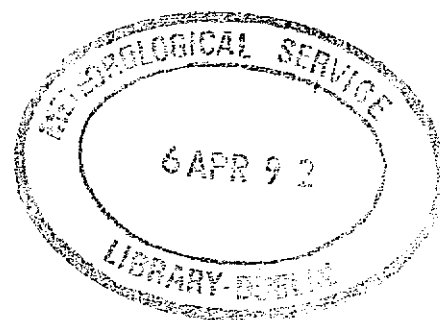


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SEMI-LAGRANGIAN METHODS

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1. INTRODUCTION

My original intention for this lecture was to present a review of semi-Lagrangian integration schemes for atmospheric models. However, a paper by Staniforth and Cote (1991) has just appeared doing exactly that. May I recommend it for its thoroughness, clarity and extensive bibliography. In order to avoid duplicating it I will refrain from giving an overview of the subject and concentrate instead on a small number of topics and treat them in more depth than is possible in a review.

The plan, therefore, is to apply semi-Lagrangian methods to simple equations in order to illustrate the fundamentals of the subject unencumbered by excessive technical detail. Hopefully, sufficient insight can be gained in this way to enable those interested to apply the methods in a more general context. Thus, in section 2 the one dimensional advection equation is used to show how the semi-Lagrangian approach works and why it should be superior to the Eulerian approach. In section 3 the barotropic vorticity equation is used to demonstrate the implementation of the scheme in practice and to trace the historical evolution of the basic ideas underpinning the method. Finally, in section 4 the one dimensional continuity equation is used to point out a potential flaw in the method, at least as presently implemented, that is, the fact that it is not exactly conserving, which may make it unsuitable for climate modelling. Possible methods of overcoming this problem are then discussed.

2. ACCURACY AND STABILITY

Consider the one dimensional linear advection equation

$$\partial\psi(x,t)/\partial t + c\partial\psi(x,t)/\partial x = 0., \quad (2.1)$$

where c is the constant advecting velocity. If it is integrated numerically using an Eulerian scheme then instabilities develop unless $c\Delta t/\Delta x \leq 1$, where Δt and Δx are the increments into which space and time have been divided for the purpose of the integration. See, for example, section 5.3 of Haltiner and Williams (1980), hereinafter called HW). As has been pointed out by Robert (1981), this condition limits Δt to a

value six times smaller than is typically required for accuracy in weather forecasting. Therefore, computer time can be saved if an alternative, equally accurate, computationally inexpensive integration method which avoids this restriction can be invented. In what follows it will be argued that the multiply-upstream semi-Lagrangian scheme fulfils these requirements.

It is founded on the 'Lagrangian' property of Eq.(2.1) that its solution at time t is given in terms of its initial value by $\psi(x, t) = \psi(x - ct, 0)$. In order to see how this can give rise to an unconditionally stable integration scheme consider what happens if Eq.(2.1) is integrated forward for one time step. The field at the arrival point $x = I\Delta x$ at time $t = (n+1)\Delta t$ is given in terms of the field at the departure point $x_* = I\Delta x - c\Delta t$ at time $t = n\Delta t$ by

$$\psi\{I\Delta x, (n+1)\Delta t\} = \psi\{x_*, n\Delta t\}. \quad (2.2)$$

Since x_* is not necessarily a grid point, some approximation method is obviously needed to interpolate to it from the known values of the fields at the grid points.

The choice of interpolation points dictates the stability of the scheme. This can be seen by looking at the linear Lagrange method, the simplest non-trivial interpolation. For any two grid points this gives ($J > K$ without loss of generality)

$$\psi(x, n\Delta t) = [(x - x_K)/(x_J - x_K)]\psi_J^n + [(x - x_J)/(x_K - x_J)]\psi_K^n, \quad (2.3)$$

where the notation $\psi_J^n = \psi(J\Delta x, n\Delta t)$ has been introduced. Assuming that Eq.(2.2) has a solution of the form $\psi_J^n = \lambda^n \exp[ikI\Delta x]$ and substituting $x = x_* = I\Delta x - c\Delta t$ in Eq.(2.3) yields

$$|\lambda|^2 = 1 + [-1 + \{-1 + 2(I - \alpha - J)/(K - J)\}^2] \sin^2[k\Delta x(J - K)/2],$$

where $\alpha = c\Delta t/\Delta x$. Inspection of this equation yields the condition $|\lambda|^2 \leq 1$ if $0 \leq 2(I - \alpha - J)/(K - J) \leq 2$, that is, if $K \leq (I - \alpha) < J$, or equivalently, $K\Delta x \leq x_* < J\Delta x$. Thus, stability is guaranteed for any c provided the grid points used in the interpolation surround the departure point. Although this has been demonstrated only for the simplest possible interpolation it will be used as a guiding principle from now on. Thus, the method avoids the CFL stability restriction by 'going multiply upstream'.

The next question to ask is whether it is as accurate as the Eulerian schemes which it seeks to supplant. Eq.(2.2) can be written as

$$[\psi\{I\Delta x, (n+1)\Delta t\} - \psi\{x_*, n\Delta t\}]/\Delta t = 0. \quad (2.4)$$

The task is to find an interpolation method which ensures that this finite difference equation approximates Eq.(2.1) at least to $O(\Delta t^2)$ and $O(\Delta x^2)$. Not surprisingly, it turns out that the Lagrange linear method is not accurate enough. Consider, therefore, a Lagrange quadratic interpolation using the three grid points closest to, and surrounding the point x :

$$\begin{aligned} \psi(x, n\Delta t) = & \{[(x - x_K)(x - x_{K+1})] / [(x_{K-1} - x_K)(x_{K-1} - x_{K+1})]\} \psi_{K-1}^n \\ & + \{[(x - x_{K+1})(x - x_{K-1})] / [(x_K - x_{K+1})(x_K - x_{K-1})]\} \psi_K^n \\ & + \{[(x - x_{K-1})(x - x_K)] / [(x_{K+1} - x_{K-1})(x_{K+1} - x_K)]\} \psi_{K+1}^n \end{aligned} \quad (2.5)$$

Let $K = I - p$, p being an integer chosen such that $(I - p - 0.5)\Delta x \leq x < (I - p + 0.5)\Delta x$ and let $\hat{\alpha}$ be defined by

$$\Delta x \hat{\alpha} = (I - p)\Delta x - x, \quad (2.6)$$

(See fig.1). Clearly, the choice of p means that $-0.5 < \hat{\alpha} \leq 0.5$. Then Eq.(2.5) becomes

$$\psi(x, n\Delta t) = 0.5\hat{\alpha}(1 + \hat{\alpha})\psi_{I-p-1}^n + (1 - \hat{\alpha})(1 + \hat{\alpha})\psi_{I-p}^n - 0.5\hat{\alpha}(1 - \hat{\alpha})\psi_{I-p+1}^n \quad (2.7)$$

If this is now substituted in Eq.(2.4) with $x = x_* = I\Delta x - c\Delta t$ it is not difficult to show this scheme is also unconditionally stable because the interpolation points surround the departure point; see Bates and McDonald (1982). How accurate is it? In order to find out, first expand ψ in a Taylor series about $(I\Delta x, n\Delta t)$ giving

$$\psi(x, n\Delta t) = \psi_I^n - (p + \hat{\alpha})\Delta x [\partial\psi/\partial x]_I^n + (p + \hat{\alpha})^2 (\Delta x^2/2) [\partial^2\psi/\partial x^2]_I^n + O(\Delta x^3), \quad (2.8)$$

where the leading $O(\Delta x^3)$ term is $(\Delta x^3/6) [\partial^3\psi/\partial x^3]_I^n W_2^3$, and

$$W_2^3(\hat{\alpha}, p) = 0.5\hat{\alpha}(1 + \hat{\alpha})(-p - 1)^3 + (1 - \hat{\alpha})(1 + \hat{\alpha})(-p)^3 - 0.5\hat{\alpha}(1 - \hat{\alpha})(-p + 1)^3. \quad (2.9)$$

With $x = x_* = I\Delta x - c\Delta t$ in Eq.(2.6) giving

$$p + \hat{\alpha} = c\Delta t/\Delta x,$$

substitution of $\psi(x, n\Delta t)$ from Eq.(2.8) in Eq.(2.4) and expansion of ψ_I^{n+1} yields

$$\{[1 + (\Delta t/2)(\partial/\partial t - c\partial/\partial x)](\partial\psi/\partial t + c\partial\psi/\partial x)\}_I^n + O(\Delta t^2) + O(\Delta x^3/\Delta t) = 0., \quad (2.10)$$

where the leading $O(\Delta x^3/\Delta t)$ term is given by $[-\Delta x^3/(6\Delta t)][\partial^3\psi/\partial x^3]_i^n W_2^3$. It is important to examine this term carefully to make sure it does not misbehave as Δt and Δx approach zero. Otherwise, the approximation is not consistent. Recall in what follows that p is always chosen so that $-0.5 < \hat{\alpha} \leq 0.5$. There are three cases to consider.

Case 1. The grid is refined in such a way that $\Delta t/\Delta x \rightarrow 0$ as Δt and $\Delta x \rightarrow 0$. Then $p \rightarrow 0$ and $\hat{\alpha} \rightarrow c\Delta t/\Delta x$. In that case $W_2^3 \rightarrow -c\Delta t/\Delta x$ and the term which seems to be $O(\Delta x^3/\Delta t)$ is seen to be $O(\Delta x^2)$.

Case 2. The grid is refined in such a way that $\Delta t/\Delta x \rightarrow g$, a constant, as Δt and $\Delta x \rightarrow 0$. Then, since $\Delta t = g\Delta x$ and $(\Delta x/\Delta t)W_2^3 \rightarrow gW_2^3(\hat{\alpha}, \hat{\alpha} - gc)$, a constant, the $O(\Delta x^3/\Delta t)$ term is again seen to be $O(\Delta x^2)$.

Case 3. The grid is refined in such a way that $\Delta x/\Delta t \rightarrow 0$ as Δt and $\Delta x \rightarrow 0$. Then $|c|\Delta t/\Delta x \gg |\hat{\alpha}|$ and $p \rightarrow c\Delta t/\Delta x$. In that case $W_2^3 \rightarrow (c\Delta t/\Delta x)^3$ and the term which seems to be $O(\Delta x^3/\Delta t)$ term is seen to be $O(\Delta t^2)$. Since $\Delta t \gg \Delta x$ in case 3, the quadratic interpolation yields an $O(\Delta x^2)$ and $O(\Delta t^2)$ accurate scheme in all three cases. Thus the scheme is consistent and attains the required accuracy. In what follows the notation $O(\Delta)$ will be used as shorthand for $O(\Delta t)$ or $O(\Delta x)$ or $O(\Delta x^2/\Delta t)$ in this sense.

There remains the important question of efficiency. Since Eq.(2.7) combined with Eq.(2.4) form a Lax Wendroff scheme when $p = 0$, (see Eq.(5-116) of HW), it is clear that in the one dimensional case the semi-Lagrangian and Eulerian methods of treating the advection equation with constant velocity are approximately equally expensive.

These results are very encouraging. Will they survive in a more hostile environment? To find out, consider the advection equation with non-constant velocity,

$$\partial\psi(x,t)/\partial t + u(x,t)\partial\psi(x,t)/\partial x = 0., \quad (2.11)$$

where $u(x,t)$ is a given function. Again, the the field is conserved following the parcel of fluid. That is, Eq.(2.4) is still valid but with x_* now obtained by solving the equation

$$dx/dt = u(x,t). \quad (2.12)$$

See Ince(1956), page 45-50, for example. Thus, a new difficulty arises , that of solving Eq.(2.12). It can also be written

$$x(t + \Delta t) - x(t) = \int_t^{t+\Delta t} u[x(\tau), \tau]d\tau. \quad (2.13)$$

This highly implicit system must be solved for the departure point $x(t) = x_*$, assuming the arrival point $x(t + \Delta t)$ to have the known value $I\Delta x$.

Consider the consequences for the accuracy of the method of using the simplest possible approximation, that is, assuming $u[x(\tau), \tau]$ to be the constant $u_j^{n+1/2}$. From Eq.(2.13), $x_* = I\Delta x - \Delta t u_j^{n+1/2}$, which on substitution in Eq.(2.6) yields $p + \hat{\alpha} = u_j^{n+1/2} \Delta t / \Delta x$. Putting this in Eq.(2.8), (again using the quadratic scheme to estimate ψ at x_*), enables one to expand $\psi\{x_*, n\Delta t\}$ about $(I\Delta x, n\Delta t)$. Subsequent substitution in Eq.(2.4) shows it causes an $O(\Delta)$ error. So this estimate is not accurate enough.

Robert(1981) suggested the following iterative method which overcomes this problem. The idea is to get as good an estimate of u at the centre of the trajectory as possible, and then approximate Eq.(2.13) as

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

thus restoring $O(\Delta^2)$ accuracy. The estimate of $x(t + \Delta t/2)$ is taken as half of the the arrival point position plus the previous best estimate of the departure point position:

$$x^{(k)}(t + \Delta t/2) = 0.5[x(t + \Delta t) + x^{(k)}(t)], \quad (2.14)$$

where Eq.(2.13) is approximated as follows to get the next estimate of $x^{(k)}$:

$$x^{(k+1)}(t) = x(t + \Delta t) - \Delta t u[x^{(k)}(t + \Delta t/2), t + \Delta t/2]. \quad (2.15)$$

Thus, for example, if the zeroth order guess for x_* is taken as

$$x_*^{(0)} = x^{(0)}(t) = I\Delta x - \Delta t u_j^{n+1/2},$$

then Eqs. (2.14) and (2.15) give the first order estimate of x_* :

$$x_*^{(1)} = I\Delta x - \Delta t u[I\Delta x - (\Delta t/2)u_j^{n+1/2}, (n + 1/2)\Delta t]. \quad (2.16)$$

This process can be continued until convergence. Defining $\hat{u}^{(0)} = u_j^{n+1/2}$, the procedure can be summarised as follows

$$\hat{u}^{(k+1)} = u[I\Delta x - \hat{u}^{(k)} \Delta t/2, (n + 1/2)\Delta t], \quad (2.17)$$

$$x_* = I\Delta x - \Delta t \hat{u}^{(k+1)}. \quad (2.18)$$

Once x_* has been found by this method, $\psi(x_*, n\Delta t)$ can be evaluated by a suitable interpolation.

In order to see whether accuracy has been improved, consider the simplest possible implementation of the procedure, using a Lagrange linear interpolation to compute the first guess of $x_i^{(1)}$ in Eq.(2.16):

$$u[I\Delta x - u_i^{n+1/2} \Delta t/2, (n+1/2)\Delta t] = (1 - \hat{\gamma})u_{i-m}^{n+1/2} + \hat{\gamma}u_{i-m-1}^{n+1/2} \quad (2.19)$$

where $\hat{\gamma} = -m + \Delta t u_i^{n+1/2} / (2\Delta x)$ and m is an integer chosen so that $0 < \hat{\gamma} < 1$. Expanding about $(I\Delta x, n\Delta t)$ and substitution in Eq.(2.16) yields

$$x_i^{(1)} = I\Delta x - \Delta t[u + (\partial u / \partial t - u \partial u / \partial x) \Delta t / 2]_i^n + O(\Delta t^2 \Delta). \quad (2.20)$$

Now, Eq.(2.20) and (2.6) give $p + \hat{\alpha} = (\Delta t / \Delta x)[u + (\partial u / \partial t - u \partial u / \partial x) \Delta t / 2]_i^n$. Using this to expand $\psi(x, n\Delta t)$ about $(I\Delta x, n\Delta t)$ in Eq.(2.8) and then substituting the result in Eq.(2.4) yields

$$[\{1 + (\Delta t / 2)(\partial / \partial t - u \partial / \partial x)\}(\partial \psi / \partial t + u \partial \psi / \partial x)]_i^n + O(\Delta^2) = 0.$$

Thus, the required accuracy has been restored.

There is a small computational cost, that of the extra linear interpolation, (2.19). In addition, as Pudykiewicz et. al. (1985) pointed out, there is a condition for the convergence of the iterative procedure, that is, $\max[\Delta t |\partial u / \partial x|] \leq 1$. In a meteorological context this is not severe since an upper bound on $\max |\partial u / \partial x|$ is $10^{-4} s^{-1}$. Hence, the method remains attractive and one is encouraged to examine it further.

Therefore, consider the following more realistic equation which contains all of the terms one meets in integrating the primitive equations of motion:

$$\partial \psi(x, t) / \partial t + u(x, t) \partial \psi(x, t) / \partial x = \xi(x, t) \quad (2.21)$$

For instance, in the momentum equation, ξ would contain the Coriolis and the pressure gradient terms, etc. What additional problems does it pose for the semi-Lagrangian approach?

Solving Eq.(2.21) is equivalent to solving the system of ordinary differential equations (see Ince(1956) p 47) $d\psi/\xi = dx/u = dt$. The solutions are given by Eq.(2.13) plus the following:

$$\psi[x(t + \Delta t), t + \Delta t] - \psi[x(t), t] = \int_t^{t+\Delta t} \xi[x(\tau), \tau] d\tau. \quad (2.22)$$

Let $\xi = L + N$ where the terms in L must be integrated implicitly to maintain stability whereas those in N are small enough to be integrated explicitly. The integral on the

right hand side of Eq.(2.22) can be approximated in a number of ways. For the L -terms a ‘Lagrangian implicit’ choice would be an obvious one (the mean of points A and B in Fig. 1):

$$\int_t^{t+\Delta t} L[x(\tau), \tau] d\tau = 0.5\Delta t [L_I^{n+1} + L(I\Delta x - \hat{u}\Delta t, n\Delta t)]. \quad (2.23)$$

For the explicitly integrated terms there are two obvious choices; the ‘centered Lagrangian explicit (1)’ (point C in Fig.1),

$$\int_t^{t+\Delta t} N[x(\tau), \tau] d\tau = \Delta t N\{I\Delta x - \hat{u}\Delta t/2, (n+1/2)\Delta t\}, \quad (2.24)$$

and the ‘centered Lagrangian explicit (2)’ (the mean of points D and E in Fig.1),

$$\int_t^{t+\Delta t} N[x(\tau), \tau] d\tau = 0.5\Delta t [N_I^{n+1/2} + N\{I\Delta x - \hat{u}\Delta t, (n+1/2)\Delta t\}]. \quad (2.25)$$

Accuracy to $O(\Delta^2)$ is again guaranteed by the ‘multiply upstream’ quadratic scheme, provided x_* is obtained by iterating once with the linear scheme as can be verified by using Eqs.(2.20), (2.6) and (2.8) in expanding the terms in Eqs.(2.23), (2.24) and (2.25) about $(I\Delta x, n\Delta t)$ to get for both explicit schemes

$$[\{1 + (\Delta t/2)(\partial/\partial t - u\partial/\partial x)\}(\partial\psi/\partial t + u\partial\psi/\partial x - L - N)]_I^n + O(\Delta^2) = 0.$$

An $O(\Delta^2)$ discretization of Eq.(2.21) using scheme (2) for N would be

$$[\psi_I^{n+1} - \psi_*^n]/\Delta t = [L_I^{n+1} + L_*^n]/2 + [N_I^{n+1/2} + N_*^{n+1/2}]/2, \quad (2.26)$$

where the * subscript means evaluation at the departure point given by Eq.(2.18). Computationally, it appears at first glance that three interpolations are now required, thus increasing the cost substantially. This is not true. All of the fields to be evaluated at the departure point can first be gathered together and then a single interpolation performed:

$$[\psi - L\Delta t/2]_I^{n+1} = [\psi^n + L^n \Delta t/2 + N^{n+1/2} \Delta t/2]_* + N_I^{n+1/2} \Delta t/2. \quad (2.27)$$

This is formally the same equation as arises in an Eulerian implicit model (see, for example, section 5-7-4 of HW). Hence, the main additional expence remains that of

iterating to find the departure point position. Notice, however, that use of scheme (1) for N would involve an extra interpolation.

As far as stability is concerned, the explicit integration of the N terms introduces a potential instability for large enough Δt . In the models constructed so far they have not been a source of difficulty, but they bear watching.

Thus, for the most general type of equation likely to be encountered an analysis in one dimension indicates that accuracy is maintained, the additional computational expense is minimal, and instability can only arise from terms that are expected to be very small in a meteorological context.

The above derivation has been for a two time level scheme. (In fact, it can also be thought of as for a three time level scheme with a time step of $\Delta t/2$ and with the fields at level $(n + 1/2)$ being known entities.) In the two time level context, the fields at level $(n + 1/2)$ must be computed. The simplest estimate which is accurate to $O(\Delta t^2)$ is

$$f(n + 1/2) = [(3f(n) - f(n - 1)]/2,$$

which must be used in Eqs.(2.17), (2.24) and (2.25). This is a minor additional computational expense.

It is now obvious how the spatial accuracy of the semi-Lagrangian scheme can be further improved, that is, use a higher order interpolation to find the fields at the departure points. For consistency these must be accompanied by additional iterations of Eq.(2.17) using appropriately higher order interpolations. See McDonald (1984) for details. In all of this, one is not restricted to the Lagrange interpolation. As far as is known, any method which surrounds the departure point is satisfactory. For instance, splines can be used.

3. APPLICATION TO A METEOROLOGICAL MODEL

Historically, the barotropic vorticity equation played a major role in the development of numerical weather prediction in general and of the semi-Lagrangian technique in particular. It might be interesting, therefore, to demonstrate the practical implementation of the methods outlined in section 2 by applying them to this equation, and in the process see how they evolved over time.

For arguments that this equation is a reasonable approximation to the primitive meteorological equations for mid-tropospheric flow see, for example, chapter 3 of HW. It is written as

$$[\partial/\partial t + \mathbf{v}(\mathbf{r}, t) \cdot \nabla] \eta(\mathbf{r}, t) = 0., \quad (3.1)$$

where \mathbf{v} is the advecting velocity, $\eta = \zeta + f$, with f equal to the Coriolis parameter and the vorticity given by $\zeta = \mathbf{k} \cdot \nabla \times \mathbf{v}$. Since the divergence is assumed to be zero, the velocity can be defined in terms of a stream function ψ by

$$\mathbf{v} = \mathbf{k} \times \nabla \psi, \quad (3.2)$$

giving

$$\eta = \nabla^2 \psi + f. \quad (3.3)$$

Generalising the arguments from section 2 to two dimensions, the solution to Eq.(3.1) is

$$\eta[\mathbf{r}(t + \Delta t), t + \Delta t] - \eta[\mathbf{r}(t), t] = 0. \quad (3.4)$$

where $\mathbf{r}(t)$ is the solution of the equation

$$\mathbf{r}(t + \Delta t) - \mathbf{r}(t) = \int_t^{t+\Delta t} \mathbf{v}[\mathbf{r}(\tau), \tau] d\tau. \quad (3.5)$$

In general, the integration of Eq.(3.1) using the Lagrangian approach proceeds as follows:

Step 1. Construct η at time $t = 0$.

Step 2. Integrate Eq.(3.5) using an appropriate approximation method dividing Δt into M increments $\Delta t/M$.

Step 3. Use Eqs. (3.4) to get the forecast value of $\eta[\mathbf{r}(t + \Delta t), t + \Delta t]$.

Step 4. Although $\eta[\mathbf{r}(t + \Delta t), t + \Delta t]$ is now known, in order to proceed to the next step $\mathbf{v}[\mathbf{r}(t + \Delta t), t + \Delta t]$ is also required. It is obtained by first of all solving the Poisson equation, (3.3), for $\psi[\mathbf{r}(t + \Delta t), t + \Delta t]$ and from that getting $\mathbf{v}[\mathbf{r}(t + \Delta t), t + \Delta t]$ from Eq.(3.2).

Step 5. Repeat steps 2-4 N times to get the forecast at time $N\Delta t$.

Fjortoft (1952) seems to have been the first to introduce the use of Lagrangian techniques in meteorology. He simplified Eq.(3.1) slightly by making the geostrophic assumption. He performed all of the steps graphically, starting from the analysed 500hPa. height field (z). Thus, step 1 resulted in a chart, at time zero, of the isolines of

$$\eta = (g/f) \nabla^2 z + f.$$

Then in steps 2 and 3, by means of a wind ruler the geostrophic wind was used to advect these lines of constant η . This was done in one step $\Delta t = 24h$. Knowing η, z was obtained via step 4, again using a graphical method combined with a set of tables.

This paper is remarkable not only because it represents the first use of Lagrangian methods in weather prediction, and not only for the ingenuity involved in carrying out the program graphically, but also for the impressive accuracy of the forecasts, the same as that obtained by the first computer model of Charney, Fjortoft, and von Neumann (1950). It is also interesting that one man could produce a 24h forecast for the whole north Atlantic area in 2-3 hours.

Further progress was made when Wiin Nielsen (1959) tried to implement Fjortoft's program on a computer. In the process he encountered a difficulty, the solution to which takes us on the next step toward our present day methodology. He wanted his arrival points to be grid points so that he could perform step 4, solving the Poisson equation, by conventional methods. He computed the departure point positions (step 2) by taking M small steps, assuming \mathbf{v} constant in time. Because he was using Lagrangian coordinates, that is, following the parcels, he found that his initially square grid embedded in the flow became so distorted as to introduce unacceptable truncation errors after 12h. He therefore introduced the idea of abandoning the strict Lagrangian approach of following the parcels for the full duration of the forecast. He suggested instead following the parcels for $\Delta t = 12h$, after which steps 3 and 4 are completed. When the cycle is restarted at step 2 he does not follow the original set of parcels but a new set which arrive at the grid points at time $2\Delta t$. He used the term quasi-Lagrangian to describe this procedure.

The next leap was made by Okland (1962) and Sawyer (1963) who decided to abandon the Lagrange coordinates and to switch parcels 'as often as possible'. Thus, they solved Eq.(3.5) in one step ($M = 1$) using a simple approximation. Robert (1981) subsequently improved this estimate of the departure point position when he invented the iterative method which, of course, is a two-dimensional generalization of Eqs.(2.17) and (2.18). This brings us up to the present where we would proceed as follows.

Let $t = n\Delta t$ and choose $\mathbf{r}(t + \Delta t)$ to be a set of grid points $\mathbf{r}_{I,J}$. Then the details of steps 2 and 3 are as follows.

2. Taking $M = 1$ solve Eq.(3.5) iteratively at each grid point using $\hat{\mathbf{v}}^{(0)} = \mathbf{v}_{I,J}^n$:

$$\hat{\mathbf{v}}^{(k+1)} = \mathbf{v}[\mathbf{r}_{I,J} - \hat{\mathbf{v}}^{(k)} \Delta t/2, (n + 1/2)\Delta t]. \quad (3.6)$$

Then the departure point position associated with each arrival point (I, J) is given by

$$\mathbf{r}(t) = \mathbf{r}_{I,J} - \hat{\mathbf{v}}^{(k+1)} \Delta t. \quad (3.7)$$

3. Since $\mathbf{r}(t)$ is now known $\eta[\mathbf{r}(t), t]$ can be found by a suitable interpolation of the known $\eta_{I,J}^n$, using, for example, a Lagrange biquadratic interpolation so enabling us to proceed with steps 4 and 5.

Robert's other contribution, Robert(1981, 1982), was to realise that semi-implicit methods could be combined with semi-Lagrangian methods to yield a discretization of the primitive equations of motion with an extremely lenient stability criterion. This was the final breakthrough which made the method attractive for modelling the evolution of the atmosphere using unapproximated equations. See Staniforth and Cote (1991) and the references therein for the rest of the story.

4. AN UNSOLVED PROBLEM

If the primitive equations of motion are integrated over the entire atmosphere a set of conservation relations can be derived. These relations have important implications as was demonstrated by Fjortoft (1953) who examined the conservation properties of the barotropic vorticity equation (3.1). He showed that mean enstrophy and mean kinetic energy are conserved and as a result that energy cannot cascade toward higher wave numbers; see section 5.11 of HW for an introduction. It is therefore felt desirable that these properties of the differential equations should also hold exactly for the finite difference equations, especially for climate models. Eulerian models have been constructed which achieve this; see chapter 7 of HW for an example of one. Doing the same for a semi-Lagrangian model has not yet been achieved. This problem will become important if it is found that prolonged integrations using the present semi-Lagrangian schemes fail to model the mean structure of the atmosphere accurately. In that case the potential increase in efficiency proffered by the method will not be available to those who might appreciate it most, climate modellers.

To demonstrate the difficulty consider a one dimensional continuity equation of the form

$$\partial\psi(x, t)/\partial t + u(x, t)\partial\psi(x, t)/\partial x + \psi(x, t)\partial u(x, t)/\partial x = 0. \quad (4.1)$$

with boundary conditions $u(0, t) = u(L, t)$ and $\psi(0, t) = \psi(L, t)$. This equation can also be written in flux form as

$$\partial\psi/\partial t + \partial(u\psi)/\partial x = 0. \quad (4.2)$$

Integration over x yields

$$\int_0^L dx \partial\psi/\partial t = 0.$$

or $\partial\bar{\psi}/\partial t = 0.$, where

$$\bar{\psi} = \int_0^L dx \psi,$$

that is, mass is conserved.

The objective, therefore, is to construct a discretization of this equation for which $\bar{\psi}^{n+1} = \bar{\psi}^n$. Before pointing out the difficulties which this poses for the semi-Lagrangian method recall the Eulerian solution to this problem. Assuming $\partial(u\psi)/\partial x$ is small enough to be integrated explicitly then a conserving discretisation Eq.(4.1) is, assuming uniform Δx (see section 5-11-2 of HW)

$$(\psi_I^{n+1} - \psi_I^n)/\Delta t = -[(\psi u)_{I+1}^{n+1/2} - (\psi u)_{I-1}^{n+1/2}]/(2\Delta x).$$

The judicious choice of spatial discretization gives a term by term cancellation on the right hand side of this equation when the summation over I is performed and the result is that mass is conserved exactly ($L = P\Delta x$):

$$\sum_{I=1}^P \psi_I^{n+1} - \sum_{I=1}^P \psi_I^n = 0. \quad (4.3)$$

Now consider what happens when the simplest possible semi-Lagrangian discretization of Eq.(4.1) is used, that is, in Eq.(2.22) put

$$-\int_t^{t+\Delta t} \psi(x, \tau) \partial u(x, \tau) / \partial x d\tau = -\Delta t [\psi \partial u / \partial x]_*^{n+1/2},$$

giving

$$\psi_I^{n+1} = [\psi^n - \Delta t (\psi \partial u / \partial x)^{n+1/2}]_*.$$

Assume p is constant first of all. Using a Lagrange linear interpolation gives

$$\psi_I^{n+1} = (1 - \hat{\alpha}_I^{n+1/2}) [\psi^n - \Delta t (\psi \partial u / \partial x)^{n+1/2}]_{I-p} + \hat{\alpha}_I^{n+1/2} [\psi^n - \Delta t (\psi \partial u / \partial x)^{n+1/2}]_{I-p-1}$$

Now, when the summation is performed there is no term by term cancellation, and mass is not conserved. This is not due to the choice of a Lagrange linear scheme for the interpolation; quadratic does not eliminate the problem.

A possible way forward is the following. Returning to Eq.(2.22) discretise the integral term in a different way,

$$-\int_t^{t+\Delta t} \psi(x, \tau) \partial u(x, \tau) / \partial x d\tau = -(\Delta t / \Delta x) \psi_{I-p}^n (\hat{u}_{I+1}^{n+1/2} - \hat{u}_I^{n+1/2}), \quad (4.4)$$

while retaining the Lagrange linear scheme for the evaluation of ψ_x^n . Then, since $p + \hat{\alpha} = \hat{u} \Delta t / \Delta x$, $\bar{\psi}$ is again conserved because the approximation (4.4) has been carefully chosen to restore conservation:

$$\psi_I^{n+1} = \psi_{I-p}^n + \hat{\alpha}_I^{n+1/2} \psi_{I-p-1}^n - \hat{\alpha}_{I+1}^{n+1/2} \psi_{I-p}^n, \quad (4.5)$$

and the term by term cancellation will once again occur when the sum over I is performed. This scheme is $O(\Delta)$ accurate. Increasing the accuracy to $O(\Delta^2)$ would not be difficult. In fact, one can make a good guess at the answer by looking at the Crowley (1969) conserving scheme. Unfortunately, there remains a problem, the solution to which may point to a different approach entirely. It is the following.

The number p was assumed to be constant when deriving Eq.(4.5) from Eq.(4.4) which, using $p_I + \hat{\alpha}_I = (\Delta t / \Delta x) \hat{u}_I$, becomes

$$\psi_I^{n+1} = (1 + p_I - p_{I+1}) \psi^n(I - p_I) + \hat{\alpha}_I^{n+1/2} \psi^n(I - p_I - 1) - \hat{\alpha}_{I+1}^{n+1/2} \psi^n(I - p_I)$$

when p varies from point to point. When the sum over I is now performed the term by term cancellation only occurs as long as $p_I = p_{I+1}$; what might be termed 'partial conservation'. Each jump in p contributes an unwanted term to the mass. For instance, if $p_I = p$ for $I = 1, N$ and $p_I = p + 1$ for $I = N + 1, M$ exact mass conservation will be violated by the additional term $\hat{\alpha}_{N+1} [\phi(N - p - 1) - \phi(N - p)]$. It is not the magnitude of p that is causing exact mass conservation to fail in this approach, but its variability. It is interesting that the property which maintains the stability of the method seems to be conspiring to prevent exact conservation.

This leads to the following question. Does there exist a clever choice of local interpolations which gives an exactly conserving scheme for non-constant p ? If not, a possible way out is to abandon local interpolation and to consider instead global interpolation, that is, to postulate a solution of the kind

$$\psi_I^{n+1} = \sum_{J=1}^P M_{I,J}(\hat{u}_I) \psi_J^n,$$

and to demand that the matrix \mathbf{M} have certain properties. The first and most important is that when \hat{u} and ψ are expanded about (I, n) then Eq.(4.1) must hold to $O(\Delta^2)$. Mass

conservation can be imposed by demanding that

$$\sum_{I=1}^P M_{I,J}(\hat{u}_I) = 1$$

These conditions are not sufficient to define M uniquely. Others are obviously needed. A first step in the direction of providing them has been taken by Bermejo(1990) who solves this problem for the simpler case of $\partial u/\partial x = 0$ using a combination of finite elements and basis splines. It would be interesting to see if the method generalises to the more important $\partial u/\partial x \neq 0$ case.

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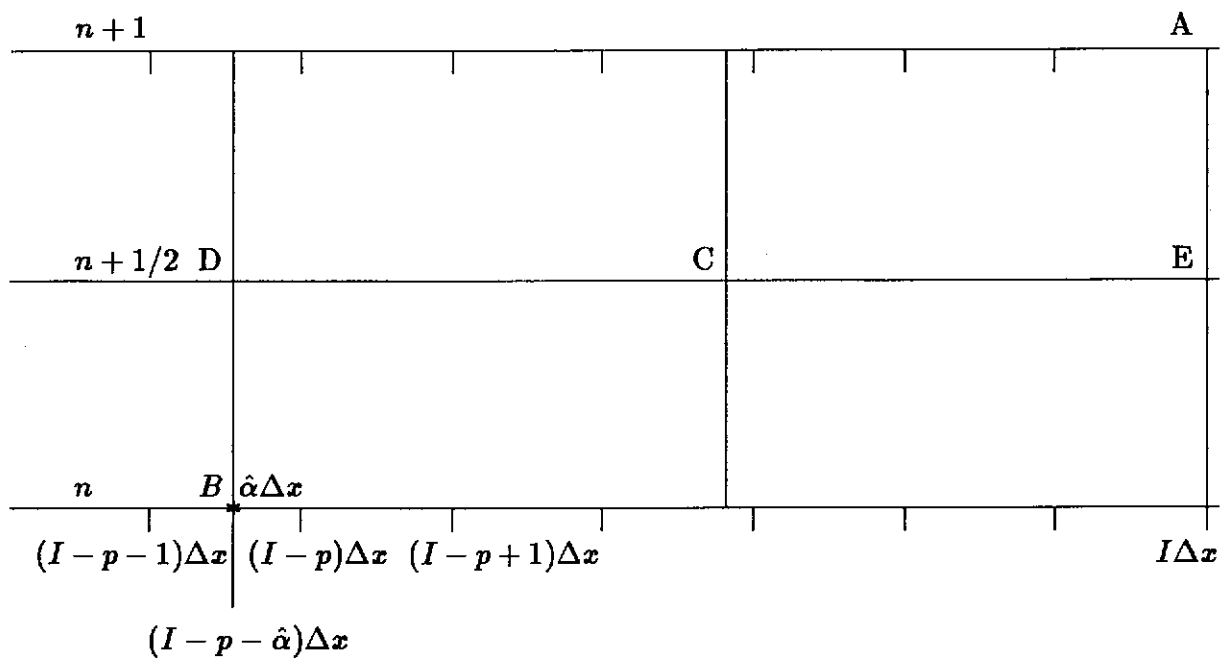


Figure 1.