UNIFIED MODEL DOCUMENTATION PAPER NUMBER 11

POSITIVE DEFINITE ADVECTION SCHEME

M.J.P.Cullen and R.T.H.Barnes

Version no. 6 dated 24/06/97

UM version 4.3

Numerical Weather Prediction
Meteorological Office
London Road
BRACKNELL
Berkshire
RG12 2SZ
United Kingdom

Modification Record

Document version	Author	Description....................	
5		30/11/90	Missing reference added
		24/10/91	Revised fully conservative version of scheme. Revisions to text.
		5/2/92	Fractional east-west timestep chosen separately at each level. Corrections to text.
		28/4/92	Entropy fix included in scheme. Option to use van Leer limiter.
6	R.T.H.Barnes	24/06/97	Appendix added: implementation on MPP computer.

1. INTRODUCTION

The unified model can be run with additional tracer variables. These will usually represent quantities which are inherently positive. The standard advection scheme described in UMDP no. 10 does not preserve positiveness. This paper describes an alternative ‘positive definite’ scheme which does. It is important to note that any such scheme includes some internal diffusion, and that Fourier filtering cannot be applied to quantities which have to be positive. Therefore, when applying the positive definite scheme in the global model, multiple short timesteps have to be used in the east-west direction at high latitudes. The scheme used is the flux redistribution method of Roe (1983). Various flux limiters can be used with this scheme. The ones available in the present implementation are the ‘Superbee’ and ‘van Leer’ limiters.

2. TRACER ADVECTION SCHEME

2.1. Requirements

The equation to be solved is

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+\dot{\eta}\frac{\partial C}{\partial \eta}=0 \qquad \textbf{(1)}$$

where C is the concentration of the tracer, x and y are standard cartesian coordinates and the vertical coordinate is $\eta=\eta(p,p_*)$ with p and p_* pressure and surface pressure respectively.

Combining this with the continuity equation (Cullen et al, 1992)

$$\frac{\partial}{\partial \eta}\left[\frac{\partial p}{\partial t}\right]+\frac{\partial}{\partial x}\left[u\frac{\partial p}{\partial \eta}\right]+\frac{\partial}{\partial y}\left[v\frac{\partial p}{\partial \eta}\right]+\frac{\partial}{\partial \eta}\left[\dot{\eta}\frac{\partial p}{\partial \eta}\right]=0 \qquad \textbf{(2)}$$

gives the conservation law

$$\frac{\partial}{\partial t}\left[C\frac{\partial p}{\partial \eta}\right]+\frac{\partial}{\partial x}\left[uC\frac{\partial p}{\partial \eta}\right]+\frac{\partial}{\partial y}\left[vC\frac{\partial p}{\partial \eta}\right]+\frac{\partial}{\partial \eta}\left[\dot{\eta}C\frac{\partial p}{\partial \eta}\right]=0 \qquad \textbf{(3)}$$

The finite difference approximation must preserve the integral of the conservation law, equation (3), i.e. the total amount of tracer is preserved. It is also required that the concentration of the tracer remains bounded by the initial values. The amount of computational smoothing introduced should be minimised.

2.2 Finite Difference Equations

Equations (1) multiplied by $\partial p/\partial \eta$ and (2) can be approximated by second order finite difference equations,

$$\frac{\partial p}{\partial \eta}\frac{\partial C}{\partial t}+\overline{\overline{U}^{y}\ \delta_{x}C}^{x}+\overline{\overline{V}^{x}\ \delta_{y}C}^{y}+\overline{E\ \delta_{\eta}C}^{\eta}=0 \qquad \textbf{(4)}$$

$$\frac{\partial}{\partial t}\left[\frac{\partial p}{\partial \eta}\right]+\delta_{x}\overline{U}^{y}+\delta_{y}\overline{V}^{x}+\delta_{\eta}\overline{E}^{\eta}=0 \qquad \textbf{(5)}$$

where $U=u\overline{\frac{\partial p}{\partial \eta}}^{xy}$, $V=v\overline{\frac{\partial p}{\partial \eta}}^{xy}$ and $E=\dot{\eta}\frac{\partial p}{\partial \eta}$

and where the Arakawa ‘B’ grid has been assumed in the horizontal.

The standard finite difference notation

$$\delta_{x}X=\frac{1}{\Delta x}\left[X\left(x+\frac{\Delta x}{2}\right)-X\left(x-\frac{\Delta x}{2}\right)\right]$$
$$\overline{X}^{x}=\frac{1}{2}\left[X\left(x+\frac{\Delta x}{2}\right)+X\left(x-\frac{\Delta x}{2}\right)\right]$$

is used.

The above equations can be combined to give

$$\frac{\partial}{\partial t}\left[C\frac{\partial p}{\partial \eta}\right]+\delta_{x}\left[\overline{U}^{y}\overline{C}^{x}\right]+\delta_{y}\left[\overline{V}^{x}\overline{C}^{y}\right]+\delta_{\eta}\left[\overline{E}^{\eta}\overline{C}^{\eta}\right]=0 \qquad (6)$$

This shows that the scheme obtained by combining (4) and (5) is conservative. Note that (6) cannot be used directly in the unified model because (5) has to be integrated with a shorter timestep than (4). In addition, if flux limiting is applied directly to (6), and (5) used unmodified as the continuity equation, then an unsatisfactory approximation to (4) is obtained by subtracting (5) from (6). It is therefore necessary to modify (4) directly to enforce the boundedness requirements on C. In (4), $C\frac{\partial p}{\partial \eta}$ is incremented equally to the left and to the right by a sum of advective fluxes, e.g. $\overline{U}^{y}\delta_{x}C$. Only the sum of the fluxes has to be preserved to retain the conservation law. Therefore the conservation law is not affected if the flux is redistributed unequally, say $(1-\alpha)$ to the left and α to the right, so that no more of the concentration C in a grid box is removed than there was initially.

Flux redistribution schemes were developed by Roe (1985) and shown to be able to satisfy boundedness requirements. The schemes described here are the "Superbee" method which Morton and Sweby (1987) have shown is a good method for linear advection, but is often thought to distort smooth waves into square waves, and the "van Leer" method which Morton and Sweby showed to be more diffusive. Other redistribution algorithms can also be used. Since we are only interested in advection, and not the general compressible flow equations, the operator splitting approach for the multi-dimensional problem is adequate. Therefore, the redistribution is applied separately in each coordinate direction. This also allows the scheme to be used near the poles of a latitude-longitude grid. The east-west sweep can be iterated using a shorter timestep than the other sweeps.

'Truly' multidimensional versions of these algorithms have been developed recently by Roe et al. (1990). These cannot be used in the global model because of the multiple east-west sweeps, but could be used in future versions of the regional models. Instead, the scheme has to be applied as a sequence of one-dimensional sweeps.

2.3. One dimensional method

1. At the point $(x+\frac{\Delta x}{2},y,\eta)$ calculate the advective flux $\overline{U}^y\delta_x C$.

2. If $\overline{U}^y>0$ subtract $\boldsymbol{B}$ from $C\frac{\partial p}{\partial\eta}$ at (x,y,η) and $(\Delta t\overline{U}^y\delta_x C-\boldsymbol{B})$ from $C\frac{\partial p}{\partial\eta}$ at $(x+\Delta x,y,\eta)$ where

$$B=B\left[\frac{1}{2}v_{x+\frac{\Delta x}{2}}(1-|v|_{x+\frac{\Delta x}{2}})(C_{x+\Delta x}-C_x),\frac{1}{2}v_{x-\frac{\Delta x}{2}}(1-|v|_{x-\frac{\Delta x}{2}})(C_x-C_{x-\Delta x})\right] \tag{7}$$

If $\overline{U}^y<0$ subtract $\boldsymbol{B}$ from $C\frac{\partial p}{\partial\eta}$ at $(x+\Delta x,y,\eta)$ and $(\Delta t\overline{U}^y\delta_x C-\boldsymbol{B})$ from $C\frac{\partial p}{\partial\eta}$ at (x,y,η) where

$$B=B\left[\frac{1}{2}v_{x+\frac{\Delta x}{2}}(1-|v|_{x+\frac{\Delta x}{2}})(C_{x+\Delta x}-C_x),\frac{1}{2}v_{x+\frac{3}{2}\Delta x}(1-|v|_{x+\frac{3}{2}\Delta x})(C_{x+2\Delta x}-C_{x+\Delta x})\right] \tag{8}$$

where $v=\frac{\overline{U}^y\Delta t}{\Delta x}$ is calculated at the appropriate value of x . .

In order to make the correct choices in situations where the velocities used to calculate n change sign, set $\sigma=+1$ if equation (7) applies and $v_{x+\frac{1}{2}\Delta x}$ and $v_{x-\frac{1}{2}\Delta x}$ have the same sign or if equation (8) applies and $v_{x+\frac{1}{2}\Delta x}$ and $v_{x+\frac{3}{2}\Delta x}$ have the same sign. Set $\sigma=-1$ otherwise. (Note that this extra logic is referred to as the 'entropy fix' in the literature referred to, because it is used to prevent unphysical expansion shock waves). For the Superbee limiter set:

$$\begin{aligned} B(b_1,b_2) &= 0 && \textit{if}\quad b_2=0\\ &= b_2\max(\sigma b_1/b_2,1) && \textit{if}\quad \frac{1}{2}<\sigma b_1/b_2<2\\ &= 0 && \textit{if}\quad \sigma b_1/b_2\leq 0\\ &= 2b_2\min(\sigma b_1/b_2,1) && \textit{otherwise} \end{aligned} \tag{9}$$

The van Leer limiter replaces equation (9) by

$$B(b_1,b_2) = 2\sigma b_1 b_2/(b_1+\sigma b_2) \qquad if\ \sigma b_1/b_2>0$$
$$= 0 \qquad if\ b_2=0\ or\ \sigma b_1/b_2 \leq 0 \qquad \textbf{(10)}$$

Other limiters that can be used are given in Roe (1983). The value of Δx used in (7) and (8) is the downwind value, Priestley (1991).

2.4 Multi-dimensional method

When the scheme is applied in global versions of the model, it is first necessary to calculate a value of n for each row and level such that

where u is the maximum zonal velocity, a the radius of the earth, λ the longitude, and ϕ the

$$\nu = \frac{u\Delta t}{n\,a\Delta\lambda\cos\phi} < 1/4$$

latitude. The east-west sweep is then performed n times for each row at each level, with the timestep reduced by a factor of n . n is not allowed to decrease towards the pole in the current implementation. Since the unified model advection scheme is applied to mass-weighted fields, the effective grid length to be used in (8) and (9) is

$(r_s^2\Delta p)_{u\ point}/(r_s^2\Delta p)_{downwind}\Delta\lambda\cos\phi$. In order to maintain conservation under time differencing, it is necessary to update the mass-weighting at each fractional step.Thus the east-west, north-south, and vertical sweeps must all be individually conservative. Set

$$\Delta p^* = \Delta p + \delta_\lambda(U)\Delta t \qquad \textbf{(11)}$$

$$\Delta p^* C^* = \Delta p^* C + U\ \delta_\lambda C^n \Delta t \qquad \textbf{(12)}$$

$U = r_s u \Delta p$. Then the mass update for the east-west sweep is

The * superscript denotes values at the end of the sweep. After the east-west sweeps are complete, the north-south sweeps are carried out using the same algorithm. The appropriate Courant number ν to be used in the flux-limiting calculation is now

$$\nu = v\frac{(r_s^2\Delta p)_{v\ point}\Delta t}{a\Delta\phi\cos(\phi+\Delta\phi/2)(r_s^2\Delta p)_{\phi+\Delta\phi/2}} \qquad \textbf{(13)}$$

when $v<0$, and a similar formula using $\cos(\phi-\Delta\phi/2)$ when $v>0$. At the pole, the correct conservation is obtained if $\cos(\phi-\Delta\phi/2)$ is replaced by $\cos(\phi)/2$, and the polar value is incremented by the sum of the increments calculated from the surrounding points. Note that each north-south sweep is periodic, crossing the poles and continuing on the opposite meridian. A mass update similar to (11) and (12) is then performed in the north-south direction. The horizontal sweeps are performed for each level in turn. After they are completed, the vertical sweeps are performed using the same algorithm. The Courant number used is

$$\nu = \dot{\eta}\frac{\Delta t}{\Delta p}$$

where the layer thickness Δp is that of the layer being updated. If the vertical advection is performed for the full depth of the model, zero vertical advective fluxes are assured at the boundaries because $\dot{\eta}$ is zero there. It is also possible to use the scheme over a limited range of the levels. At the lower boundary, an advective flux is calculated using a prescribed value of C at the layer below that being updated. The resulting increment is only applied to the layer within those being updated and so conservation is not satisfied. At the upper boundary, the advective flux is applied to the layers both above and below the top layer boundary. This is the only update applied to the value above the top layer boundary by the advection scheme, and conservation is satisfied.

REFERENCES

Cullen M.J.P., Davies T., Mawson M.H., Unified Model Doc. Paper no. 10 (1992)

Morton K.W. and Sweby P.K., J. Comp. Phys. **73**, 203 (1987)

Priestley.A., S Division Technical note no. 66, June (1991)

Roe, P.L., Large Scale Computations in Fluid Mechanics, Lectures in Applied Maths, **22**, 163 (1985)

Roe, P.L., Deconinck, H. and Struijs, R.J., von Karman Institute preprint 1990-32/AR (1990)

APPENDIX.

Tracer Advection - Implementation of parallelisation on CRAY T3E.

1. Scope of task.
The work applies to Unified Model Section 11_1A, in which there are 5 decks, comprising 5 routines plus the UK-specific boundary function BDRYV. The routines SET_TRAC,_ADV & TRAC_VERT_ADV may be run in either global or LAM configurations, and have different treatments for meridian wraparound or boundary points respectively. TRBDRY is specific to UK Mes at present, whereas TRSRCE is also used, for instance, in the sulphur cycle code.

2. Discussion.
TRAC_VERT_ADV and TRSRCE have no lateral dependencies and work virtually as written on the standard decomposition grid. In principle the polar points need a broadcast update after TRAC_VERT_ADV, but it is assumed the calculation can be done for a polar point in each processor with a polar row to avoid having to broadcast.

TRBDRY has no lateral dependencies but in MPP mode we need to know which processors have boundary points and which points they are. This is done using IF(at_top/base/left/right_of_LPG) THEN blocks, requiring *IF DEF,MPP directives within the routine.

TRAC_ADV contains 2 distinct sections. The 2nd, N-S sweep of horizontal advection, requires only one sweep and uses adjacent points only, so standard decomposition with halo works fine, provided halo points are up-to-date before this code is run. Although only adjacent points appear to be used, in fact there is some differencing or averaging of fields that have been calculated using halo points, so additional N-S SWAPBOUNDS are required for these fields. These are
MW & COURANT in section 2.1,
FLUX_DELTA_T in section 2.2, and
B_TERM at the end of section 2.4.
The most complicated work for parallelisation the NS sweep is in sections 2.3, 2.6 & 2.7 for the Global case (but not used for the LAM/Mes case). The increments for polar points are an average of all polar points, so a rowise reproducible sum using GCG_RVECSUMR is needed for the polar rows. Moreover, before that is done, a cross-polar value is calculated involving values 180 degrees round the polar rows. This can be done in MPP mode by using the GCG_RVECSHIFT vector shift routine.

The 1st section of TRAC_ADV, the E-W sweep of horizontal advection, uses only adjacent points but may require several sweeps, with an EW exchange of halo points between each sweep if on standard decomposed grid. 1 or 2 sweeps is sufficient for Mes runs, but because of the polar convergence of longitude lines, a few rows near the poles in Global runs may require 8-10 at climate resolution and up to 60-70 sweeps at operational global resolution, eg. for polar night jet, Again there is some "differencing/averaging of differences/averages" so additional E-W SWAPBOUNDS are required for the following fields
MW & COURANT in section 1.1, before the loop over 1,max_sweeps, and for
FLUX_DELTA_T in section 1.2,
and B_TERM at end of section 1.4 in side the loop over sweeps,
as well as of FIELD after each sweep
and full SWAPBOUNDS of FIELD, RS_SQUARED_DELTAP &
RS_SQUARED_DELTAP_RECIP
after all E-W sweeps are completed before going on the N-S sweep.
SWAPBOUNDS must be called by all processors together, so even those not doing any further

sweeps still have to call it, resulting in global synchronisations and a breaking up of the code structure with IF blocks inside *IF DEF,MPP blocks, compared with the non-MPP code.
Load imbalance could be a big problem with this approach, but for the current main users of tracer advection (the operational UK mesoscale model and climate resolution global model) this simple approach has similar relative costs to those on the C90. Extensive use at higher global resolution is likely to require recoding using a more efficient domain decomposition.
The semi-independent treatment of the 2 hemispheres would have been difficult to reproduce in MPP mode, particularly if a decomposition with an odd value for nproc_y were chosen. Therefore the algorithm for finding the one or two sets of rows still needing processing has been recoded to work for any grid decomposition.

3. A comment on performance so far.
The passive advection of a multi-level aerosol in the mesoscale model, with only a couple of E-W sweeps required, it is at least as fast as it was on the C90. However, first reports from the Hadley Centre, using it for Sulphur cycle advection in a global climate model indicate it is somewhat more expensive. If it were used in higher resolution global models, the effect of the polar convergence of longitude lines on the maximum number of sweeps required might make it prohibitive. A follow-on task is probably required to try an alternate zonal decomposition, with rows assigned to processors on the basis of number of sweeps required. This will be similar to how fourier filtering is treated already.

4. Error found in the existing code for LAM configuration.
While testing in LAM configuration it became apparent that bit comparison could not be achieved because the existing (non-MPP) non-Global code used "wraparound" values for some of its differencing because of the "differences of differences" in the code, as noted above. Study of the code and this documentation paper (UMDP 11), shows that there is indeed a weakness/error in the formulation when applied to a limited area model. The simplest way to avoid using "wraparound" values, and thus also to get bit comparison between MPP & non MPP runs, is to set the East- and Westmost values of B2 to zero. Because of the B-grid staggering, the first interior East points have to be set to zero, not just the Eastern edge points.

5. Implementation of the code on MPP machine.
SET_TRAC is done the simple way and seems not to cost too much. It must compute how many E-W sweeps are needed for each row and level TRACER_EW_SWEEPS(P_ROWS,P_LEVELS) to satisfy CFL criterion. This involves a MAX of ABS of the Courant number along each row of the full grid, followed by a constraint that the number of sweeps must increase monotonically from the equator to the pole in each hemisphere. This is done on the standard decomposed grid and basically follows SET_FIL where similar things are done.
The max(abs(courant)) is computed for local rows and from that the number of EW sweeps required. Then GCG_IMAX is used to find the rowise max of these and returned to all processors of the row group. These are then broadcast to all the other processors N & S of this PE so that each PE has the full set of TRACER_EW_SWEEPS values and can apply the equator to pole monotonically increasing constraint on each processor. If the loop over levels is split and the global array of EW_SWEEPS declared as (levels,rows), then the data for GC_IBCAST are contiguous in memory and one call per row group with length p_levels*(p_rows-2*Offy) is all that is required. The global values of TRACER_EW_SWEEPS are saved and returned through the argument list for use in TRAC_ADV, because each processor needs to know the maximum number of sweeps for each level (because SWAP_BOUNDS has to be called the same number of times by all processors).

6. Summary of Implementation Strategy.

To recap, we treat SET_TRAC like SET_FIL using GCG_IMAX and GC_IBCAST.
For TRAC_ADV and TRAC_VERT_ADV, the standard horizontal decomposition can be used.
E-W SWAPBOUNDS after each EW sweep are required in the 1st section of TRAC_ADV.
Other SWAPBOUNDS are needed within the structure of TRAC_ADV owing to the "differencing/averaging of differences/averages".
Rowise reproducible sums are needed for polar increments.
As much as possible the new set of pointers in ARGFLDPT is used to minimise the amount of different loop constructs under *IF DEF,MPP directives.

7. Testing.

The new code was tested for bit comparison over typical real data, using the tracer advection of thetal & qt option in climate resolution global runs as well as passive aerosol tracers in Mesoscale (LAM) runs, for executables compiled with MPP code and run over many processor elements (2x2 up to 6x6 PEs) and compiled without MPP code and run on a single PE.