Lagrangian treatment of advection.

In our review of the semi-Lagrangian literature we have endeavored to present the strengths and weaknesses of the method, particularly with respect to accuracy, stability, and efficiency. This is not to say that we believe that the semi-Lagrangian approach outperforms traditional schemes in each and every respect; e.g., conservation properties. We endorse the suggestion of one of the referees that it would be valuable for the numerical modeling community to compare the performance of various semi-Lagrangian and Eulerian schemes for the solution of a given set of problems. Such an activity is presently being organized (Williamson et al. 1991) within the framework of the CHAMMP (computer hardware, applied mathematics, model physics) initiative.

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