An introduction to semi - Lagrangian methods for geophysical scale flows

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Introduction

The semi-Lagrangian method is a numerical solution technique for the partial differential equations describing the advection process. It accounts for the Lagrangian nature of the transport process but, at the same time, it allows to work on a fixed computational grid. Starting from the first proposals to in the meteorological literature, which focussed on the advection of vorticity in simplified models of large scale flow, it has developed into a mature discretization approach for the complete equations of atmospheric flows. The semi-Lagrangian is also related (and, in some cases, entirely equivalent) to similar methods developed in other modelling communities, such as for example the modified method of characteristics, the Eulerian-Lagrangian method and the characteristic Galerkin method.

A comprehensive review of the semi-Lagrangian method in the meteorological literature until 1990 is provided by [67]. Reviews of the developments concerning the related methods in other modelling areas can be found e.g. in [15], [43], [56].

The outline of the present introductory paper is now described. In section 2, the basic concept of the semi-Lagrangian method is presented, the simple context of the linear, one dimensional advection equation. Furthermore, the difference and relationship to purely Lagrangian methods are highlighted. In section 3, the special role of the advection process for large scale atmospheric flow is reviewed on the basis of classical scaling analysis. In section 4, the development of semi-Lagrangian methods is briefly outlined, along with some of the parallel developments in other scientific communities. In section 5, some of the possible choices for the implementation of the key steps in the semi-Lagrangian method are reviewed and discussed. In section 6, results of simple numerical tests for passive advection in one and two dimensions are presented, in order to show how the method can perform in practice. Furthermore, results are compared with those of some Eulerian schemes. In section 7, the stability and convergence of the semi-Lagrangian method will be discussed.

The first version of this review of semi-Lagrangian methods was made possi-

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ble by an invitation at the Seminar for Applied Mathematics of ETH Zurich to give a series of talks on this topic in the framework of the ERCOFTAC programme in July 2004. I would like to thank prof. Rolf Jeltsch and William Sawyer for supporting this invitation and the basic concept of this review.

My personal experience with semi-Lagrangian methods has begun in 1993, during my PhD thesis work with prof. Vincenzo Casulli (University of Trento, Italy). I would like to thank him for introducing me to this fascinating topic and to the world of real-life numerical modelling as well. Various conversations with dr. Andrew Staniforth (Met Office, UK) have been equally important for the development of my understanding of these methods and, more generally, of numerical issues in NWP.

My experience with semi-Lagrangian has also benefited from discussions and collaboration with many friends and colleagues. I would like to thank them all for their help and advice.

The semi - Lagrangian method for the linear advection equation

In order to introduce the semi-Lagrangian method in a simple context, consider the one dimensional linear advection equation

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0 \tag{2.1}$$

with constant coefficient u and with initial datum $c_0(x)$, $x \in \mathbf{R}$. It is well known

$$c(x,t) = c_0(x - ut) \tag{2.2}$$

Consider now discretizations of equation 2.1 on a uniform one dimensional mesh with spacing Δx and time step Δt . Nodes of the mesh are denoted by i and discrete time levels by n, so that the grid spacetime locations are denoted by $x_i = i\Delta x$, $t^n = n\Delta t$ and the approximate values computed by a numerical solution are denoted by $c_i^n \approx c(x_i, t^n)$. Standard finite difference methods based on approximation of differential operators by finite difference quotients. Let us consider some typical examples. One of the most basic is the upwind method, in which one-sided finite difference quotients are used to approximate the

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u \frac{c_i^n - c_{i-1}^n}{\Delta x} = 0$$
 (2.3)

Here, it was assumed that u>=0 and the direction. The upwind method has a truncation error of order one both in space and time. For higher order versions of the upwind scheme, see e.g. [12]. The leapfrog method employs instead centered finite differences in space and time

$$\frac{c_i^{n+1} - c_i^{n-1}}{2\Delta t} + u \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} = 0.$$
 (2.4)

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The resulting method has a truncation error of order two in space and time. Employing a more accurate approximation of the spatial derivative can yield schemes of high accuracy in space and time. For example, taking centered differences in time and a fourth order accurate approximation of the derivative in x (see e.g. [14] yields

$$\frac{c_i^{n+1} - c_i^{n-1}}{2\Delta t} + u \left[\frac{4}{3} \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} - \frac{1}{3} \frac{c_{i+2}^n - c_{i-2}^n}{4\Delta x} \right] = 0.$$
 (2.5)

These are three time level methods, so they require the use of a different approximation to compute the first time step. A two time level method that has truncation error of order two is for example the Lax-Wendroff method

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u \frac{c_i^n - c_{i-1}^n}{2\Delta x} - \frac{u^2 \Delta t}{2} \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2} = 0,$$
 (2.6)

which can be also interpreted as a stabilized version of the (unstable) scheme

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} = 0$$
 (2.7)

obtained adding a special form of numerical dissipation (see e.g. [56]). It is well known that the stability of these methods depends in an essential way on the parameter $C = u\Delta t/\Delta x$, also known as the Courant number. A general condition for stability is in fact $|C| \leq 1$, which is also known as the Courant - Friedrichs - Lewy (CFL) condition (see [10]).

Lagrangian and semi-Lagrangian methods exploit instead the special feature of the advection equation, that is the representation of the exact solution in terms of the initial datum. In particular, considering without loss of generality the case of u>0, it can be observed that the following two equations hold:

$$c(x_i, t^n) = c_0(x_i - un\Delta t)$$

$$= c_0(x_i + u\Delta t - u(n+1)\Delta t) = c(x_i + u\Delta t, t^{n+1})$$
(2.8)

$$c(x_i, t^{n+1}) = c_0(x_i - u(n+1)\Delta t)$$

$$= c_0(x_i - u\Delta t - un\Delta t) = c(x_i - u\Delta t, t^n)$$
(2.9)

Equation (2.9) provides the basis for purely Lagrangian methods. The special nature of the exact solution of (2.1) allows to use the knowledge of the solution at a mesh point at time n to derive the value of the solution at time n + 1 at points of a mesh that has moved with the flow. Due to the fact that the mesh must be changed at each time step, practical application of Lagrangian methods is not

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straightforward and these techiques have never been turned into operational tools in weather forecasting or large scale atmospheric simulation.

Equation (2.10) provides instead the basis for the semi-Lagrangian method. Again, the special nature of the exact solution of (2.1) is used to express the value of the solution at time n+1 at the mesh points in terms of the solution values at time n at points of a mesh that within a single time step will be transported by the flow onto the computational mesh. This has the practical advantage that the mesh does not change in time, which is the one of the fundamental reasons for the much more widespread use of semi-Lagrangian rather than purely Lagrangian methods. Discrete definition of the semi-Lagrangian method can then be obtained from equation (2.10) as

$$c_i^{n+1} = c_{i-u\frac{\Delta t}{\Delta x}}^n = c_{i-k-\alpha}^n \qquad u\frac{\Delta t}{\Delta x} = k + \alpha \quad k = \left[u\frac{\Delta t}{\Delta x}\right]. \tag{2.10}$$

k and α are often called the integral and the fractional Courant numbers, respectively. The expression $c^n_{i-k-\alpha}$ is to be interpreted as the value obtained from the approximate c^n values at the point $i\Delta x - u\Delta t$ by some interpolation procedure. Two interesting facts can be noticed immediately if simple linear interpolation is applied, so that

$$c_i^{n+1} = \alpha c_{i-k-1}^n + (1-\alpha)c_{i-k}^n.$$
(2.11)

First of all, if $C = u\Delta t/\Delta x < 1$, then one has in (2.11) $k = 0, C = \alpha$ and the resulting method is easily seen to be identical to the upwind method (2.3). Furthermore, it is clear that (2.11) holds for any value of the Courant number and that, since the values of the solution at the new time level n + 1 are obtained by a linear interpolation of the values at time level n with nonnegative coefficients, the discrete maximum principle holds, i.e.

$$\min_{i} c_{i}^{0} \le \min_{i} c_{i}^{n} \le \max_{i} c_{i}^{n} \le \max_{i} c_{i}^{0}$$
 (2.12)

for any n. This also implies stability in the maximum norm for an arbitrary Courant number. Thus, at least in a simple case the semi-Lagrangian method appear to have a great advantage over the previously reviewed Eulerian methods, since no stability condition restricts the choice of the timestep.

The semi-Lagrangian method can be easily generalized to the multidimensional case. If a constant velocity field $\mathbf{u} \in \mathbf{R}^d$ and and initial datum $c_0(x), \mathbf{x} \in \mathbf{R}^d$ are considered, the multidimensional linear advection equation is given by

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = 0. \tag{2.13}$$

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As in the one dimensional case, the analytic solution is given by

$$c(\mathbf{x}, t) = c_0(\mathbf{x} - \mathbf{u}t), \tag{2.14}$$

and the semi-Lagrangian approach can be derived as in the one dimensional case, by replacing one dimensional interpolation with multidimensional interpolation techniques.

In the more general case of a space and time dependent velocity field $\mathbf{u}(\mathbf{x},t) \in \mathbf{R}^d$, one has

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \mathbf{u}(\mathbf{x}, t) \cdot \nabla c = 0$$
 (2.15)

where the usual notation dc/dt for the Lagrangian derivative has been introduced. Under some regularity assumptions on the velocity field (which has to be Lipschitz continuous, see e.g. [56]), it can be proved that streamline or characteristic line functions exist. These are defined as the solutions $\mathbf{X}(t; s, \mathbf{x})$ of the ordinary differential equations

$$\frac{d}{dt}\mathbf{X}(t; s, \mathbf{x}) = \mathbf{u}(\mathbf{X}(t; s, \mathbf{x}), t)$$
 (2.16)

with initial datum at time s given by $\mathbf{X}(t; s, \mathbf{x}) = \mathbf{x}$. For smooth initial data, by the chain rule it is then possible to prove that

$$c(\mathbf{x},t) = c_0(\mathbf{X}(0;t,\mathbf{x})). \tag{2.17}$$

This shows that the same derivation as above holds for a numerical method based on the semi-Lagrangian approach, provided that a numerical solution to equation (2.16) is computed. Thus, to sum things up, using the representation formula (2.17) the semi-Lagrangian methods reduces the approximation of the advection equation (2.15) to the following key steps:

- at a given time level n, compute for each mesh point \mathbf{x} an approximate solution of (2.16) to determine an estimate $\mathbf{X}^*(t^n;t^{n+1},\mathbf{x})$
- compute an approximation of (2.17) by interpolating the mesh point values at time level n at the points $\mathbf{X}^*(t^n;t^{n+1},\mathbf{x})$.

This implies that solution of the PDE (2.15) is reduced to solution of a large set of mutually independent ODEs and to performing a multidimensional interpolation. For each of these steps, a number of classical and well studied methods is available.

The role of advection in geophysical scale flows

The Euler equations in a rotating coordinate system can be written as

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u} \tag{3.1}$$

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u}$$

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p - 2\mathbf{\Omega} \times \mathbf{u} - \nabla \Phi$$
(3.1)

$$c_v \frac{dT}{dt} = -p\nabla \cdot \mathbf{u}. \tag{3.3}$$

For large scale atmospheric motion, the horizontal spatial scale $L = \mathcal{O}(10^7)m$ is much larger than the vertical one $D = \mathcal{O}(10^4)m$. Thus, the hydrostatic assumption is a good approximation (see e.g. [24], [49] for a complete derivation of the scale analysis). Furthermore, many key dynamical features of the solution to the full system are retained by simplified models that can be obtained by the barotropic assumption $p = p(\rho)$ and by considering the vertical average of equations over a homogeneous layer of fluid of variable depth. This is again justified by the fact that L >> D and leads to a two dimensional model, the so called shallow water equations

$$\frac{dh}{dt} = -h\nabla \cdot \mathbf{v} \tag{3.4}$$

$$\frac{d\mathbf{v}}{dt} = -g\nabla h - f\mathbf{k} \times \mathbf{v}. \tag{3.5}$$

$$\frac{d\mathbf{v}}{dt} = -g\nabla h - f\mathbf{k} \times \mathbf{v}. \tag{3.5}$$

where $f = 2\Omega \sin \theta$, θ is latitude and the orographic profile has been taken to be constant. Taking the curl of the momentum equation and combining the result with the continuity equation, one obtains the so called potential vorticity equation

$$\frac{d}{dt}\left(\frac{\zeta+f}{h}\right) = 0. {(3.6)}$$

It is well acknowledged (see e.g. [49]) that equation (3.6) admits as solutions most of the large scale waves (Rossby waves) which represent large meteorological systems. Further simplification can even lead to the quasigeostrophic model, in which a variant of equation (3.6) is actually the only prognostic equation, all other evolution equations having been replaced by approximate balance equations. Starting from the pioneering work of [8], early models for numerical weather forecasting (see e.g. [24], [73]) employed this simplified system for a number of computational reasons. An accurate solution of equation (3.6) (or of equivalent formulations of vorticity advection) is one of the necessary features for models that are aimed at simulating large scale atmospheric flows. It was in this context that the semi-Lagrangian methods were first developed and became over the years a widely used numerical technique.

It should also be remarked that, beyond the conceptual reasons, there have been also many practical motivations for the success of semi-Lagrangian methods in meteorology. On the standard cartesian grids in spherical coordinates, convergence of meridians at the poles leads to very high Courant numbers even at resolutions that are quite coarse elsewhere. This so called *pole problem* leads to the need for special treatment of the polar caps in many global models. Semi-Lagrangian methods, being unconditionally stable, do not pose any special stability problem with this respect, although they still require appropriate treatment of the coordinate singularity in the trajectory computation and in the interpolation in cells close to the poles.

The historical development of semi - Lagrangian methods

The first papers which are concerned with methods for the advection equation using the propagation along characteristics are the well known work of Courant, Isaacson and Rees [11] on the numerical solution of hyperbolic systems and, in the meteorological literature, a graphical integration technique proposed by R. Fjørtoft [20]. A more detailed analysis was carried out by A. Wiin-Nielsen in [73]. In this paper, the focus is again on the barotropic vorticity equation, which represented the only model for which at the time a practically feasible numerical forecast could be carried out. The method was then applied and rephrased in a formulation more similar to that of the present day in [48]. A first application to the primitive equation model was presented in [28] and the first evidence that longer time steps could be used without numerical instabilities was provided by J. Sawyer in [63]. Further development of the method of characteristic was provided in [1], while further analyses and tests in the meteorological literature were carried out in [30], [12]. It is to be remarked that one of the features which presently is most closely associated with semi-Lagrangian methods, i.e. being stable for any value of the Courant number, still had not been clearly recognized at that time (see e.g. [30],[53]).

In the early eighties, various contributions established the role of semi-Lagrangian or characteristic based methods in different modelling approaches. In the context of finite elements, the papers by Pironneau and Douglas [50], [27] have been extremely influential. In the context of finite volume approaches, a variant of the method of characteristics was proposed by G. Moretti in [41] and the concept of characteristic Galerkin methods was introduced by K.W. Morton in [42], [45]. In the meteorological context, the key contribution was that of A.Robert in [59], [60], where the numerical method by Sawyer was revisited and coupled to the semi-implicit discretization technique, thus demonstrating the full potential of

semi-Lagrangian methods in allowing the use of much longer time steps. The underlying unconditional stability was proven by J.R. Bates and A. McDonald in [3] for linear and quadratic interpolation on cartesian grids. The stability analysis of [53] for cubic spline interpolation on cartesian grids was extended to the case of Courant numbers higher than one by J. Pudykiewicz and A. Staniforth [52]. Two time level schemes were proposed by A. McDonald and J.R. Bates in [38] and by A. Staniforth and C. Temperton in [70]. The coupling of semi-Lagrangian techniques to spectral methods for the primitive equations of motion was pioneered by H.Ritchie, [57],[58]. A general stability and convergence analysis for the variable coefficient advection case was presented in [16] in the context of the finite element formulation.

The situation around the year 2000 is that a number of operational centers are employing semi-Lagrangian models for their daily forecasts, such as for example the IFS model at ECMWF [71], the GEM model at RPN Canada [9] and the Unified Model at the Met Office [72].

The practice of semi - Lagrangian methods

As it was shown at the end of section 2, the semi-Lagrangian methods reduces the approximation of the advection equation (2.15) to performing the following key steps:

- at a given time level n, compute for each mesh point \mathbf{x} an approximate solution of (2.16) to determine an estimate $\mathbf{X}^*(t^n;t^{n+1},\mathbf{x})$
- compute an approximation of (2.17) by interpolating the mesh point values at time level n at the points $\mathbf{X}^*(t^n;t^{n+1},\mathbf{x})$.

It will now be discussed how the solution to each of these steps can be implemented so as to achieve the greatest accuracy and efficiency in the resulting numerical method.

5.1 Trajectory approximation techniques

An approximation of the equations

$$\frac{d}{dt}\mathbf{X}(t;t^{n+1},\mathbf{x}) = \mathbf{u}(\mathbf{X}(t;t^{n+1},\mathbf{x}),t)$$
(5.1)

with initial datum at time t^{n+1} given by $\mathbf{X}(t;t^{n+1},\mathbf{x})=\mathbf{x}$ is essentially an ODE solver which yields the approximate Lagrangian backward trajectories which will get at the meshpoints. It is important to notice that the solution of (5.1) requires, in general, knowledge of the velocity field at points which do not belong to the spacetime computational mesh. For application to realistic models, this implies that some interpolation or in some cases, as far as the time dependence is concerned,

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some extrapolations are necessary. Traditionally, three main strategies have been proposed and implemented for the approximation of the particle trajectories.

- fixed point iteration approach
- substepping with explicit ODE solvers
- Taylor expansion of the parametric representation for the trajectory

The fixed point iteration technique was introduced in its best known form in [59], although an iterative technique had also been used in [36]. It is quite widely (if not almost exclusively) the technique of choice in atmospheric modelling. Defining the displacement $\mathbf{a} = \mathbf{x} - \mathbf{X}(t^n; t^{n+1}, \mathbf{x})$ as the unknown quantity to be determined, Robert's method consists of formulating the displacement equation

$$\mathbf{a} = \Delta t \mathbf{u} (\mathbf{x} - \mathbf{a}, t^*), \tag{5.2}$$

where t^* is a time at which the velocity field has been frozen for the purposes of the trajectory computation. Depending on the value of t^* , a more or less accurate time discretization is achieved, see e.g. the discussion in []. For example, in order to have a second order accurate time discretization, in the context of a two time level scheme, one should choose $t^* = t^{n+\frac{1}{2}}$, which leads to the need for a time extrapolation in case the velocity fields are only known up to time t^n . The advantage of the iterative technique is that it is unconditionally stable and that the iterations can be proven to converge under conditions that are relatively mild for atmospheric flows, see e.g. [52], [65].

The trajectory methods have been instead more popular in the finite element and coastal modelling community, see e.g. [50], [7], [56], [16], [40], although applications to atmospheric models have are also reported in the literature, see e.g. [6], [22]. In order to guarantee that the approximated trajectories do not cross each other, shorter time steps have to be used in general for their approximation, whenever the Courant number is larger than one.

The Taylor expansion technique was introduced instead by [39] for cartesian grids and extended in [21] to triangular finite element grids. It is based on the Taylor expansion in time of $\mathbf{X}(t^n;t^{n+1},\mathbf{x})$ and on an approximate reconstruction of the time derivatives involved. The advantage over the previous techniques is that no interpolations or extrapolations are required. On the other hand, the approximated time derivative require extra storage and the derivation of the approximation is entirely heuristic and not generally valid for arbitrary flows.

Another possible approach is that proposed by R.J. Purser and L.M. Leslie in [55], which employs forward in time trajectories.

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5.2 Interpolation techniques

The other key ingredient in the implementation of a semi-Lagrangian method is the interpolation procedure employed in each timestep to reconstruct the solution values at the departure point of the streamline. Most of the work on evaluation of interpolation algorithms has been done for cartesian grids, due to the context in which the methods were developed. Linear interpolation produces quite diffusive solutions, as it will be shown in section 6. In the case of one dimensional flow with Courant numbers smaller than one, it is easy to see that in fact the upwind method is recovered. Quadratic interpolation was used in [3]. Cubic Lagrange interpolation was used already in [63] and cubic spline was first applied in [53]. Cubic Lagrange interpolation was also used in the fundamental work of Robert [59], [60] and analyzed in [52]. This is the interpolation technique most widely used in atmospheric applications. In general, it was shown by McCalpin in [37] that different properties are obtained depending on whether odd or even order polynomials are used in the interpolation. The so called cascade interpolation method was also proposed by R.J. Purser in [54] and an improved cascade interpolation technique is presented in [46].

On unstructured meshes typical of finite element models, the finite element interpolators are generally used. However, successful attempts to achieve higher accuracy by means of kriging or radial basis function interpolators have been reported in [61],[62], [4].

It is well known that the maximum principle discussed in section 2 for the linear interpolation case cannot be proven for higher order interpolators. This is similar to what happens for many other numerical schemes for the advection equation, see e.g. [32], [56]. The issue was considered in [74], where various monotonic interpolation techniques based on Hermite interpolation were compared. A general prescription to overcome the intrinsic lack of monotonicity of all higher order interpolation and to monotonize a semi-Lagrangian method was given [5], along with a proof of the monotonicity of the resulting scheme. This approach is also the most widely followed in operational implementations. In all the tests performed in section 6, smooth solutions were considered (for which undershoots and overshoots are minimized) and no monotonization procedure was employed.

Numerical tests: one and two dimensional passive tracer transport

In this section, the results of some numerical tests will be presented, in order to give an idea of how the semi-Lagrangian method performs and of the different accuracy that can be achieved by varying the interpolation and trajectory approximation algorithm. Results obtained in the same tests with some Eulerian schemes will also be shown, for the purpose of some general comparison of the two approaches. It should be stressed that good results in computation of specific idealized test cases are a necessary, but not sufficient condition for the general applicability of a numerical method. Furthermore, unsatisfactory results do not rule out the applicability in special cases different than the ones considered and it is not always possible to draw general conclusion from the particular cases considered. Last but not least, evaluation of the efficiency of a specific method can in our view be done only in a very approximate way, since the effective execution time is so strongly dependent on many things that have little to do with the numerical method itself (i.e., its specific coding and the machine architecture). Although these considerations are pure good common sense, they are sometimes overlooked when different modelling philosophies are compared against each other in a simplified framework.

6.1 One dimensional advection

The one dimensional tests have been performed considering equation (2.1) on the interval [0,2] of the real line and taking as initial datum a \mathcal{C}^1 , compactly supported, bell shaped function with a maximum value of 10. The advection velocity was taken to be u=1/2 and the spatial resolution was $\Delta x=1/100$. For the first tests, the timestep was taken to be $\Delta t=0.05$, so that a Courant number of C=2.5 was

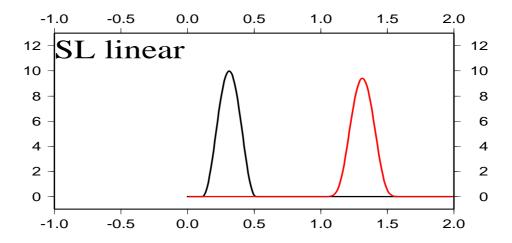


Figure 6.1: Semi-Lagrangian method, exact trajectories, linear interpolation.

obtained. The test was run up to time T=2. The results obtained with the semi-Lagrangian method using linear, quadratic or cubic spline interpolation are shown in figures 6.1, 6.2, 6.3, respectively (black lines are used for the initial datum, gray lines for the profile at the final time). It should be remarked that in this test the exact value for the trajectory departure point was used, since all basic integration schemes would have given the exact result in the simple case of velocity constant in time and space.

A more quantitative analysis is given in table 6.1. here, the relative l_1 and l_2 errors are given, which at time level n are computed as

$$e_1^{rel} = \frac{\sum_{i=1}^{N} |c_i^n - ex_i|}{\sum_{i=1}^{N} |ex_i|}$$
 (6.1)

$$e_1^{rel} = \frac{\sum_{i=1}^{N} |c_i^n - ex_i|}{\sum_{i=1}^{N} |ex_i|}$$

$$e_2^{rel} = \frac{\sqrt{\sum_{i=1}^{N} (c_i^n - ex_i)^2}}{\sqrt{\sum_{i=1}^{N} ex_i^2}}$$
(6.1)

where c(x,t) is the analytic solution, $ex_i = c(x_i,t^n)$ and N is the total number of gridpoints in the computational domain. The dispersion and diffusion errors are also given. These quantities were introduced in [69] and can be defined as

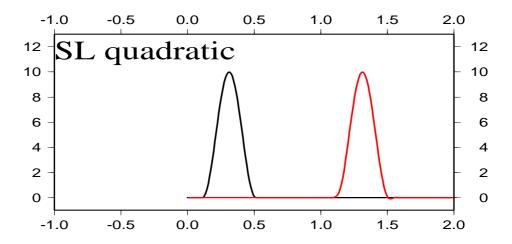


Figure 6.2: Semi-Lagrangian method, exact trajectories, quadratic interpolation.

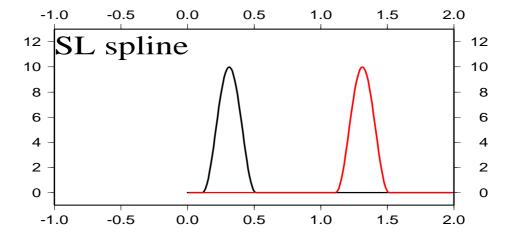


Figure 6.3: Semi-Lagrangian method, exact trajectories, cubic spline interpolation.

Method	e_2^{rel}	e_1^{rel}	Dispersion	Diffusion	Minimum
Linear	6.31e-2	7.40e-2	3.84e-2	2.13e-2	0.0
Quadratic	7.98e-3	9.38e-3	9.55e-4	4.36e-7	-0.1
Spline	5.02e-4	3.60e-4	3.77e-6	3.57e-9	-9.5e-3

Table 6.1: Errors of semi-Lagrangian method for the one dimensional test.

Dispersion error
$$= 2 \left[\sigma(c^n) \sigma(ex) - \frac{1}{N^2} \sum_{i,j=1}^N (c_i^n - \bar{c})(ex_j - \bar{ex}) \right]$$
Dissipation error
$$= [\sigma(c^n) - \sigma(ex)]^2 + (\bar{c}^n - \bar{ex})^2, \tag{6.3}$$

where one has defined, for a generic mesh functions ϕ_i ,

$$ar{\phi} = rac{1}{N} \sum_{i=1}^{N} \phi_i \quad \ \sigma(\phi)^2 = rac{1}{N} \sum_{i=1}^{N} (\phi_i - ar{\phi})^2.$$

They have the property that

$$\sum_{i=1}^{N} (c_i^n - ex_i)^2 = \text{Dispersion error} + \text{Diffusion error}, \tag{6.4}$$

so that the total l_2 error can be decomposed in two terms. One accounts for the difference in the first two moments of the computed and analytic solutions. This term is called diffusion error because the largest contribution to these differences are given by the numerical diffusion of the considered method. The other term measures the difference between the correlation of the computed and analytic solution and the product of their variances. If the deviation from the mean of the computed and analytic solution were independent random variables, this term would be zero. Thus, values different from zero denote a spatial correlation between these deviations and therefore a certain amount of phase shift between the computed and analytic solution. These quantities are quite useful for an accurate evaluation of the properties of a numerical method for the advection equation. Finally, the minimum of the computed solution is also shown, to highlight the fact that undershoots (or overshoots) may occur.

6.2 Two dimensional advection

For two dimensional passive advection, the most basic and best known test case was considered, namely solid body rotation. The rotation takes place around

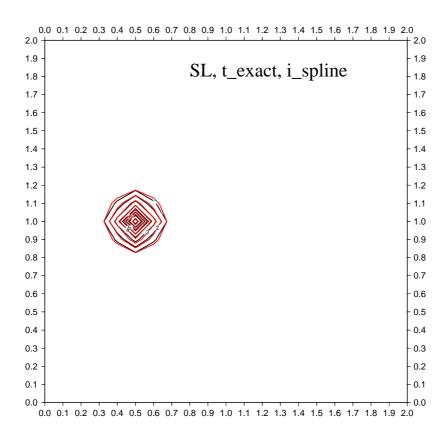


Figure 6.4: Semi-Lagrangian method, exact trajectories, cubic spline interpolation.

the center of the domain interval $[0,2] \times [0,2]$ and taking as initial datum a \mathcal{C}^1 , compactly supported, bell shaped function with a maximum value of 10. The rotation period was taken to be was taken to be T=1000 and the spatial resolution was $\Delta x=1/25$. For the first tests, the timestep was taken to be $\Delta t=5.0$. Maximum one dimensional Courant numbers of C=0.78 were obtained, so that a CFL condition is actually still satisfied everywhere. The test was run up to time T=1000. First of all, the results obtained with the semi-Lagrangian method using cubic spline interpolation and the exact trajectories are shown in figure 6.4.

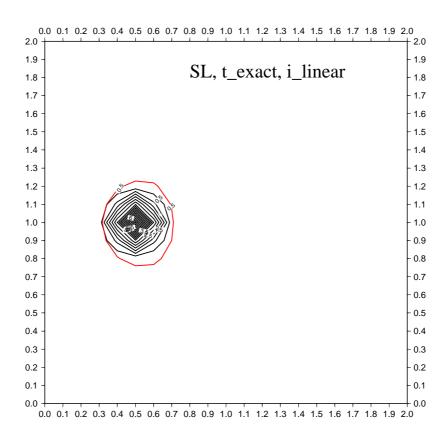


Figure 6.5: Semi-Lagrangian method, exact trajectories, bilinear interpolation.

Method	e_2^{rel}	e_1^{rel}	Dispersion	Diffusion	Minimum
Bilinear	0.89	1.51	0.49	0.75	0.0
Cubic	0.21	0.35	4.31e-2	2.76e-3	-0.98

Table 6.2: Errors of semi-Lagrangian method with exact integration of trajectories in solid body rotation test.

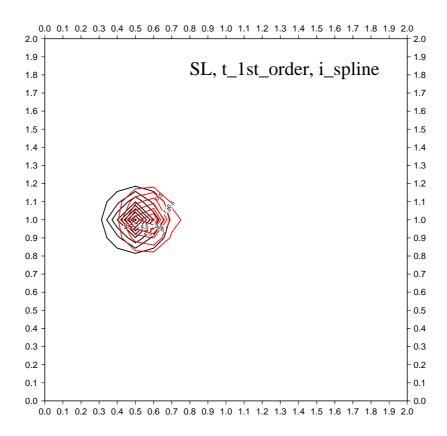


Figure 6.6: Semi-Lagrangian method, Euler method for trajectories, spline interpolation.

Method	e_2^{rel}	e_1^{rel}	Dispersion	Diffusion	Minimum
Cubic, 1st	0.62	0.75	0.54	4.58e-2	-0.27
Cubic, 1st, $\Delta t/5$	0.19	0.31	5.06e-2	3.62e-3	-0.43
Cubic, 2nd	0.14	0.23	2.93e-2	2.84e-3	-0.23

Table 6.3: Errors of semi-Lagrangian method with approximate integration of trajectories in solid body rotation test.

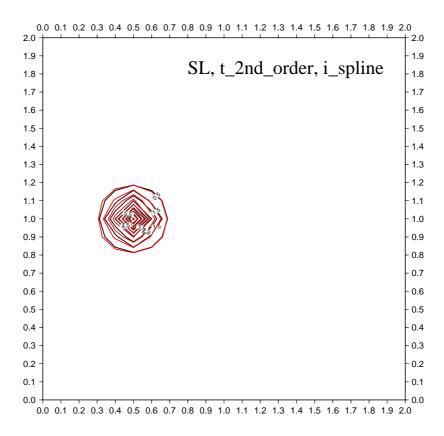


Figure 6.7: Semi-Lagrangian method, second order Runge Kutta method for trajectories, spline interpolation.

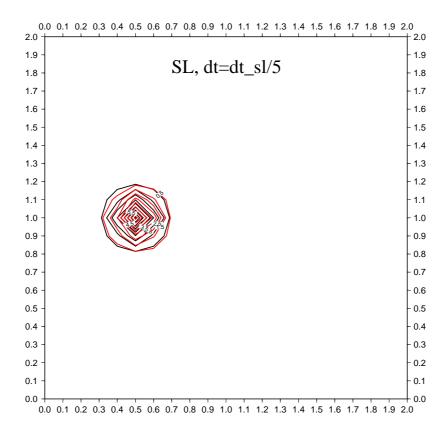


Figure 6.8: Semi-Lagrangian method, Euler method for trajectories with $\Delta t/5$, spline interpolation.

Method	e_2^{rel}	e_1^{rel}	Dispersion	Diffusion	Minimum
upwind	0.23	0.29	0.54	0.3	0.0
leapfrog	3.62e-2	4.94e-2	1.96e-2	8.25e-11	-0.33
Lax Wendroff	3.47e-2	4.44e-2	1.8e-2	1.18e-5	-0.3
Crowley	2.48e-3	2.23e-3	9.25e-5	1.7e-9	-4.2e-2
leapfrog, 4th order in x	1.18e-2	1.54e-2	2.11e-3	3.57e-10	-0.13

Table 6.4: Errors of Eulerian methods for the one dimensional test.

Method	e_2^{rel}	e_1^{rel}	Dispersion	Diffusion	Minimum
Crowley $\Delta t/5$	0.55	1.4	0.46	2.75e-3	-2.73
Crowley $\Delta t/10 \ \Delta x/2$	0.16	0.27	4.03e-2	3.95e-4	-0.65

Table 6.5: Errors of Eulerian methods in solid body rotation test.

6.3 A comparison with simple Eulerian schemes

The issue of whether semi-Lagrangian schemes are to be preferred to Eulerian schemes for the treatment of advection has been quite widely debated. Here, just a small contribution to this long and often heated debate is given, with the aim of providing a few examples of typical results obtained when applying the two techniques in standard tests.

First of all, the results of basic one dimensional advection schemes are shown for the same passive advection test discussed in section 6.1. Here, the Courant number was taken to be C=1/2 in order to comply with the CFL criterion. The advection schemes reviewed in section 2 were used. The two dimensional fourth order Crowley scheme obtained by simple discretization with the same approach of the derivatives in the x and y direction was then used in the solid body rotation test, at various space and time resolutions. Timesteps shorter than the semi-Lagrangian one had to be used to achieve acceptable results, the timestep fraction indicated in the legends refers to the timestep used for the semi-Lagrangian runs.

No final conclusions can be drawn from a such limited and non exhaustive comparison. However, in the opinion of the author of this review, some considerations are possible. First of all, the reduction of the dispersion error provided by accurate upstream based methods is apparent. This can be seen in the one dimensional tests both for Eulerian upwind schemes such as the Crowley method and for the semi-Lagrangian method. The (upwind based) Crowley scheme and the leapfrog, fourth order scheme (2.5) are both formally of the same order of accuracy in space, but the upstream methods appear to produce better results in this respect.

It is also clear that one dimensional comparisons are not really sufficient,

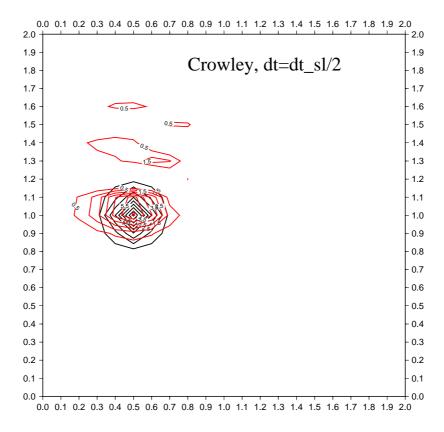


Figure 6.9: Eulerian method (Crowley) with $\Delta t/2$.

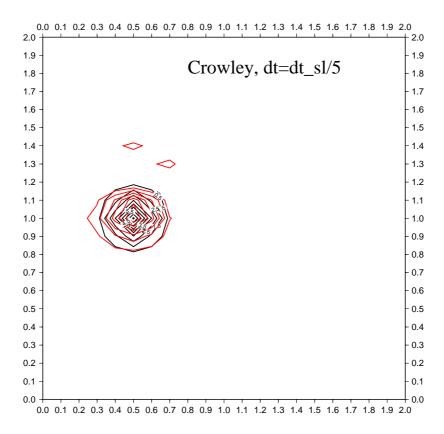


Figure 6.10: Eulerian method (Crowley) with $\Delta t/5$.

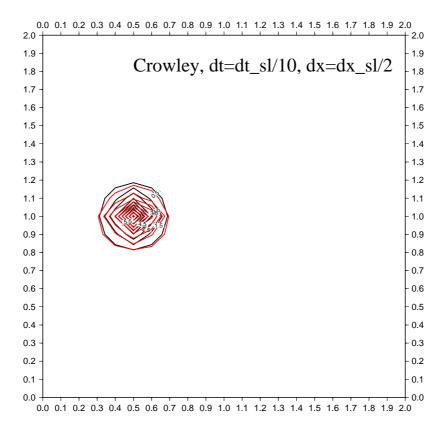


Figure 6.11: Eulerian method (Crowley) with $\Delta t/10$ and $\Delta x/2$.

since another key point appears to be the natural multidimensionality of semi-Lagrangian methods. In one dimension, the Crowley scheme is formally of the same order of accuracy of the cubic spline, first order trajectory semi-Lagrangian method. However, the straightforward generalization to two dimensions is clearly less accurate. Fully multidimensional, accurate Eulerian schemes are available (see e.g. among many others [32], [64], [66]), but the computational cost and complexity required appear to be roughly of the same order of magnitude (at least) as those required by standard semi-Lagrangian approaches.

These considerations are completely independent of the unconditional stability of semi-Lagrangian schemes and of the resulting issue. Clearly, being able to run a model at high Courant numbers is a very attractive feature, especially for weather prediction models using latitude-longitude cartesian meshes, where convergence of meridians at the poles naturally leads to severe CFL restrictions for Eulerian schemes. On the other hand, abusing of the unconditional stability can also lead to other accuracy problems, as discussed e.g. in [2], [26].

Putting all this together, it seems possible that, replacing the *Eulerian vs semi-Lagrangian* controversy with a *naively vs fully multidimensional* controversy could make some sense. In view of the rather general framework proposed e.g. in [43], this seems also justified with respect to the related controversy on the mass conservation issue. The efficiency issue would require much more careful and complex comparisons (whose results may possibly yield contradicting answers, depending on the target application). However, it should be observed that, as pointed out in [26], the Courant numbers are often smaller than one in large portions of the computational domain. Thus, it is especially a gain in robustness that is provided by semi-Lagrangian methods, by enabling *cum grano salis* runs with Courant numbers larger than one somewhere.

The theory of semi - Lagrangian methods: convergence and stability analysis

It is remarkable that one of the features that are presently most closely associated with semi-Lagrangian methods, i.e. being stable for any value of the Courant number, was not been clearly recognized in the early stages of the development of these methods (see for example, [30],[53]). Motivated by the results of A.Robert in [59], [60], the unconditional von Neumann stability was proven in [3] for linear and quadratic interpolation and in [52] for cubic spline interpolation, thus extending previous results of [53]. A general convergence and stability analysis for the variable coefficient advection case was presented in [16]. Characteristic Galerkin approaches were analyzed in [44], [68] and a general framework for the analysis of characteristic based methods on unstructured grids was proposed in [43].

The stability analysis in [16] extends the previous results to more general interpolation procedures, in particular those natural for finite element approaches. The convergence analysis is performed for a finite element formulation of the semi-Lagrangian method using Runge-Kutta methods for the approximation of the trajectories in the case for which a single step is sufficient (i.e., Courant number smaller than one). One of the main results in [16] can be summarized and reformulated as follows in the context of the finite difference formulation outlined in 2:

Theorem: Assuming that the trajectory approximation method is $\mathcal{O}(\Delta t^p)$, that the error in the spatial interpolation procedure is $\mathcal{E}(\Delta x)$, and that a time interval [0,T] is considered such that $\Delta t = T/N$, under mild regularity assumptions it holds

$$\max_{n=1,N} \max_{i} |c(x_i, t^n) - c_i^n| \le C \left[\mathcal{O}(\Delta t^p) + N \mathcal{E}(\Delta x) \right]. \tag{7.1}$$

	l_2 error	l_2 error $\Delta t/2, \Delta x/2$	Order
SL, cubic	1.96e-2	4.72e-3	2.2
Lax Wendroff	0.13	3.58e-2	1.8

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Table 7.1: Convergence test for semi-Lagrangian and Lax Wendroff method (one dimensional advection).

	l_2 error	l_2 error $\Delta t/2$	Order
SL, cubic	1.96e-2	2.27e-2	-0.5
SL, cubic $\Delta x/2$	3.19e-4	4.72e-3	-3.9
Order	5.9	2.2	

Table 7.2: Convergence test for semi-Lagrangian and (one dimensional advection).

Here, x_i are the nodes of a cartesian discretization mesh in \mathbf{R}^d . It can be seen that this upper bound of the error in the l_{∞} norm grows proportionally to the number of timesteps used. Although this is not necessarily a strict upper bound, error accumulation can be easily observed in simple advection tests. For a clear demonstration of the impact of the interpolation error $\mathcal{E}(\Delta x)$, see e.g. the results in figures 6.4,6.5. A consequence of this property is that convergence tests give rather awkward, if not quite disappointing results, see e.g. table 6.2, the results presented in [16] and the discussion in [26]. As an example, simple convergence tests performed with the semi-Lagrangian scheme and the Lax Wendroff scheme are reported in table 7. Here, one dimensional advection was considered and the space and time steps were halved simultaneously. While the Lax Wendroff scheme displays a convergence rate approximaly corresponding to the expected one, the convergence rate of the (formally fourth order in space) semi-Lagrangian scheme is barely around 2. These results can be confronted with those in table 7, where the same test was repeated halving space and time steps independently. It can be seen that increase in spatial resolution leads to a consistent decrease in the discretization error, even beyond the expected convergence rate, while halving the time step leads actually to an error increase (hence the negative convergence rates), whose magnitude, however, depends on the spatial resolution.

Semi - Lagrangian methods versus the method of characteristics: semi implicit semi - Lagrangian methods for low Froude number regimes

The semi-Lagrangian method and the method of characteristics are very similar in many respects. For example, the method of Courant, Isaacson and Rees [11] applied to the scalar advection equation yields a variant of the semi-Lagrangian method. On the other hand, if the applications to hyperbolic systems are considered, the way in which the semi-Lagrangian approach is generally applied to the atmospheric equations of motion in the meteorological literature is quite different from the method of characteristics. In this section, the method of characteristics will be briefly reviewed and the differences with semi-implicit, semi-Lagrangian methods willbe highlighted.

The literature on method of characteristics will not be reviewed here fully, some relevant references with closer relationship to semi-Lagrangian methods are for example [17],[18], [19], [41], [42],[44]. Consider a one dimensional, linear hyperbolic system

$$\frac{\partial \mathbf{c}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{c}}{\partial x} = 0 \tag{8.1}$$

where hyperbolic means that A has real and distinct eigenvalues and the invertible matrix T whose columns are the eigenvectors of A is such that $T^{-1}AT = \Lambda$, where Λ is the diagonal matrix of the eigenvalues of A. For definiteness and for the purpose of the following discussion, consider the linear shallow water equations, for which

$$\mathbf{c} = \begin{bmatrix} h \\ u \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} U & H \\ g & U \end{bmatrix}$$

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so that

$$\mathbf{\Lambda} = \begin{bmatrix} U + \sqrt{gH} & 0 \\ 0 & U - \sqrt{gH} \end{bmatrix} \quad \mathbf{T} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{\frac{H}{g}} \\ \frac{1}{2} & -\frac{1}{2}\sqrt{\frac{H}{g}} \end{bmatrix} \quad \mathbf{T}^{-1} = \begin{bmatrix} 1 & 1 \\ \sqrt{\frac{g}{H}} & -\sqrt{\frac{g}{H}} \end{bmatrix}$$

Setting d = Tc and performing this change of variables in equation (8.1) one obtains

$$\frac{\partial \mathbf{d}}{\partial t} + \mathbf{\Lambda} \frac{\partial \mathbf{d}}{\partial x} = 0. \tag{8.2}$$

The resulting system consists now of two decoupled, one dimensional advection equations. The method of Courant, Isaacson and Rees [11] solves them, at each timestep, by tracking back the characteristic line and interpolating at the foot of the characteristic. The values of the original variables can then be recovered as $\mathbf{c} = \mathbf{T}^{-1}\mathbf{d}$. In the linear case, this procedure yields back

$$h_{i}^{n+1} = \frac{1}{2} h_{i-\frac{(U+\sqrt{gH})\Delta t}{\Delta x}}^{n} + h_{i-\frac{(U-\sqrt{gH})\Delta t}{\Delta x}}^{n}$$

$$u_{i}^{n+1} = \frac{1}{2} u_{i-\frac{(U+\sqrt{gH})\Delta t}{\Delta x}}^{n} + u_{i-\frac{(U-\sqrt{gH})\Delta t}{\Delta x}}^{n}$$

$$(8.3)$$

Here, the same notation as in section 2 has been used.

Since the Euler and shallow water equations also constitute hyperbolic systems, it is possible in principle to apply the method of characteristics directly to atmosperic modelling. However, a number of peculiarities of the atmospheric equations of motion (3.1)-(3.3) have lead instead to rather different developments in atmospheric modelling. The scale analysis sketched in section 3 shows that large scale atmospheric flows are in approximate geostrophic balance away from the tropics. This also holds for simplified two dimensional models such as the shallow water equations, for which geostrophic balance can be expressed as

$$-g\nabla h - f\mathbf{k} \times \mathbf{v} \approx 0. \tag{8.4}$$

Thus the Coriolis force is very important part of the equations, but since it is just a zero order term, it does not show up in the associated hyperbolic system and does not influence its characteristics. Furthermore, the rotational component of the typical large scale flow is about one order of magnitude larger than the divergent component (see e.g. [24], [49]). As a result, further simplified models can be developed, such as quasigeostrophic models or models based on the barotropic

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vorticity equation, which still capture the basic observable features of large scale dynamics. In these models, gravity waves (i.e., the solutions to the shallow water equations whose features are related to the characteristics of the associated hyperbolic system) are not present any more. Some of the most relevant physical quantities which determine atmospheric flows (i.e. potential vorticity) are simply advected by the velocity field, rather than propagating along the characteristics. In the case of the full Euler equations (3.1)-(3.3), the solutions determined by the characteristics of the associated hyperbolic problem (i.e., the sound waves) would in general be unresolved even on very high resolution meshes. Furthermore, the previous analysis shows that they are not the most relevant term for the prediction of large scale flow. Even for the prediction of mesoscale features, they are much less relevant than internal gravity waves produced by buoyancy effects, which also depend mostly on therms that do not contribute to the characteristics of the Euler equations. It should also be considered that typical atmospheric applications are concerned with flows at low Mach number and in the quasi-incompressible regime, i.e., in the context of the linear shallow water equations, regimes for which

$$\frac{|U|}{\sqrt{gH}} << 1. \tag{8.5}$$

Thus, the characteristics derived from the hyperbolic system are quite different from the streamlines of the flow, along which the relevant quantities are actually advected. On top of all these issues, most standard implementations of the method of characteristics must satisfy a Courant-Friedrichs-Lewy stability restriction of the type

$$\frac{|U \pm \sqrt{gH}|\Delta t}{\Delta x}.$$
 (8.6)

Thus, these time discretizations for the gravity wave propagation are quite inefficient if (8.5) holds.

The semi-implicit, semi-Lagrangian methods proposed by Robert in [60] do not suffer from this stability restriction, which explains their widespread (although by no means universal) use, especially for weather forecasting models. In the semi-implicit, semi-Lagrangian approach, the Lagrangian derivatives e.g. in equations (3.4)-(3.5) are approximated by a finite difference along an approximated streamline, while the terms responsible for the gravity wave propagation are discretized implicitly in time to avoid the stability restriction (8.6). More precisely, using the notation introduced in section 2, consider for each generic point x in the computational domain the ODE

$$\frac{d}{ds}\mathbf{X}(s; s + \Delta t, \mathbf{x}) = \mathbf{u}(\mathbf{X}(s; s + \Delta t, \mathbf{x}), s)$$
(8.7)

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and set $\mathbf{x}_* = \mathbf{X}(t; t + \Delta t, \mathbf{x})$. Furthermore, denote by ϕ_* a generic quantity interpolated at the point \mathbf{x}_* . A semi-implicit semi-Lagrangian discretization of the shallow water equations is given by

$$\frac{h^{n+1} - h_*^n}{\Delta t} = -\frac{1}{2} [h^n \nabla \cdot \mathbf{v}^{n+1} + h_*^n \nabla \cdot \mathbf{v}_*^n]$$
(8.8)

$$\frac{\mathbf{v}^{n+1} - \mathbf{v}_*^n}{\Delta t} = -\frac{g}{2} [\nabla h^{n+1} + \nabla h_*^n] - \frac{f \mathbf{k} \times \mathbf{v}^{n+1} + f_* \mathbf{k} \times \mathbf{v}_*^n}{2}.$$
 (8.9)

As previously remarked, the Lagrangian derivatives have been approximated by backward finite differences along the streamlines, while the terms responsible for the propagation of gravity and inertia-gravity waves (see e.g. [49]) have been averaged in time along the streamlines. The implicit discretization algorithm resulting from (8.8)- (8.9) entails substitution of equation (8.9) into (8.8) to obtain an elliptic equation for h^{n+1} , which has to be solved at each time step. Once this value is computed, it is then backsubstituted in (8.9) to complete the time discretization algorithm. The von Neumann analysis of the corresponding linearised equations shows that this time discretization is unconditionally stable. Furthermore, it can be extended successfully to the full Euler equations.

Mass conservative and flux form semi-Lagrangian methods

Semi-Lagrangian methods, in the generally applied formulation that was presented here, are not mass conservative. As an example, consider the one and two dimensional tests discussed previously. The ratios between the total mass of the computed solution and that of the initial datum are shown in tables 9,9, respectively.

A number of approaches have been proposed to overcome the lack of mass conservation of semi-Lagrangian methods. In many practical applications, *a posteriori* mass restoration is performed to keep the mass of the atmosphere constant. The methods proposed in [23], [51] impose mass conservation as a global constraint, which is however still achieved via redistributions of the mass gains or losses among all mesh points. Neither of these simpler approaches guarantees local mass conservation, i.e., changes in the solution at a given mesh point do not necessarily depend on the values in the neighbouring mesh points.

In order two achieve also local mass conservation, two main strategies have been pursued. On one hand, the advection equation

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = 0 \tag{9.1}$$

can be integrated over a volume $\Omega(t)$ that is moving with the flow, so as to obtain

	Linear	Quadratic	Spline
Computed/exact mass	1.00002384	1.00293481	1.00027871

Table 9.1: Errors of semi-Lagrangian method with respect to mass conservation in one dimensional test (Courant number 2.5).

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	Linear, exact traj.	Spline, 1st order traj.	Spline, 2nd order traj.
Computed/exact mass	0.7668	0.8828	1.1059

Table 9.2: Errors of semi-Lagrangian method with respect to mass conservation in two dimensional test (Courant number 0.7).

$$\frac{d}{dt} \int_{\Omega(t)} c dx = 0. {(9.2)}$$

Taking $\Omega(t + \Delta t)$ to coincide with a mesh control volume, as in the non conservative semi-Lagrangian approach, a simple time discretization of (9.2) yields

$$\int_{\Omega(t+\Delta t)} c dx = \int_{\Omega(t)} c dx, \tag{9.3}$$

where $\Omega(t)$ is now an upstream control volume which will evolve into the $\Omega(t+\Delta t)$ within the timestep Δt . Equation (9.3) is then discretized by approximate reconstruction the upstream control volume and approximate computation of the integral on the right hand side. This approach has been sometimes called conservative remapping, or cell integrated semi-Lagrangian method. The idea of remapping goes back at least as far as [25]. Mass conserving variants of the semi-Lagrangian method based on this concept of remapping were introduced for example in [29], [34], [35], [13], [47].

An alternative path to local conservation is more similar in spirit to Eulerian finite volume methods. Equation (9.1) is rewritten as conservation law

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = 0 \tag{9.4}$$

by means of the continuity equation (for simplicity, constant density, incompressible flow is considered here). Equation (9.4) is then integrated in space over a fixed mesh control volume Ω and the divergence theorem is applied as usual. The resulting equation is then integrated in time over a generic time step, so as to obtain

$$\int_{\Omega} c(x, t + \Delta t) dx = \int_{\Omega} c(x, t) dx - \int_{t}^{t + \Delta t} ds \int_{\partial \Omega} c(x, s) \mathbf{u}(x, s) \cdot \mathbf{n}$$
 (9.5)

Equation (9.5) is then discretized by approximate reconstruction of the flux through the domain boundaries over the time step Δt . Semi-Lagrangian backward trajectories that reach a number of points along $\partial\Omega$ at time $t+\Delta t$ are computed and used for the approximation of the fluid portion that is advected through the boundaries.

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Some form of polynomial reconstruction is then used at these points to discretize the space time integral on the right hand side. We will refer loosely to methods which can be described in this way as flux form semi-Lagrangian methods. Examples of these have been introduced for example in [17], [18], [19], [31], [33]. In [43], these approaches were described in a wider context as generalized Godunov methods and a stability analysis of the method was outlined. It should be remarked that this approach can also be interpreted as a natural generalization of the so called wave propagation methods, see e.g. [32].

Conclusions

The semi-Lagrangian method for the solution of the advection equation was introduced, as it has developed in the context of atmospheric modelling over the last 50 years. Its basic implementation features were discussed and analyses of the underlying theorical properties were reviewed. In particular, it was attempted to put the methods developed for atmospheric modelling in the broader perspective of advanced finite volume and finite element methods, along the lines of the framework proposed by K.W. Morton in [43]. Possibly, in this way many controversies on the relative merits of Eulerian and Lagrangian schemes could be reconciled by the understanding of the strong similarities among advanced, fully multidimensional advection schemes.

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