IFS DOCUMENTATION CY28r1

III: DYNAMICS AND NUMERICAL PROCEDURES

(Operational implementation 9 March 2004)

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will be made which is inappropriate to their scientific basis.

Part III: DYNAMICS AND NUMERICAL PROCEDURES

CHAPTER 1 Introduction

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1.1 OVERVIEW

Since the original demonstration of the efficiency advantage of the semi-Lagrangian semi-implicit method over a decade ago by André Robert, this numerical integration scheme is being used in an increasing range of atmospheric models. Most of the applications have been in grid-point models. Shallow-water-equations studies have included three-time-level versions by *Robert* (1981, 1982) and *Staniforth and Temperton* (1986), and two-time-level schemes by *Temperton and Staniforth* (1987), *Purser and Leslie* (1988), *McDonald and Bates* (1989), and *Côté and Staniforth* (1990). There also have been various applications in baroclinic grid-point models. Three-time-level sigma-coordinate versions have been presented by *Robert et al.* (1985) and *Tanguay et al.* (1989), and the extension of the three-time-level approach to a non-hydrostatic coordinate has been demonstrated by *Tanguay et al.* (1990) . *Bates and McDonald* (1982), *McDonald* (1986), *Leslie and Purser* (1991), *McDonald and Haugen* (1992), and *Bates et al.* (1993) have developed two-time-level sigma-coordinate schemes, *McDonald and Haugen* (1993) have presented the two-time-level extension to a hybrid vertical coordinate, and *Golding* (1992) has applied a split two-time-level semi-Lagrangian scheme in a non-hydrostatic model.

For spectral models, a semi-Lagrangian semi-implicit shallow-water equation model was presented by *Ritchie* (1988) for a three-time-level version, and adapted by *Côté and Staniforth* (1988) for a two-time-level scheme. Baroclinic three-time-level spectral model formulations have been demonstrated by *Ritchie* (1991) for operational numerical weather prediction in a sigma-coordinate model, and recently by *Williamson and Olson* (1994) for climate simulations with a hybrid coordinate model.

In a broader context, the semi-Lagrangian scheme, as incorporated in spectral numerical weather prediction models, may be considered as an economical variant of the spectral Lagrange-Galerkin method (*Süli and Ware*, 1991).

Experience at ECMWF (*Simmons et al.*, 1989) suggests that the accuracy of medium-range forecasts has steadily improved with increasing resolution. Consequently, in its four-year plan for the period 1989-1992, ECMWF proposed development of a high-resolution version of its forecast model. A target resolution of a spectral representation with a triangular truncation of 213 waves in the horizontal and 31 levels in the vertical (T213/L31) was set, entailing a doubling of the horizontal resolution and an approximate doubling of the vertical resolution in the troposphere compared to the T106/L19 configuration that was operational at the time (*Simmons et al.*, 1989). In view of the anticipated computer resources, it was clear that major efficiency gains would be necessary in order to attain this objective. These gains have been provided by the introduction of the semi-Lagrangian treatment of advection permitting a substantial increase in the size of the time-step, the use of a reduced Gaussian grid giving a further advantage of about 25%, the introduction of economies in the Legendre transforms, and improvements to the model's basic architecture.

The layout for the remainder of the document is as follows. In Chapter 2 'Basic equations and discretization' we present the reformulation of the Eulerian model in order to transform the vorticity–divergence formulation into a momentum-equation version in preparation for a subsequent semi-Lagrangian vector treatment of the equations of motion. The vertical discretization of the ECMWF hybrid coordinate on a staggered grid is also considered. The semi-Lagrangian treatment is discussed in some detail in Chapter 3 'Semi-Lagrangian formulation' , including the adaptation to accommodate the reduced Gaussian grid.

Part III: DYNAMICS AND NUMERICAL PROCEDURES

CHAPTER 2 Basic equations and discretization

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2.1 EULERIAN REFORMULATION OF THE CONTINUOUS EQUATIONS

Following *Ritchie* (1988,1991), the first step in developing a semi-Lagrangian version of the ECMWF spectral model was to convert the existing Eulerian ζ–D (vorticity–divergence) model to a $U-V$ formulation, where U and V are the wind images defined by $U = u\cos\theta$, $V = v\cos\theta$ (u and v are the components of the horizontal wind in spherical coordinates, and θ is latitude). In this section we describe the Eulerian $U-V$ model.

First we set out the continuous equations in (λ, θ, η) coordinates, where λ is longitude and η is the hybrid vertical coordinate introduced by *Simmons and Burridge* (1981); thus $\eta(p, p_{\mathrm{surf}})$ is a monotonic function of the pressure p, and also depends on the surface pressure p_{surf} in such a way that

$$\eta(0, p_{\mathrm{surf}}) = 0 \text{ and } \eta(p_{\mathrm{surf}}, p_{\mathrm{surf}}) = 1 .$$

The momentum equations are

$$\frac{\partial U}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial U}{\partial\lambda} + v\cos\theta\frac{\partial U}{\partial\theta}\right\} + \dot{\eta}\frac{\partial U}{\partial\eta} \\ (-fv) + \frac{1}{a}\left\{\frac{\partial\phi}{\partial\lambda} + R_{\mathrm{dry}}T_{\mathrm{v}}\frac{\partial}{\partial\lambda}(\ln p)\right\} = P_U + K_U \tag{2.1}$$

$$\frac{\partial V}{\partial t}+\frac{1}{a\cos^2\theta}\left\{U\frac{\partial V}{\partial\lambda}+V\cos\theta\frac{\partial V}{\partial\theta}+\sin\theta(U^2+V^2)\right\}+\dot{\eta}\frac{\partial V}{\partial\eta}$$
$$+fU+\frac{\cos\theta}{a}\left\{\frac{\partial\phi}{\partial\theta}+R_{\mathrm{dry}}T_{\mathrm{v}}\frac{\partial}{\partial\theta}(\ln p)\right\}=P_V+K_V \quad , \tag{2.2}$$

where a is the radius of the earth, $\dot{\eta}$ is the η-coordinate vertical velocity ($\dot{\eta}=\mathrm{d}\eta/\mathrm{d}t$), ϕ is geopotential, R_{dry} is the gas constant for dry air, and T_{v} is the virtual temperature defined by

$$T_{\mathrm{v}}=T[1+\{R_{\mathrm{vap}}/(R_{\mathrm{dry}}-1)\}q]$$

where T is temperature, q is specific humidity and R_{vap} is the gas constant for water vapour. P_U and P_V represent the contributions of the parametrized physical processes, while K_U and K_V are the horizontal diffusion terms.

The thermodynamic equation is

$$\frac{\partial T}{\partial t}+\frac{1}{a\cos^2\theta}\left\{U\frac{\partial T}{\partial\theta}+V\cos\theta\frac{\partial T}{\partial\theta}\right\}+\dot{\eta}\frac{\partial T}{\partial\eta}-\frac{\kappa T_{\mathrm{v}}\omega}{(1+(\delta-1)q)p}=P_T+K_T \tag{2.3}$$

where $\kappa=R_{\mathrm{dry}}/\mathrm{c}_{p_{\mathrm{dry}}}$ ($c_{p_{\mathrm{dry}}}$ is the specific heat of dry air at constant pressure), ω is the ρ-coordinate vertical velocity ($\omega=\mathrm{d}p/\mathrm{d}t$), and $\delta=c_{p_{\mathrm{vap}}}/c_{p_{\mathrm{dry}}}$ ($c_{p_{\mathrm{vap}}}$ is the specific heat of water vapour at constant pressure).

The moisture equation is

$$\frac{\partial q}{\partial t}=\frac{1}{a\cos^2\theta}\left\{U\frac{\partial q}{\partial\lambda}+V\cos\theta\frac{\partial q}{\partial\theta}\right\}=\eta\frac{\partial q}{\partial\eta}=P_q+K_q \tag{2.4}$$

In (2.2) and (2.3), P_T and P_q represent the contributions of the parametrized physical processes, while K_T and K_q are the horizontal diffusion terms.

The continuity equation is

$$\frac{\partial}{\partial t}\left(\frac{\partial p}{\partial\eta}\right)+\nabla.\left(\mathbf{v}_{\mathrm{H}}\frac{\partial p}{\partial\eta}\right)+\frac{\partial}{\partial\eta}\left(\dot{\eta}\frac{\partial p}{\partial\eta}\right)=0 \tag{2.5}$$

where ∇ is the horizontal gradient operator in spherical coordinates and $\mathbf{v}_{\mathrm{H}}=(u,v)$ is the horizontal wind.

The geopotential ϕ which appears in (2.1) and (2.2) is defined by the hydrostatic equation

$$\frac{\partial\phi}{\partial\eta}=\frac{R_{\mathrm{dry}}T_{\mathrm{v}}}{p}\frac{\partial p}{\partial\eta} \tag{2.6}$$

while the vertical velocity ω in (2.3) is given by

$$\omega=-\int_0^{\eta}\nabla.\left(\mathbf{v}_{\mathrm{H}}\frac{\partial p}{\partial\eta}\right)\mathrm{d}\eta+\mathbf{v}_{\mathrm{H}}.\nabla p \tag{2.7}$$

Expressions for the rate of change of surface pressure, and for the vertical velocity $\dot{\eta}$, are obtained by integrating (2.5), using the boundary conditions $\dot{\eta} = 0$ at $\eta = 0$ and at $\eta = 1$

$$\frac{\partial p_{\mathrm{surf}}}{\partial t} = -\int_0^1 \nabla.\left(\mathbf{v}_{\mathrm{H}}\frac{\partial p}{\partial \eta}\right)\mathrm{d}\eta \tag{2.8}$$

$$\dot{\eta}\frac{\partial p}{\partial \eta} = -\frac{\partial p}{\partial \eta} - \int_0^{\eta} \nabla.\left(\mathbf{v}_{\mathrm{H}}\frac{\partial p}{\partial \eta}\right)\mathrm{d}\eta \tag{2.9}$$

Since we use $\ln(p_{\mathrm{surf}})$ rather than p_{surf} as the surface pressure variable, it is convenient to rewrite (2.8) as

$$\frac{\partial}{\partial t}(\ln p_{\mathrm{surf}}) = -\frac{1}{p_{\mathrm{s}}}\int_0^1 \nabla.\left(\mathbf{v}_{\mathrm{H}}\frac{\partial p}{\partial \eta}\right)\mathrm{d}\eta \tag{2.10}$$

2.2 DISCRETIZATION

2.2.1 Vertical discretization

To represent the vertical variation of the dependent variables U, V, T and q, the atmosphere is divided into $NLEV$ layers. These layers are defined by the pressures at the interfaces between them (the 'half-levels'), and these pressures are given by

$$p_{k+1/2} = A_{k+1/2} + B_{k+1/2}p_{\mathrm{surf}} \tag{2.11}$$

for $0 \le k \le NLEV$. The $A_{k+1/2}$ and $B_{k+1/2}$ are constants whose values effectively define the vertical coordinate and p_{surf} is the surface pressure field.

The values of the $A_{k+1/2}$ and $B_{k+1/2}$ for all $0 \le k \le NLEV$ are stored in the GRIB header of all fields archived on model levels to allow the reconstruction of the 'full-level' pressure p_k associated with each model level (middle of layer) from $p_k = \frac{1}{2}(p_{k-1/2} + p_{k+1/2})$ $(1 \le k \le NLEV)$by using (2.11) and the surface pressure field.

The prognostic variables are represented by their values at 'full-level' pressures p_k. Values for p_k are not explicitly required by the model's vertical finite-difference scheme, which is described below.

The discrete analogue of the surface pressure tendency equation (2.10) is

$$\frac{\partial}{\partial t}(\ln p_{\mathrm{surf}}) = -\frac{1}{p_{\mathrm{surf}}}\sum_{k=1}^{NLEV} \nabla.(\mathbf{v}_{\mathrm{H}}\Delta p_k) \tag{2.12}$$

where

$$\Delta p_k = p_{k+1/2} - p_{k-1/2} \quad . \tag{2.13}$$

From (2.11) we obtain

$$\frac{\partial}{\partial t}(\ln p_{\text{surf}}) = -\sum_{k=1}\left\{\frac{1}{p_{\text{surf}}}D_k\Delta p_k + (\mathbf{v}_k.\nabla\ln p_{\text{surf}})\Delta B_k\right\} \tag{2.14}$$

where D_k is the divergence at level k,

$$D_k = \frac{1}{a\cos^2\theta}\left(\frac{\partial U_k}{\partial\lambda} + \cos\theta\frac{\partial V_k}{\partial\theta}\right) \tag{2.15}$$

and

$$\Delta B_k = B_{k+1/2} - B_{k-1/2} \ . \tag{2.16}$$

The discrete analogue of (2.9) is

$$\left(\dot{\eta}\frac{\partial p}{\partial\eta}\right)_{k+1/2} = -\frac{\partial p_{k+1/2}}{\partial t} - \sum_{j=1}^{k}\nabla.(\mathbf{v}_j\Delta p_j) \tag{2.17}$$

and from (2.11) we obtain

$$\left(\dot{\eta}\frac{\partial p}{\partial\eta}\right)_{k+1/2} = -p_{\text{surf}}\left[B_{k+(1/2)½}\frac{\partial}{\partial t}(\ln p_{\text{surf}}) + \sum_{j=1}^{k}\left\{\frac{1}{p_{\text{surf}}}D_j\Delta p_j + (\mathbf{v}_j.\nabla\ln p_{\text{surf}})\Delta B_j\right\}\right] \tag{2.18}$$

where $\partial/\partial t(\ln p_{\text{surf}})$ is given by (2.14).

Vertical advection of a variable X is now given by

$$\left(\dot{\eta}\frac{\partial x}{\partial\eta}\right)_k = \frac{1}{2\Delta p_k}\left\{\left(\dot{\eta}\frac{\partial p}{\partial\eta}\right)_{k+1/2}(X_{k+1} - X_k) + \left(\dot{\eta}\frac{\partial p}{\partial\eta}\right)_{k-1/2}(X_k - X_{k-1})\right\} \tag{2.19}$$

The discrete analogue of the hydrostatic equation (2.6) is

$$\phi_{k+1/2} - \phi_{k-1/2} = -R_{\text{dry}}(T_{\text{v}})_k\ln\frac{p_{k+1/2}}{p_{k-1/2}} \tag{2.20}$$

which gives

$$\phi_{k+1/2} = \phi_{\text{surf}} + \sum_{j=k+1}^{NLEV} R_{\text{dry}}(T_{\text{v}})\ln\frac{p_{j+1/2}}{p_{j-1/2}} \tag{2.21}$$

where ϕ_{surf} is the geopotential at the surface. Full-level values of the geopotential, as required in the momentum equations (2.1) and (2.2), are given by

$$\phi_k = \phi_{k+1/2} + \alpha_k R_{\mathrm{dry}}(T_{\mathrm{v}})_k \tag{2.22}$$

where $\alpha_1 = \ln 2$ and, for $k > 1$,

$$\alpha_k = 1 - \frac{p_{k-1/2}}{\Delta p_k} \ln\left(\frac{p_{k+1/2}}{p_{k-1/2}}\right), \tag{2.23}$$

The remaining part of the pressure gradient terms in (2.1) and (2.2) is given by

$$R_{\mathrm{dry}}(T_{\mathrm{v}}\nabla \ln p)_k = \frac{R_{\mathrm{dry}}(T_{\mathrm{v}})_k}{\Delta p_k} = \left\{\ln\left(\frac{p_{k+1/2}}{p_{k-1/2}}\right)\nabla p_{k-1/2} + \alpha_k \nabla(\Delta p_k)\right\} \tag{2.24}$$

with α_k given by (2.23) for all .

Finally, the energy conversion term in the thermodynamic equation (2.3) is discretized as

$$\frac{\kappa T_{\mathrm{v}}\omega}{(1+(\delta-1)q)p} =$$

$$\frac{\kappa(T_{\mathrm{v}})_k}{1+(\delta-1)q_k}\left(-\frac{1}{\Delta p_k}\left((\ln\frac{p_{k+1/2}}{p_{k-1/2}})\sum_{j=1}^{k-1}(D_j\Delta p_j + p_{\mathrm{surf}}(\mathbf{v}_j.\nabla \ln p_{\mathrm{surf}})\Delta B_{jj})\right.\right. \tag{2.25}$$

$$\left.\left. +\alpha_k(D_k\Delta p_k + p_{\mathrm{surf}}(\mathbf{v}_k.\nabla \ln p_{\mathrm{surf}})\Delta B_k)\right\}\right) \left(+ \frac{p_{\mathrm{surf}}}{\Delta p_k}\left\{\Delta B_k + \frac{C_k}{\Delta p_k}\ln\frac{p_{k+1/2}}{p_{k-1/2}}\right\}(\mathbf{v}_k.\nabla \ln p_{\mathrm{surf}})\}\right)$$

where $\alpha_1 = \ln 2$, α_k, is defined by (2.23) for $k > 1$, and

$$C_k = A_{k+1/2}B_{k-1/2} - A_{k-1/2}B_{k+1/2}. \tag{2.26}$$

The reasons behind the various choices made in this vertical discretization scheme are discussed by *Simmons and Burridge* (1981); basically the scheme is designed to conserve angular momentum and energy, for frictionless adiabatic flow.

2.2.2 Finite-element vertical discretization

In CY24R3 the vertical discretization has been changed in the operational model from the finite-difference discretization in Lorenz staggering described in the previous subsection to a finite-element discretization using cubic B-splines as basis functions.

For the finite-element (FE) discretization, all variables (even pressure) are kept at the same levels (full levels), i.e. the values of pressure at full levels and not at half levels are required. Also, the values of the derivatives $\mathrm{d}A/\mathrm{d}\eta$ and $\mathrm{d}B/\mathrm{d}\eta$ at full levels are now needed, from which the vertical derivative of pressure can be computed according to $\partial p/\partial\eta = (\mathrm{d}A/\mathrm{d}\eta) + (\mathrm{d}B/\mathrm{d}\eta)p_{\mathrm{s}}$. In the semi-Lagrangian version of the evolution equations these are the only vertical derivatives required. They are constant in time and linked to the definition of the vertical coordinate. It is therefore convenient to change the definition of the vertical coordinate and supply $(\mathrm{d}A/\mathrm{d}\eta)_k$ and $(\mathrm{d}B/\mathrm{d}\eta)_k$ at full levels (instead of $A_{k+1/2}$ and $B_{k+1/2}$ at half levels) such that

$$\left(\frac{\partial p}{\partial \eta}\right)_k = \left(\frac{\mathrm{d}A}{\mathrm{d}\eta}\right)_k + \left(\frac{\mathrm{d}B}{\mathrm{d}\eta}\right)_k p_s \tag{2.27}$$

and

$$\int_0^1 \frac{\mathrm{d}A}{\mathrm{d}\eta}\mathrm{d}\eta = 0 \quad , \quad \int_0^1 \frac{\mathrm{d}B}{\mathrm{d}\eta}\mathrm{d}\eta = 1 \tag{2.28}$$

The two conditions of Eq.(2.28) above ensure that the integral of pressure from the top of the atmosphere to the surface yields exactly the surface pressure . These conditions have to be fulfilled to a good approximation with the numerical integration scheme used. Pressure at any full level can then be obtained by integrating Eq. (2.27) from the top of the atmosphere to the level in question.

The only operation in the vertical which has to be evaluated is the vertical integration. An integral operator based on a finite-element representation will be derived next.

Most of the integrals we have to evaluate are integrals from the top of the atmosphere to the individual model levels and to the surface. We therefore derive an operator in finite-element representation for this type of integral, i.e. an operator which returns the integral from the top of the atmosphere to each of the model levels η_k and to the surface $(\eta = 1)$. The vertical integral in the hydrostatic equation (i.e. from the surface upwards) can be constructed by taking the difference of the integral from the top of the atmosphere to the model level in question minus the integral from the top to the surface.

Let $\{d_i(\eta)\}_{i=K_1}^{K_2}$ and $\{e_i(\eta)\}_{i=M_1}^{M_2}$ be two sets of linearly independent functions of compact support which can be used as basis functions to expand any function of the vertical coordinate η given in the domain [0,1].

The vertical integral

$$F(\eta) = \int_0^\eta f(x)\mathrm{d}x$$

can then be approximated as

$$\sum_{i=K_1}^{K_2} C_i d_i(\eta) = \sum_{i=M_1}^{M_2} c_i \int_0^\eta e_i(x)\mathrm{d}x \tag{2.29}$$

where C_i are the coefficients of the expansion of $F(\eta)$ as a linear combination of the basis functions $\{d_i(\eta)\}$ and c_i are the coefficients of the expansion of $f(\eta)$ as a linear combination of the basis functions $\{e_i(\eta)\}$.

We can then apply the Galerkin procedure to Eq. (2.29) by multiplying both sides of this equation by each function from a complete set of "test functions" $\{t_j\}_{j=N_1}^{N_2}$ and integrating over the vertical domain:

$$\sum_{i=K_1}^{K_2} C_i \int_0^1 \mathrm{d}_i(x) t_j(x) dx = \sum_{i=M_1}^{M_2} c_i \int_0^1 \left[t_j(x) \int_0^x e_i(y) \mathrm{d}y \right] \mathrm{d}x$$

In matrix form this can be expressed as $A\tilde{C} = B\tilde{c}$ => $\tilde{C} = A^{-1}B\tilde{c}$.

Incorporating into the above expression also the transformations from physical space to finite-element space and back, i.e. $\tilde{c} = S^{-1}\tilde{f}$ and $\tilde{F} = P\tilde{C}$, we obtain $\tilde{F} = PA^{-1}BS^{-1}\tilde{f} \equiv I\tilde{f}$. Here $\tilde{f}$ and $\tilde{F}$ denote vectors in physical space composed mainly of the values of f and F , respectively, at the model levels: $f_i = f(\eta_i)$, $F_i = F(\eta_i)$, $1 \le i \le N$. The set of values F also includes the value at the surface of the model. Details of the basis functions chosen to implement the scheme as well as how to compute the projection matrices S and P are given in *Untch and Hortal* (2002) .

Matrix $I \equiv PA^{-1}BS^{-1}$ is the integration operator in finite-element formulation which, applied to a function given at full model levels, yields the integrals of this function from the top of the atmosphere to each individual full model level and to the surface. All the finite sums on the vertical levels in subsection 2.2.1 are replaced by vertical integrals computed by applying the matrix integration operator *I*. Moreover the quantities α_k are no longer needed as the integration operator gives directly the value of the integral at the model levels (the half levels do not have any meaning in the FE discretization).

2.2.3 Time discretization

To introduce a discretization in time, together with a semi-implicit correction, we define the operators

$$\delta_t X = (X^+ - X^-)/\,2\Delta\,\mathrm{t}\ ,$$

$$\Delta_{tt} X = (X^+ - 2X + X^-)$$

where X represents the value of a variable at time t, X^+ the value at time $(t + \Delta t)$, and X^- the value at $(t - \Delta t)$. In preparation for the semi-Lagrangian treatment to be developed in section 3, we also introduce the three-dimensional advection operator

$$A(X) = \frac{1}{a\cos^2\theta}\left(U\frac{\partial x}{\partial \lambda} + V\cos\theta\frac{\partial x}{\partial \theta}\right) + \dot{\eta}\frac{\partial x}{\partial \eta} \tag{2.30}$$

Introducing the semi-implicit correction terms, Eqs. (2.1)–(2.4) become:

$$\begin{aligned} &\delta_t U + A(U) - fV + \frac{1}{a}\left\{\frac{\partial \phi}{\partial \lambda} + R_{\mathrm{dry}} T_{\mathrm{v}} \frac{\partial}{\partial \lambda}\ln p\right\} = \\ &P_U + K_U - \frac{\beta}{2a}\,\Delta_{tt}\left\{[\gamma]\frac{\partial T}{\partial \lambda} + R_{\mathrm{dry}} T^{\mathrm{ref}} \frac{\partial}{\partial \lambda}(\ln p_{\mathrm{surf}})\right\} \end{aligned} \tag{2.31}$$

$$\delta_t V + A(V) + \frac{\sin\theta}{a\,\cos^2\theta}(U^2+V^2) + fU + \frac{\cos\theta}{a}\left\{\frac{\partial\phi}{\partial\theta} + R_{\text{dry}}T_{\text{v}}\frac{\partial}{\partial\theta}(\ln p)\right\} = \\ P_V + K_V - \frac{\beta\cos\theta}{2a}\,\Delta_{tt}\left([\gamma]\frac{\partial T}{\partial\theta} + R_{\text{dry}}T^{\text{ref}}\frac{\partial}{\partial\theta}(\ln p_{\text{surf}})\right) \tag{2.32}$$

$$\delta_t T + A(T) - \frac{\kappa T_{\text{v}}\omega}{(1+(\delta-1)q)p} = P_T + K_T - \frac{\beta}{2}\,\Delta_{tt}([\tau]D) \tag{2.33}$$

$$\delta_t q + A(q) = P_q + K_q \tag{2.34}$$

where β is a parameter of the semi-implicit scheme; the classical scheme (*Robert* 1969) is recovered with $\beta = 1$. The semi-implicit correction terms are linearized versions of the pressure gradient terms in (2.1)–(2.2) and the energy conversion term in (2.3). Thus T^{ref} is a reference temperature (here chosen to be independent of vertical level), while $[\gamma]$ and $[\tau]$ are matrices such that

$$([\gamma]\mathbf{T})_k = \alpha_k^{\text{ref}}R_{\text{dry}}T_k + \sum_{j=k+1}^{NLEV} R_{\text{dry}}T_j\,\ln\left(\frac{p_{j+1/2}^{\text{ref}}}{p_{j-1/2}^{\text{ref}}}\right), \tag{2.35}$$

$$([\tau]\mathbf{D})_k = \kappa T^{\text{ref}}\left\{\frac{1}{\Delta p_k^{\text{ref}}}\ln\left(\frac{p_{k+1/2}^{\text{ref}}}{p_{k-1/2}^{\text{ref}}}\right)\sum_{j=1}^{k-1}(D_j\Delta p_j^{\text{ref}}) + \alpha_k^{\text{ref}}D_k\right\}. \tag{2.36}$$

where the half-level pressures appearing in (2.35) and (2.35) are reference values obtained from (2.11) by choosing a reference value $p_{\text{surf}}^{\text{ref}}$ of p_{surf}, and the coefficients α_k^{ref} are based on these reference values. The reference values adopted for the semi-implicit scheme are $T^{\text{ref}} = 300\ \text{K}$ and $p_{\text{surf}}^{\text{ref}} = 800\ \text{hPa}$.

The integrated surface pressure tendency equation (2.14) becomes

$$\delta_t(\ln p_{\text{surf}}) + \sum_{k=1}^{NLEV}\left\{\frac{1}{p_{\text{surf}}}D_k\,\Delta p_k + (\mathbf{v}_k.\nabla\ \ln p_{\text{surf}})\,\Delta B_k\right\} = -\frac{\beta}{2}\,\Delta_{tt}[\nu]D \tag{2.37}$$

where

$$[\nu]D = \frac{1}{p_{\text{surf}}^{\text{ref}}}\sum_{j=1}^{NLEV} D_j\Delta p_{\text{surf}}^{\text{ref}} \tag{2.38}$$

2.2.4 Horizontal grid

A novel feature of the model is the optional use of a reduced Gaussian grid, as described by *Hortal and Simmons* (1991). Thus, the number of points on each latitude row is chosen so that the local east–west grid length remains approximately constant, with the restriction that the number should be suitable for the FFT ($N = 2^p3^q5^r$). After some experimentation, the 'fully reduced grid' option of *Hortal and Simmons* was implemented; all possible wavenumbers (up to the model's truncation limit) are used in the Legendre transforms. A small amount of noise in the immediate vicinity of the poles was removed by increasing the number of grid points in the three most northerly and southerly rows of the grid (from 6, 12 and 18 points in the original design of the T213 grid to 12, 16 and 20 points respectively). *Courtier and Naughton* (1994) have very recently reconsidered the design of reduced Gaussian grids.

2.2.5 Time-stepping procedure

The time-stepping procedure for the Eulerian $U-V$ version of the model follows closely that outlined by *Temperton* (1991) for the shallow-water equations. At the start of a time-step, the model state at time $(t-\Delta t)$ is defined by the values of U, V, T, q and $\ln p_{\mathrm{surf}}$ on the Gaussian grid. To compute the semi-implicit corrections, the $(t-\Delta t)$ values of divergence D, $\partial P/\partial\lambda$ and $\partial P/\partial\mu$ are also held on the grid, where $\mu = \sin\theta$ and

$$P = [\gamma]T + R_{\mathrm{dry}}T^{\mathrm{ref}}\ln p_{\mathrm{surf}} \quad . \tag{2.39}$$

The model state at time t is defined by the spectral coefficients of ζ, D, T, q and $\ln p_{\mathrm{surf}}$. Legendre transforms followed by Fourier transforms are then used to compute ζ, D, U, V, T, $\partial T/\partial\mu$, $\ln p_{\mathrm{surf}}$ and $\partial(\ln p_{\mathrm{surf}})/\partial\mu$ at time t on the model grid. Additional Fourier transforms are used to compute the corresponding values of $\partial U/\partial\lambda$, $\partial V/\partial\lambda$. $\partial T/\partial\lambda$, $\partial q/\partial\lambda$ and $\partial(\ln p_{\mathrm{surf}})/\partial\lambda$. The meridional gradients of U and V are obtained using the relationships

$$\begin{aligned} \cos\theta\frac{\partial V}{\partial\theta} &= aD\cos^2\theta - \frac{\partial U}{\partial\lambda} \\ \cos\theta\frac{\partial U}{\partial\theta} &= \frac{\partial V}{\partial\lambda} - \zeta\cos^2\theta \end{aligned} \quad .$$

All the information is then available to evaluate the terms at time t on the left-hand sides of (2.31)–(2.34) and (2.37), and thus to compute ‘provisional’ tendencies of the model variables. These tendencies (together with values of the variables at $(t-\Delta t)$ are supplied to the physical parametrization routines, which increment the tendencies with their respective contributions. The semi-implicit correction terms evaluated at time-levels $(t-\Delta t)$ and t are then added to the tendencies. Ignoring the horizontal diffusion terms (which are handled later in spectral space), and grouping together the terms which have been computed on the grid, (2.31)–(2.34) and (2.37) can be written in the form

$$U^+ + \frac{\beta\Delta t}{a}\frac{\partial p^+}{\partial\lambda} = R_1 \tag{2.40}$$

$$V^+ + \frac{\beta\Delta t}{a}\cos\theta\frac{\partial p^+}{\partial\theta} = R_2 \tag{2.41}$$

$$T^+ + \beta\,\Delta t\,[\tau]D^+ = R_3 \tag{2.42}$$

$$q^+ = R_4 \tag{2.43}$$

$$(\ln p_{\mathrm{surf}})^+ + \beta\,\Delta t\,[\nu]D^+ = R_5 \tag{2.44}$$

The right-hand sides $R_1 - R_5$ are transformed to spectral space via Fourier transforms followed by Gaussian integration. The curl and divergence of (2.40) and (2.41) are then computed in spectral space, leading to

$$\zeta^{+} = \text{curl}\,(R_1, R_2) \tag{2.45}$$

$$D^{+} + \beta\,\Delta t\,\nabla^2 p^{+} = \text{div}(R_1, R_2)\,. \tag{2.46}$$

Eqs. (2.42), (2.44) and (2.46) can then be combined with the aid of (2.39) to obtain an equation of the form

$$\left([I] + \frac{n(n+1)}{a^2}[\Gamma]\right)(D_n^m)^{+} = (\tilde{D})_n^m \tag{2.47}$$

for each zonal wavenumber m and total wavenumber n, where the matrix

$$[\Gamma] = \beta^2(\Delta t)^2([\gamma][\tau] + R_{\text{dry}}T^{\text{ref}}[\nu]) \tag{2.48}$$

couples all the $NLEV$ values of $(D_n^m)^{+}$ in a vertical column. Once D^{+} has been found, the calculation of T^{+} and $(\ln p_{\text{surf}})^{+}$ can be completed, while q^{+} and ζ^{+} have already been obtained from (2.43) and (2.45).

Finally, a 'fractional step' approach is used to implement the horizontal diffusion of vorticity, divergence, temperature and specific humidity. A simple linear diffusion of order $2r$ is applied along the hybrid coordinate surfaces:

$$K_X = -(-1)^r K \nabla^{2r} X \tag{2.49}$$

where $X = \zeta$, D or q. It is applied in spectral space to the $(t + \Delta t)$ values such that if X_n^m is the spectral coefficient of X prior to diffusion, then the diffused value $\bar{X}_n^m$ is given by

$$\bar{X}_n^m = \left\{1 + 2\Delta t\,K\left(\frac{n(n+1)}{a^2}\right)^r\right\}^{-1} X_n^m \tag{2.50}$$

A modified form of (2.50) is also used for the temperature T, to approximate diffusion on surfaces of constant pressure rather than on the sloping hybrid coordinate surfaces (*Simmons,* 1987). The operational version of the model uses fourth-order horizontal diffusion $(r = 2)$

2.2.6 Time filtering

To avoid decoupling of the solutions at odd and even time steps, a Robert filter (*Asselin* 1972) is applied at each timestep. The time-filtering is defined by

$$X_{\text{f}} = X + \varepsilon\,(X_{\text{f}}^{-} - 2X + X^{+}) \tag{2.51}$$

where the subscript f denotes a filtered value, and X^{-}, X and X^{+} represent values at $(t - \Delta t)$, t and $(t + \Delta t)$, respectively.

Because of the scanning structure of the model, it is convenient to apply the time-filtering in grid-point space, and to split (2.51) into two parts:

$$\tilde{X}_{\text{f}} = X + \varepsilon(X_{\text{f}}^{-} - 2X) \tag{2.52}$$

$$X_{\mathrm{f}} = \tilde{X}_{\mathrm{f}} + \varepsilon X^{+} \tag{2.53}$$

The 'partially filtered' values computed by (2.52) are stored on a grid-point work file and passed from one time-step to the next. Thus, the information available after the transforms to grid-point space consists of partially filtered values at time $(t-\Delta t)$ together with unfiltered values at time t. The filtering of the $(t-\Delta t)$ fields can then be completed via (2.53), which after shifting by one timestep becomes:

$$X_{\mathrm{f}}^{-} = \tilde{X}_{\mathrm{f}}^{-} + \varepsilon\, X\ . \tag{2.54}$$

The computations described in Section 2.2.5 are performed using these fully filtered values at time $(t-\Delta t)$ and the unfiltered values at time t. Once (2.54) has been implemented, values of X_{f}^{-} are also available to implement (2.52) for the partially filtered values to be passed on to the next timestep.

2.2.7 Remarks

Ritchie (1988*)* noted that for a spectral model of the shallow-water equations, the $U-V$ form and the $\zeta-D$ form gave identical results (apart from round-off error). In extending this work to a multi-level model, *Ritchie* (1991) found that this equivalence was not maintained. This was in fact a result of some *analytic* manipulations in the vertical, used to eliminate between the variables in solving the equations of the semi-implicit scheme, which were not exactly matched by the finite-element vertical discretization of Ritchie's model.

In the case of the model described here, the corresponding elimination between the variables is purely algebraic, and the equivalence between the $U-V$ form and the $\zeta-D$ form is maintained apart from one small exception due to the use of the hybrid vertical coordinate. In the $U-V$ model, the gradients of the geopotential ϕ are computed in grid-point space (from the spectrally computed gradients of T, q and $\ln p_{\mathrm{surf}}$), while in the $\zeta-D$ model ϕ itself is computed and transformed separately into spectral space, where its Laplacian is added into the divergence equation. Since ϕ is not a quadratic function of the model variables there is some aliasing, which is different for the two versions of the model. In practice the differences between the $\zeta-D$ model and the $U-V$ model were found to be very small, and in the case of a pure sigma-coordinate the two models would be algebraically equivalent.

The $U-V$ model is nevertheless considerably more economical than its $\zeta-D$ counterpart in terms of the number of Legendre transforms required. In addition to the transform of ϕ referred to above, four Legendre transforms are saved in the treatment of the wind fields using the procedures described by *Temperton* (1991) for the shallow-water equations. The number of multi-level Legendre transforms is thereby reduced from 17 to 12 per time-step.

2.2.8 T_{v} as spectral variable

In preparation for a further reduction in the number of Legendre transforms required by the semi-Lagrangian version of the model, the modified Eulerian version includes an option to keep the virtual temperature T_{v}, rather than the temperature T, as the spectral variable. In the time-stepping procedure, Legendre transforms followed by Fourier transforms are used to compute T_{v}, $\partial T_{\mathrm{v}}/\partial\mu$ and $\partial T_{\mathrm{v}}/\partial\lambda$ at time t on the model grid; the corresponding values of T, $\partial T/\partial\mu$ and $\partial T/\partial\lambda$ are then computed using the corresponding values of q, $\partial q/\partial\mu$ and $\partial q/\partial\lambda$. The thermodynamic equation (2.3) is then stepped forward in time exactly as before. After the physical parametrization routines, the 'provisional' value of $T(t+\Delta t)$ is combined with $q(t+\Delta t)$ to compute a provisional value of $T_{\mathrm{v}}(t+\Delta t)$. The semi-implicit correction terms evaluated at time-levels $(t-\Delta t)$ and $T_{\mathrm{v}}(t+\Delta t)$ are then added to the provisional value of $T_{\mathrm{v}}(t+\Delta t)$, just before the transform back to spectral space.

There are corresponding slight changes in the semi-implicit correction terms. The linearized hydrostatic matrix $[\gamma]$

in (2.31)–(2.32) and (2.39) now operates on T_{v} rather than on T. From the point of view of the semi-implicit scheme, (2.33) has implicitly been replaced by an equation of the form

$$\delta_t T_{\mathrm{v}} = \ldots - \frac{\beta}{2}\Delta_{tt}([\tau]D) \tag{2.55}$$

although as explained above it is not necessary to formulate or compute the missing terms explicitly. Hence, (2.42) is replaced by

$$T_{\mathrm{v}}^{+} + \beta\Delta t[\tau]D^{+} = R_3' \tag{2.56}$$

and the solution of the semi-implicit equations in spectral space proceeds just as before.

This change of spectral variable results in only insignificant changes to a 10-day model forecast, but permits useful economies in the semi-Lagrangian version to be described in the next chapter.

IFS documentation

Part III: DYNAMICS AND NUMERICAL PROCEDURES

CHAPTER 3 Semi-Lagrangian formulation

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3.1 GENERAL DESCRIPTION

The general form of the model equations is

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \frac{\partial X}{\partial t} + A(X) = R = L + N \tag{3.1}$$

where the three-dimensional advection operator A was defined in (2.30), L is the linearized part of R and N is the remainder or “non-linear terms”. An explicit three-time-level semi-Lagrangian treatment of (3.1) is obtained by finding the approximate trajectory, over the time interval $[t-\Delta t, t+\Delta t]$, of a particle which arrives at each grid point $\underset{\sim}{x}$ at time $(t+\Delta t)$. Equation (3.1) is then approximated by

$$\frac{X^+ - X^-}{2\Delta t} = R^0 \tag{3.2}$$

where the superscripts $+$, 0 and $-$, respectively denote evaluation at the arrival point $(\underset{\sim}{x},\ t+\Delta t)$, the mid-point of the trajectory $(x-\alpha,\, t)$, and the departure point $(x-2\alpha,\, t-\Delta t)$. Since the mid-point and the departure point will not in general coincide with model grid points, X^- and R^0 must be determined by interpolation.

It is more economical (and, as discussed later, gives better results in some circumstances; see also *Tanguay et al.*, 1992) to evaluate the right-hand side of (3.2) as

$$R^0 = \frac{1}{2}\{R(\underset{\sim}{x}-2\underset{\sim}{\alpha},\, t)+R(\underset{\sim}{x},\, t)\} \tag{3.3}$$

since only a single interpolation (of the combined field $X(t-\Delta t)+\Delta t R(t)$ at the point $(\underset{\sim}{x}-2\underset{\sim}{\alpha})$) is then required in order to determine X^+.

The right-hand sides of the time-discretized model equations also contain semi-implicit correction terms, which in the Eulerian model took the form

$$\Delta_{tt}X = (X^+ - 2X^0 + X^-)$$

where the superscripts refer to time-levels, and to a single common grid point. In the semi-Lagrangian version of the model, the semi-implicit correction terms take the form

$$\Delta_{tt}X = (X(\underset{\sim}{x},\, t+\Delta t)-X(\underset{\sim}{x},\, t))+(X(\underset{\sim}{x}-2\underset{\sim}{\alpha},\, t-\Delta t)-X(\underset{\sim}{x}-2\underset{\sim}{\alpha},\, t)) \tag{3.4}$$

and again the terms to be evaluated at the departure point $(\underset{\sim}{x}-2\underset{\sim}{\alpha})$ can be added to other right-hand side terms before interpolation. Notice that the evaluation of $\Delta_{tt}X$, and both ways of evaluating R^0, are all centred in space and time.

To obtain accurate results from a semi-Lagrangian integration scheme, it is necessary to choose the order of interpolation carefully (see for example *Staniforth and Côté*, 1991). In practice it has been found (for the model described here) that linear interpolation is adequate for the terms evaluated at the midpoint of the trajectory, but that cubic interpolation is essential for the terms evaluated at the departure point. Cubic interpolation in three dimensions is expensive, and fortunately a 'quasi-cubic' interpolation (suggested by Courtier) was found to give essentially equivalent results. The technique can be illustrated by two-dimensional interpolation on a regular grid. The target point is at $(x_I+\alpha,\, y_J+\beta)$. In the first step, four interpolations are performed in the x-direction: *linear* (rather than the usual cubic) interpolations to the points $(x_I+\alpha,\, y_{J-1})$ and $(x_I+\alpha,\, y_{J+2})$, and *cubic* interpolations to the points $(x_I+\alpha,\, y_J)$ and $(x_I+\alpha,\, y_{J+1})$. In the second step, one cubic interpolation is performed in the y-direction, to evaluate the field at the target point. The number of 'neighbours' contributing to the result is reduced from 16 to 12. The generalization to three dimensions is straightforward and results in a significant saving, the number of neighbours being reduced from 64 to 32, and the computation being reduced from 21 one-dimensional cubic interpolations to 7 cubic plus 10 linear one-dimensional interpolations.

For the reduced Gaussian grid described in Subsection 2.2.4, the mesh is no longer regular. However, it is easily seen that the extra complication is relatively minor provided that the first step in the interpolation is performed in the λ-direction.

The order of the interpolation in the vertical is reduced to linear when the evaluation point lies between the two highest model levels, or between the lowest two model levels. Extrapolation beyond the top or bottom levels is not allowed.

All the cubic interpolations, except for the vertical interpolations in the thermodynamic and the momentum equations are quasi-monotone interpolations. That means that, after the interpolation itself, the interpolated value is compared with the values of the interpolated function at the two closest points used in the interpolation. The interpolated value is then restricted to stay within the interval defined by the values at these two points. If it is larger that both of them it is reset to the larger value and if it is smaller than both it is reset to the lower value.

3.2 FINDING THE DEPARTURE POINT

Extending the procedure of *Robert* (1981) to three dimensions, the midpoint $(\tilde{x} - \tilde{\alpha})$ and the departure point $(\tilde{x} - 2\tilde{\alpha})$ of the trajectory for each arrival point $\tilde{x}$ are found by iteratively solving the equation

$$\tilde{\alpha} = \Delta t \mathbf{v}(\tilde{x} - \tilde{\alpha},\, t) \tag{3.5}$$

where $\mathbf{v}$ in (3.5) is the *three*-dimensional wind field $(u, v, \dot{\eta})$. Since $\dot{\eta}$ was never explicitly required in the Eulerian version of the model (see Eqs. (2.18)–(2.19) for the Eulerian discretization of vertical advection), it is necessary to construct this field for the trajectory calculations. As $\dot{\eta}$ is already specified at the upper and lower boundaries ($\dot{\eta} = 0$, at $\eta = 0$ and at $\eta = 1$) it would be natural to construct $\dot{\eta}$ at the half-levels (i.e. vertically staggered with respect to u and v), and indeed a preliminary version of the model was coded that way. However, it is more convenient to hold the three velocity components at the same set of points (which also coincide with the arrival points), so the formulation was changed to use $\dot{\eta}$ at the 'full' levels. Thus, the vertical velocity used in (3.5) is defined by

$$\dot{\eta}_k = \frac{\frac{1}{2}\left[\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k-\frac{1}{2}} + \left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}}\right]}{\left(\frac{\partial p}{\partial \eta}\right)_k} \tag{3.6}$$

where $\dot{\eta}\partial p/\partial\eta$ is already defined by (2.18) and

$$\left(\frac{\partial p}{\partial \eta}\right)_k = \frac{\Delta p_k}{\Delta \eta_k} = p_{\mathrm{surf}}\frac{\Delta A_k/p_{\mathrm{surf}} + \Delta B_k}{\Delta A_k/p_0 + \Delta B_k} \tag{3.7}$$

In deriving (3.7) we have used (2.11) together with a formal definition of η itself (which again was not required by the discretized Eulerian dynamics):

$$\eta_{k+½} = A_{k+½}/p_0 + B_{k+½} \tag{3.8}$$

where p_0 is a constant pressure (chosen to be $1013.25\ \mathrm{hPa}$).

The iterative procedure for solving (3.5) is analogous to that used by *Ritchie* (1991) in a σ-coordinate model. Given an estimate $\tilde{\alpha}^{(k)}$ after k iterations, the next iteration is given by

$$\tilde{\alpha}^{(k+1)} = \Delta t \mathbf{v}(\tilde{x} - \tilde{\alpha}^{(k)},\, t) \tag{3.9}$$

where the vertical (η) component of the displacement is found first. The vertical component of $\tilde{\alpha}^{(k)}$ on the right-hand side of (3.9) is then updated before the horizontal components are found taking into account the spherical geometry following *Ritchie* (1987, 1988). The first guess is given by

$$\tilde{\alpha}^{(0)} = \Delta t \mathbf{v}(\tilde{x},\, t) \tag{3.10}$$

The calculations include approximations to the spherical geometry away from the poles, following *Ritchie and Beaudoin* (1994). In agreement with previous work (reviewed by *Staniforth and Côté*, 1991), little sensitivity was found to the order of interpolation used in the trajectory calculations, and linear interpolation appears to be sufficiently accurate. After providing a first guess via (3.10), a single further iteration was found to be adequate.

Once the midpoint $(x-\alpha)$ of the trajectory has been found, the departure point $(x-2\alpha)$ is immediately obtained (in the horizontal, the backward extension of the trajectory is along a great circle). In the vertical, if the departure point is then above the first (or below the last) mode level, it is modified to lie on the first (last) level.

In solving (3.9), it is necessary to convert between a displacement in terms of the spatial coordinates and the corresponding displacement in terms of ‘grid lengths’, in order to select the correct three-dimensional block of points for the interpolation routine. This is simple in the horizontal, since the mesh length is constant in the λ -direction (at a given latitude), and almost constant in the θ -direction. It is more difficult in the vertical, where the grid spacing changes rapidly, and the conversion algorithm for the vertical displacement makes use of an auxiliary grid defined with high uniform resolution.

At high horizontal resolutions a positive feedback mechanism, between the computation of the departure point of the trajectories and the solution of the momentum equations, can lead to instability, which results in noisy forecast fields in the winter stratosphere. In order to break the positive feedback loop, a smoothing interpolation is applied to the vertical velocity in the computation of the trajectory. This smoothing interpolation uses the same set of points around the departure point as the cubic interpolation, but the horizontal interpolations are substituted by least squares linear fits to the corresponding four points. The procedure is applied to both the arrival and the departure points of the trajectory. As the procedure is not an interpolatory procedure, the value at the arrival point is substituted by a smoothed value, as is also the case for the value at the departure point.

3.3 ‘NON-INTERPOLATING’ SCHEME IN THE VERTICAL

An alternative formulation of the semi-Lagrangian scheme in three dimensions was suggested by *Ritchie* (1991). Equation (3.1) can be rewritten as

$$\frac{\mathrm{d_H}X}{\mathrm{d}t}+\dot{\eta}^*\frac{\partial X}{\partial\eta} = R-\dot{\eta}\frac{\partial X}{\partial\eta}+\dot{\eta}^*\frac{\partial X}{\partial\eta} \tag{3.11}$$

where

$$\frac{\mathrm{d_H}X}{\mathrm{d}t} = \frac{\partial X}{\partial t}+A_\mathrm{H}(X)$$

and A_H is the horizontal part of the advection operator defined in (2.30). In (3.11), $\dot{\eta}^*$ is defined to be a vertical velocity which would lead to the departure point of the trajectory at time $(t-\Delta t)$ lying exactly on a model level. This model level is chosen to be the one closest to the true departure point. Equation (3.11) is then approximated by

$$\frac{X^+-X^-}{2\Delta t} = \left(R-\dot{\eta}\frac{\partial X}{\partial\eta}\right)^0+\dot{\eta}^*\left(\frac{\partial X}{\partial\eta}\right)^0 \tag{3.12}$$

where the superscripts $+$, 0, $-$ respectively denote evaluation at the arrival point $(x,\ t+\Delta t)$, the midpoint $(x-\alpha,\ t)$ and the departure point $(x-2\alpha,\ t-\Delta t)$ of the *modified* trajectory. Since the modified departure point lies by definition on a model level, no vertical interpolation is required to evaluate X^-. As discussed in Subsection

3.1 above, it is also possible to evaluate the terms on the right-hand side of (3.12) by averaging the values at $(x - 2\alpha, t)$ and (x, t); in this case no vertical interpolation at all is required. Notice that a separate interpolation is required to evaluate the second term on the right-hand side of (3.12) since the quantity $\dot{\eta}^*$, defined by

$$\dot{\eta}^* = \frac{\eta^+ - \eta^-}{2\Delta t} \tag{3.13}$$

where η^+ and η^- are respectively the arrival and departure levels of the modified trajectory, is meaningful only at each grid point.

If the vertical velocity (or the time-step) is sufficiently small, then the modified departure point lies on the same model level as the arrival point, $\dot{\eta}^*$ is zero and the treatment of vertical advection becomes purely Eulerian. In general there is an Eulerian treatment of the advection by the 'residual vertical velocity' $(\dot{\eta} - \dot{\eta}^*)$, which is small enough to guarantee that the Eulerian CFL criterion for vertical advection is respected. Thus, the 'non-interpolating' scheme maintains the desirable stability properties of the 'fully interpolating' scheme.

There is a subtle, but important, difference in the way the iterative scheme (3.9) is implemented to determine the modified trajectory in the non-interpolating scheme. As before, the first step at each iteration is to update the estimate of the vertical component of the displacement.The implied updated departure point is then moved to the closest model level. In the second step, the horizontal components are then updated using the winds evaluated at the midpoint of the *modified* trajectory. Notice that this gives a result different from that obtained by simply carrying out the trajectory calculation of the fully interpolating scheme and then projecting the departure point to the nearest model level. The modified procedure described above is easily seen to be more consistent by considering the case in which the vertical velocity is not zero, but is small enough for the *modified* trajectory to be horizontal ($\dot{\eta}^* = 0$). The discretization is then equivalent to a purely two-dimensional semi-Lagrangian scheme, the trajectory being computed using the horizontal wind field evaluated on a single model level.

An incidental advantage of the 'non-interpolating' scheme over the 'fully interpolating' scheme is that it resolves any ambiguities about the treatment of departure points above the top model level or below the bottom model level; the modified departure points automatically lie on the top or bottom level. The treatment of vertical advection becomes Eulerian, which is well-defined at the top and bottom levels. Thus, the non-interpolating scheme removes the need for artificial 'nudging' of the departure points or the extrapolation of quantities to points above or below the domain of the model levels.

Smolarkiewicz and Rasch (1991) have extended the principle of the 'non-interpolating' semi-Lagrangian formulation to generate a broader class of stable and accurate advection schemes.

3.4 SEMI-LAGRANGIAN DISCRETIZATION

Here we describe in detail only the fully interpolating version of the semi-Lagrangian discretization; the modifications necessary for the 'non-interpolating in the vertical' version become evident by comparing the right-hand side of (3.12) with that of (3.2).

Following *Ritchie* (1988, 1991), the momentum equations are integrated in *vector* form to avoid an instability of the metric term near the poles. Using the notation of (3.2) and defining the horizontal wind vector $\mathbf{v}_{\mathrm{H}} = (u, v)$, the semi-Lagrangian equivalent of (2.31)–(2.32) is

$$\frac{\mathbf{v}_{\mathrm{H}}^{+} - \mathbf{v}_{\mathrm{H}}^{-}}{2\Delta t} + [f\mathbf{k} \times \mathbf{v}_{\mathrm{H}} + \nabla\phi + R_{\mathrm{dry}}T_{\mathrm{v}}\nabla\ln p]^0 = P_{\mathbf{v}} + K_{\mathbf{v}} - \frac{\beta}{2}\Delta_{tt}\nabla\{[\gamma]T + R_{\mathrm{dry}}T_{\mathrm{v}}\ln p_{\mathrm{surf}}\} \tag{3.14}$$

where $\mathbf{k}$ is the vertically directed unit vector and ∇ is the horizontal gradient operator in spherical coordinates. On the right-hand side of (3.14), P_{v} and K_{v} respectively denote the contributions of the physical parametrization schemes and horizontal diffusion, to be discussed in Subsection 3.6, while the semi-implicit correction terms are evaluated as in (3.4). For the momentum equations, it was found advantageous to evaluate the time-level t terms $[\ ]^0$ as an average between the values at the departure and arrival points of the trajectory, as in (3.3). The pressure gradient terms are discretized in exactly the same way as for the Eulerian model (see Subsection 2.2.1).

Since (3.14) is in vector form, it is important to account for the change in the orientation of the coordinate system as the particle follows the trajectory; the manipulations required are as set out by *Ritchie* (1988) and simplified by *Ritchie and Beaudoin* (1994).

The thermodynamic and moisture equations (2.33)–(2.34) become

$$\frac{T^+ - T^-}{2\Delta t} + -\left\{\frac{\kappa T_{\mathrm{v}}\omega}{(1+(\delta-1)q)p}\right\}^0 = P_T + K_T - \frac{\beta}{2}\Delta_{tt}([\tau]D) \tag{3.15}$$

$$\frac{q^+ - q^-}{2\Delta t} = P_q + K_q \tag{3.16}$$

In (3.15), the $\{\ \}^0$ term is discretized as in (2.25), and evaluated at the midpoint of the trajectory, while the semi-implicit correction terms are evaluated as in (3.4).

The η-coordinate continuity equation (2.5) can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial p}{\partial \eta}\right) + \frac{\partial p}{\partial \eta}\left(D + \frac{\partial \dot{\eta}}{\partial \eta}\right) = 0 \tag{3.17}$$

Setting

$$p = A(\eta) + B(\eta)p_{\mathrm{surf}}$$

and noting that

$$\frac{\partial}{\partial t}\left(\frac{\partial A}{\partial \eta}\right) = \nabla.\left(\frac{\partial A}{\partial \eta}\right) = \frac{\partial p_{\mathrm{surf}}}{\partial \eta} = 0\ ,$$

we also have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial p}{\partial \eta}\right) = \frac{\partial B}{\partial \eta}\frac{\mathrm{d}p_{\mathrm{surf}}}{\mathrm{d}t} + \dot{\eta}\frac{\partial}{\partial \eta}\left(\frac{\partial p}{\partial \eta}\right). \tag{3.18}$$

Combining (3.17) and (3.18).

$$\frac{\partial B}{\partial \eta}\frac{\mathrm{d}p_{\mathrm{surf}}}{\mathrm{d}t} + \frac{\partial p}{\partial \eta}D + \frac{\partial}{\partial \eta}\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right) = 0\ . \tag{3.19}$$

Now introducing the vertical discretization, (3.19) becomes

$$\Delta B_k \frac{\mathrm{d}p_{\mathrm{surf}}}{\mathrm{d}t} + \Delta p_k D_k + \left(\dot{\eta}\,\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}} - \left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k-\frac{1}{2}} = 0\ . \tag{3.20}$$

the vertical discretization of $\dot{\eta}\partial p/\partial\eta$ having been defined in (2.18).

Changing the prognostic variable to $\dot{\eta}\partial p/\partial\eta$,

$$\Delta B_k \frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{surf}}) + \frac{1}{p_{\mathrm{surf}}}\left\{\Delta p_k D_k + \left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}} - \left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}}\right\} = 0 \tag{3.21}$$

Combining (3.21) with the discrete definition of $\dot{\eta}\partial p/\partial\eta$ given by (2.18),

$$\Delta B_k \frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{surf}}) - \Delta B_k\left\{\frac{\partial(\ln p_{\mathrm{surf}})}{\partial t} + \mathbf{v}_k.\nabla \ln p_{\mathrm{surf}}\right\} = 0 \tag{3.22}$$

where $\partial(\ln p_{\mathrm{surf}})/\partial t$ is given by (2.14).

Noting that

$$\sum_{k=1}^{NLEV} \Delta B_k = 1\ ,$$

and including the semi-implicit correction terms, the semi-Lagrangian discretization of the continuity equation finally becomes

$$(\ln p_{\mathrm{surf}})^{+} = \sum_{k=1}^{NLEV} \Delta B_k \left[(\ln p_{\mathrm{surf}})^{-} + 2\Delta t\left\{\frac{\partial(\ln p_{\mathrm{surf}})}{\partial t} + \mathbf{v}_k.\nabla \ln p_{\mathrm{surf}}\right\}^{0} - \frac{\beta\Delta t}{p_{\mathrm{surf}}^{\mathrm{ref}}}\,\Delta_{tt}\left\{\sum_{j=1}^{NLEV}(\Delta p_j^{\mathrm{ref}} D_j)\right\}\right] \tag{3.23}$$

(Since there is no vertical advection term in (3.23), no modification is required for the vertically non-interpolating scheme). It is important to bear in mind that each contribution to the sum on the right-hand side of (3.23) involves a different trajectory. The interpolations for $(\ln p_{\mathrm{surf}})^{-}$ and the semi-implicit correction terms are however two-dimensional, since these quantities are independent of vertical level. The $\{\ \}^{0}$ term is evaluated at the midpoint of the trajectory, and requires a three-dimensional interpolation.

In summary, the semi-Lagrangian discretization is given by Equations (3.14)–(3.16)together with (3.23).

3.5 Comparison with other schemes

The semi-Lagrangian formulation presented above differs in some respects from those proposed by other authors. Perhaps the most notable difference lies in the treatment of the conversion ω term in the thermodynamic equation (3.15), and of the right-hand side of the continuity equation (3.23). Both involve terms of the form $\mathbf{v}.\nabla \ln p_{\mathrm{surf}}$, which in our scheme are computed in a purely Eulerian fashion. This may appear somewhat inconsistent; indeed *McDonald and Haugen* (1993) state as a specific design objective of their scheme that the operator $\mathbf{v}.\nabla$ should not appear explicitly. The alternative approach, also taken by *Williamson and Olson* (1994), is to use the continuity equation in its semi-implicit semi-Lagrangian form to derive a consistent equation for *predicting* $\dot{\eta}\partial p/\partial\eta$, which can then be used to eliminate the $\mathbf{v}.\nabla \ln p_{\mathrm{surf}}$ terms. In the σ-coordinate system, *Bates et al*. (1993) and *McDonald and Haugen* (1992) used a similar approach to derive a prognostic equation for $\dot{\sigma}$. A possible disadvantage of such an approach is that $\dot{\eta}\partial p/\partial\eta$ (or $\dot{\sigma}$) then follows an independent evolution, no longer satisfying a diagnostic relationship of the form (2.18). Our 'Eulerian' treatment of the $\mathbf{v}.\nabla \ln p_{\mathrm{surf}}$ terms avoids this disadvantage and seems to work well, but further study is required to determine whether this difference in formulation is important or not.

Another aspect of our semi-Lagrangian discretization of the continuity equation, which differs from that in other models, concerns the definition of the trajectory; in our scheme this is the same (three-dimensional) trajectory as used for the other variables. In the continuous form of the equation, (3.19), the advective part of the total derivative $\mathrm{d}p/\mathrm{d}t$ may be regarded either as two-dimensional or as three-dimensional (since $\partial p_{\mathrm{surf}}/\partial\eta$ is zero). However the vertically discretized form, (3.20), is well-defined only at discrete model levels, implying that for consistency the semi-Lagrangian discretization (3.23) should be based on horizontal trajectories. Correcting this inconsistency in our scheme by computing horizontal trajectories for the continuity equation, based on the horizontal wind at each model level, made very little difference to the results, and for the time being we have allowed the inconsistency to remain. (As discussed later, in the case of the 'vertically non-interpolating' scheme the modified trajectories are nearly always horizontal anyway.) In the case of the fully interpolating scheme, recomputing the trajectories represents a significant expense; *Bates et al.* (1993) and *McDonald and Haugen* (1992) used a simple projection of the three-dimensional trajectory onto the model level of the arrival point. In our model this approach resulted in poor mass conservation, though *Bates et al.* (1993) came to the opposite conclusion. Again, the importance or otherwise of these differences in formulation is not yet firmly established.

3.6 TIME-STEPPING PROCEDURE

The general outline of the time-stepping procedure for the semi-Lagrangian version is similar to that described for the Eulerian model in Subsection 2.2.5. Thus at the start of a timestep, the model state at time $(t-\Delta t)$ is defined by the values of U, V, T, q and $\ln p_{\mathrm{surf}}$ on the Gaussian grid. To complete the semi-implicit corrections, the $(t-\Delta t)$ values of D, $\partial p/\partial\lambda$ and $\partial p/\partial\mu$ are also held on the grid. The model state at time t is defined by the spectral coefficients of ζ, D, T, q and $\ln p_{\mathrm{surf}}$. Legendre transforms followed by Fourier transforms are then used to compute D, U, V, T, $\partial T/\partial\mu$, q, $\partial q/\partial\mu$, $\ln p_{\mathrm{surf}}$, and $\partial(\ln p_{\mathrm{surf}})/\partial\mu$ at time t on the model grid; additional Fourier transforms are used to compute the corresponding values of $\partial T/\partial\lambda$, $\partial q/\partial\lambda$, and $\partial(\ln p_{\mathrm{surf}})/\partial\lambda$. Since ζ and the horizontal gradients of U and V are no longer required on the model grid, one multi-level Legendre transform and three multi-level Fourier transforms are saved in comparison with the Eulerian version.

Since the advection of moisture is handled by the semi-Lagrangian discretization (3.16), the horizontal gradients of q are only needed in order to compute the horizontal gradients of the virtual temperature T_{v} (which in turn are required to compute the $\nabla\phi$ term in (3.14)). If T_{v} is chosen as the spectral variable as in Subsection 2.2.8, these gradients are available directly, and there is then no need to transform $\partial q/\partial\mu$ (or $\partial q/\partial\lambda$) to the model grid. The number of multi-level Legendre transforms per time-step is further reduced to 10. In passing, all the ingredients are then in place for a semi-Lagrangian treatment in which the moisture field is never transformed to spectral space (*Williamson and Rasch*, 1994), and only 8 multi-level Legendre transforms are required per time-step (compared with 17 in the original $\zeta-D$ Eulerian model).

After the transforms to the model grid, all the information is then available to compute the trajectories for each grid point, and to evaluate the 'dynamical' contributions to the semi-Lagrangian discretization. Ignoring for a moment the contributions of the physical parametrization schemes and of the horizontal diffusion, each equation is either of the form

$$\tilde{X}^{+}(\tilde{x}) = \tilde{X}^{-}(\tilde{x}-2\tilde{\alpha}) + \Delta t\{\tilde{R}^{0}(\tilde{x}-2\tilde{\alpha}) + \tilde{R}^{0}(\tilde{x})\} + \tilde{S}^{-}(\tilde{x}-2\tilde{\alpha}) + \tilde{S}^{+}(\tilde{x}) \quad . \tag{3.24}$$

or

$$X^{+}(x) = X^{-}(x-2\alpha) + 2\Delta t R^{0} + S^{-}(x-2\alpha) + S^{+}(x) \tag{3.25}$$

depending on whether the R^0 terms are averaged between the end points of the trajectory or evaluated at the mid-points. In (3.24) and (3.25), the S terms represent the semi-implicit corrections; S^- includes contributions from time-levels $(t-\Delta t)$ and t, while S^+ includes contributions from time-levels t and $(t+\Delta t)$.

In the first part of the calculation for equations of the form (3.24), the combined field $X^+ + \Delta t R^0 + S^-$ is computed, and the value of this combined field at each departure point $(x-2\alpha)$ is then found by interpolation. Adding the (uninterpolated) value of $\Delta t R^0$ results in a provisional value of $\tilde{X}^+$ at each grid point, incorporating all the terms in (3.24) except for S^+. The calculation for equations of the form (3.25) proceeds similarly, except that two interpolations are required, one for $X^- + S^-$ at $(x-2\alpha)$, and one for $2\Delta t R^0$ at $(x-\alpha)$

A provisional value X^+ is now available at each grid point for each variable, and is used together with X^- at the same grid point to compute an 'Eulerian' tendency. These fields and their tendencies are then supplied to the physical parametrization routines, which increment the tendencies with their respective contributions, just as in the Eulerian version (except that, to avoid extra interpolations, the S^- terms have been included in the supplied dynamical tendencies). If T_{v} is chosen as the spectral variable, a provisional value of T_{v}^{+} is computed at this point.

The contributions from the S^- terms at time t are now added in, resulting in a set of equations of the form

$$U^{+} + \frac{\beta\Delta t}{a}\frac{\partial p^{+}}{\partial\lambda} = Q_1 \tag{3.26}$$

$$V^{+} + \frac{\beta\Delta t}{a}\cos\theta\frac{\partial p^{+}}{\partial\theta} = Q_2 \tag{3.27}$$

$$T^{+} + \beta\Delta t[\tau]D^{+} = Q_3 \tag{3.28}$$

$$q^{+} = Q_4 \tag{3.29}$$

$$(\ln p_{\mathrm{surf}})^{+} + \beta\Delta t[\nu]D^{+} = Q_5 \tag{3.30}$$

where the right-hand sides $Q_1 - Q_5$ include all the terms which have been computed on the grid, and T_{v}^{+} replaces T^+ if T_{v} is the spectral variable. Equations (3.26)–(3.30) have exactly the same form as Eqs. (2.40)–(2.44) of the Eulerian model and are solved in exactly the same way, by first transforming to spectral space. After finding the new spectral coefficients at time $(t+\Delta t)$, horizontal diffusion is also applied in the same way as for the Eulerian version.

The implementation of the time-filtering for the semi-Lagrangian model is identical to that for the Eulerian version, as described in Subsection 2.2.6

3.7 Optimization of vertically non-interpolating scheme

In the 'vertically non-interpolating' scheme, the departure point of each modified trajectory lies on a model level. For the set of arrival points on each model level, it is of interest to determine the frequency distribution of the corresponding departure points. The results of an experiment run to collect these statistics led to a significant optimization of the code for the vertically non-interpolating scheme.

The statistics were obtained from a 10-day forecast using the model in its operational configuration: T213, 31 levels, with a 15-minute timestep. The results are summarized in Table 3.1, which shows that the vast majority (99.67% overall) of modified trajectories are horizontal; no departure point was ever more than three model levels away from its corresponding arrival point.

The implication of these results is that a great deal of redundant calculation was being performed in the vertically non-interpolating scheme. For each horizontal modified trajectory, the interpolation of the horizontal winds in the trajectory calculation itself becomes two-dimensional rather than three-dimensional, as do the interpolations of 'right-hand side' terms at the mid point of the trajectory, while the additional interpolations to calculate terms of the form $\dot{\eta}^*(\partial X/\partial\eta)^0$ in (3.12) are not required at all. Consequently, special routines were written to perform interpolations which are two-dimensional everywhere except at a set of 'flagged' points where they become three-dimensional, and similarly to perform two- or three-dimensional interpolations at the flagged points while skipping all other points. The use of these special routines reduced the 'semi-Lagrangian overhead' for the vertically non-interpolating scheme by about 30%.

TABLE 3.1 FREQUENCY DISTRIBUTION (%) OF DEPARTURE POINTS IN THE 'VERTICALLY NON-INTERPOLATING' SCHEME

Arrival level k	Departure levels			
	k	$k \pm 1$	$k \pm 2$	$k \pm 3$
1–6	100.00			
7–9	100.00	*		
10	99.99	0.01	*	
11	99.96	0.04	*	
12	99.89	0.11	*	
13	99.76	0.24	*	*
14	99.60	0.40	*	*
15	99.43	0.57	*	*
16	99.28	0.72	*	
17	99.16	0.83	0.01	
18	99.08	0.92	*	
19	99.05	0.94	0.01	
20	99.05	0.94	0.01	*
21	99.09	0.91	*	*
22	99.14	0.85	0.01	*
23	99.22	0.78	*	
24	99.31	0.69	*	
25	99.44	0.56	*	
26	99.60	0.40	*	
27	99.78	0.22	*	
28	99.92	0.08	*	
29	99.99	0.01		
30	100.00	*		
31	100.00			

Asterisks indicate less than 0.005% frequency

3.8 MODIFIED SEMI-LAGRANGIAN EQUATIONS

3.8.1 Momentum equations

The momentum equations are treated in vector form (Eq. (3.14)). Following Rochas (1990) and Temperton (1997), the Coriolis terms can be incorporated in the semi-Lagrangian advection. Thus, the advected variable becomes $\underset{\sim}{v}_H + 2\underset{\sim}{\Omega} \times \underset{\sim}{r}$ where Ω is the earth's rotation and r is the radial position vector, while the Coriolis terms are dropped from the right-hand side. As described by Temperton (1997), this reformulation is beneficial provided that the spherical geometry is treated accurately in determining the departure point and in rotating the vectors to account for the change in the orientation of the coordinate system as the particle follows the trajectory.

The discretization of the momentum equations in the notation of Eq. (3.1) is then:

$$X = \underset{\sim}{v}_{\mathrm{H}} + 2\underset{\sim}{\Omega} \times \underset{\sim}{r} \tag{3.31}$$

$$L = -\underset{\sim}{\nabla}(\underline{\gamma} T_{\mathrm{v}} + R_{\mathrm{dry}} T_{\mathrm{ref}} \ln p_{\mathrm{surf}}) \tag{3.32}$$

$$N = -(\nabla\phi + R_{\mathrm{dry}} T_{\mathrm{v}} \nabla \ln p) - L \tag{3.33}$$

where R_{dry} is the gas constant for dry air, T_{ref} is a reference temperature, ϕ is geopotential and $\underline{\gamma}$ is the linearized hydrostatic integration matrix defined in Eq. (2.32) of Ritchie (1995).

In component form, $2\Omega \times r$ is just $(2\Omega a \cos\theta,\ 0)$ where a is the earth's radius and θ is latitude. Since the latitude of the departure point is known, the term $2\Omega \times r$ in the advected variable X is computed analytically rather than interpolated. An alternative semi-implicit treatment of the Coriolis terms has also been developed (Temperton 1997).

3.8.2 Continuity equation

Modelling flow over mountains with a semi-Lagrangian integration scheme can lead to problems in the form of a spurious resonant response to steady orographic forcing. The mechanism was clarified by Rivest et al. (1994). Strictly speaking, the problem has little to do with the semi-Lagrangian scheme itself; rather, it is a result of the long time steps permitted by the scheme, such that the Courant number becomes greater than 1. Recently, Ritchie and Tanguay (1996) proposed a modification to the semi-Lagrangian scheme which alleviates the problem. It turned out that their suggestion was easy to implement in the ECMWF model, and had additional benefits besides improving the forecast of flow over orography.

Although Ritchie and Tanguay start by introducing a change of variables in the semi-implicit time discretization, this is not necessary and a slightly different derivation is presented here. The continuity equation is written in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{surf}}) = [RHS] \tag{3.34}$$

where $[RHS]$ represents right-hand-side terms. The total derivative on the left-hand side is discretized in a semi-Lagrangian fashion, and the final form of the discretized equation involves a vertical summation.

Now split $\ln p_s$ into two parts:

$$\ln p_{\mathrm{surf}} = l^* + l' \tag{3.35}$$

where the time-independent part l^* depends on the underlying orography ϕ_{surf}:

$$l^* = (-\phi_{\mathrm{surf}})/(R_{\mathrm{dry}}\bar{T}) \tag{3.36}$$

and $\bar{T}$ is a reference temperature. This choice gives

$$\nabla\phi_{\mathrm{surf}} + R_{\mathrm{dry}}\bar{T}\nabla l^* = 0 \tag{3.37}$$

so that l^* is (to within an additive constant) the value of $\ln p_{\mathrm{surf}}$ appropriate for an isothermal state at rest with underlying orography.

Using (3.35) and (3.36),

$$\frac{\mathrm{d}}{\mathrm{d}t}((\ln p_{\mathrm{surf}})) = \frac{\mathrm{d}l'}{\mathrm{d}t} - \left(\frac{1}{R_{\mathrm{dry}}\bar{T}}\underset{\sim}{v}_{\mathrm{H}} \cdot \nabla\phi_{\mathrm{surf}}\right) \tag{3.38}$$

The second term on the right-hand side is computed in an Eulerian manner and transferred to the right-hand side of the continuity equation (3.34), which becomes

$$\frac{\mathrm{d}l'}{\mathrm{d}t} = [RHS] + \frac{1}{R_{\mathrm{dry}}\bar{T}}\underset{\sim}{v}_{\mathrm{H}} \cdot \nabla\phi_{\mathrm{surf}} \tag{3.39}$$

The new advected variable is much smoother than the original, since the influence of the underlying orography has been subtracted out; hence, the semi-Lagrangian advection is presumably more accurate.

3.8.3 Thermodynamic equation

As mentioned above, the semi-Lagrangian treatment of the continuity equation is improved by changing the advected variable to a smoother quantity which is essentially independent of the underlying orography. A similar modification has been implemented in the thermodynamic equation, borrowing an idea from the treatment of horizontal diffusion. To approximate horizontal diffusion on pressure surfaces, thereby avoiding spurious warming over mountain tops in sigma or hybrid vertical coordinates, the diffused quantity is $(T - T_{\mathrm{c}})$, with

$$T_c = \left(p_{\mathrm{surf}}\frac{\partial p}{\partial p_{\mathrm{surf}}}\frac{\partial T}{\partial p}\right)_{\mathrm{ref}} \ln p_{\mathrm{surf}} \tag{3.40}$$

where the subscript 'ref' denotes a reference value which is a function only of model level. For the purposes of the semi-Lagrangian advection $\ln p_{\mathrm{surf}}$ is replaced by a time-independent value as in Eq. (3.36) above, to define a "temperature" T_{b} which depends only on the model level and the underlying orography:

$$T_b = -\left(p_{\mathrm{surf}}\frac{\partial p}{\partial p_{\mathrm{surf}}}\frac{\partial T}{\partial p}\right)_{\mathrm{ref}} \cdot \phi_{\mathrm{surf}}/(R_{\mathrm{dry}}\bar{T}) \tag{3.41}$$

The semi-Lagrangian advection is now applied to the quantity $(T - T_{\mathrm{b}})$, while a compensating expression

$$-\underset{\sim}{v}_{\mathrm{H}} \cdot \nabla T_{\mathrm{b}} - \dot{\eta}\frac{\partial T_{\mathrm{b}}}{\partial \eta} \tag{3.42}$$

appears on the right-hand side of the equation and is computed in an Eulerian fashion (note that this time it includes a vertical advection term).

3.9 Two-time-level semi-Lagrangian scheme

Formally, a two-time-level scheme may be written in the notation of Eq.(3.2) as:

$$\frac{X_A^+ - X_D^-}{\Delta t} = \frac{1}{2}(L_D^- + L_A^+) + \frac{1}{2}(N_D^* + N_A^*) \tag{3.43}$$

where

$X_A^+ = X(\underset{\sim}{x}, t + \Delta t)$ is the value at the "arrival" gridpoint at $(t + \Delta t)$

$X_D^- = X(\underset{\sim}{x} - \underset{\sim}{\alpha}, t)$ s the value interpolated at the "departure" point at time t;

L_A^+ and L_D^- are the linear terms defined similarly;

N^* are the non linear terms, obtained by extrapolation in time to $\left(t + \frac{1}{2}\Delta t\right)$

$$N^* = \frac{3}{2}N(t) - \frac{1}{2}N(t - \Delta t) \tag{3.44}$$

The displacement equation becomes

$$\underset{\sim}{\alpha} = \Delta t \underset{\sim}{V}^*\left(\underset{\sim}{x} - \frac{1}{2}\underset{\sim}{\alpha}, t + \frac{1}{2}\Delta t\right) \tag{3.45}$$

where the three-dimensional wind field V^* is also extrapolated in time:

$$\underset{\sim}{V}^* = \frac{3}{2}\underset{\sim}{V}(t) - \frac{1}{2}\underset{\sim}{V}(t - \Delta t) \tag{3.46}$$

The iterative scheme and first-guess for solving (3.45) are exactly analogous to those for solving (3.5).

The choices for the variables X and for the interpolation schemes remain exactly as for the three-time-level scheme.

The semi-implicit equations to be solved in spectral space have the same form as for the three-time-level scheme, except that Δt is replaced by $\Delta t / 2$.

In principle a two-time-level scheme should have no $2\Delta t$ computational mode, and a time-filtering procedure is no longer needed.

3.9.1 Stable Extrapolation Two-Time-Level Scheme (SETTLS)

An alternative second-order accurate scheme to solving (3.45) can be derived by expanding the position vector $\vec{R}$ of the parcel of air as a Taylor series around the departure point of the semi-Lagrangian trajectory:

$$\vec{R}_{\mathrm{A}}^{t+\Delta t} \approx \vec{R}_{\mathrm{D}}^{t} + \Delta t \cdot \left[\frac{\mathrm{d}}{\mathrm{d}t}\vec{R}\right]_{\mathrm{D}}^{t} + \frac{\Delta t^2}{2} \cdot \left[\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\vec{R})\right]_{\mathrm{AV}} \tag{3.47}$$

Here subscript AV indicates some average value along the semi-Lagrangian trajectory.

Substituting the time derivative of $\vec{R}$ by the velocity vector $\vec{V}$, we find

$$\vec{R}_{\mathrm{A}}^{t+\Delta t} \approx \vec{R}_{\mathrm{D}}^{t} + \Delta t \cdot \vec{V}_{\mathrm{D}}^{t} + \frac{\Delta t^2}{2} \cdot \left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]_{\mathrm{AV}} \tag{3.48}$$

This equation describes an uniformly accelerated movement. The trajectories can no longer be considered as straight lines on a plane or as arcs of a great circle in spherical geometry as is traditionally done in semi-Lagrangian schemes and the position of the middle point of the trajectory is no longer an average between the departure and the arrival points.

To proceed, one has to estimate the quantity

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]_{\mathrm{AV}} \tag{3.49}$$

To estimate (3.49) the first possibility explored was to use an average along the trajectory of the explicit estimate of the r.h.s. of the momentum equations as the horizontal part of expression (3.49) and the expression

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(W)\right]_{\mathrm{AV}} \approx \frac{W_{\mathrm{A}}^{t} - W_{\mathrm{D}}^{t-\Delta t}}{\Delta t} \tag{3.50}$$

for the vertical part.

After exploring many other possibilities, the following estimate was adopted:

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]_{\mathrm{AV}} \approx \left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]^{t-\frac{\Delta t}{2}} \approx \frac{\vec{V}_{\mathrm{A}}^{t} - \vec{V}_{\mathrm{D}}^{t-\Delta t}}{\Delta t} \tag{3.51}$$

using the departure point of the semi-Lagrangian trajectory corresponding to the present time step instead of the departure point of the trajectory corresponding to the previous time step. Here D means the position at time t of the parcel of air which will arrive to gridpoint A at time t+Δt.

This estimate assumes that the total time derivative of the velocity is constant with time, following Durran's suggestion of "extrapolating along the trajectory", but the estimate uses only the arrival and departure points of the present trajectory and is therefore compatible with the semi-implicit treatment of the evolution equations. This scheme should therefore be also stable according to linear stability analysis and has accordingly been named "Stable Extrapolation Two-Time-Level Scheme" or SETTLS.

Substituting (3.51) into (3.48) we obtain:

$$\vec{R}_{\mathrm{A}}^{t+\Delta t} = \vec{R}_{\mathrm{D}}^{t} + \frac{\Delta t}{2} \cdot \left(\left[2\vec{V}^{t} - \vec{V}^{t-\Delta t}\right]_{\mathrm{D}} + \vec{V}_{\mathrm{A}}^{t}\right) \tag{3.52}$$

and a similar expression can be used in every evolution equation to treat the non-linear terms of the r.h.s.

3.10 NUMERICAL COUPLING OF THE PHYSICAL PARAMETERIZATIONS TO THE "DYNAMICAL" EQUATIONS (SLAVEPP)

Due to the diffusive nature of the mostly parabolic equations in the physics the contributions of the physical parameterizations are computed separately from the "dynamical" equations. The coupling of these two parts can use the *SLAVEPP* (*Semi-Lagrangian Averaging of Physical Parameterizations)* method which is described and discussed in detail by *Wedi* (1999).

In equation (3.14)-(3.16) the contribution of the physical parameterizations are denoted as P indicating an evaluation of the parameterizations at the arrival point only. In the two time level scheme as described in section 3.9 this is replaced by a partly second order accurate coupling of the parameterizations in time and space, which is achieved by evaluating part of the "physics" at the arrival point and the remainder at the departure point of the semi-Lagrangian trajectory. Due to the different nature of the parameterized processes the contributions of radiation, convection and cloud parameterization are averaged "along" the semi-Lagrangian trajectory while the contributions of vertical diffusion and parameterized gravity waves are taken at the arrival point only. Equation (3.43) becomes then

$$\frac{X_{\mathrm{A}}^{+} - X_{\mathrm{D}}^{-}}{\Delta t} = \frac{1}{2}(L_{\mathrm{D}}^{-} + L_{\mathrm{A}}^{+}) + \frac{1}{2}(N_{\mathrm{D}}^{*} + N_{\mathrm{A}}^{*}) + \frac{1}{2}(P_{\mathrm{D,\,rad+conv+cloud}}^{-} + P_{\mathrm{A,\,rad+conv+cloud}}^{+}) + P_{\mathrm{A,\,vdif+gwdrag}}^{+} \qquad (3.53)$$

Part of the implicit calculations of the physical parameterizations use the following tendency:

$$\tilde{D}_{\mathrm{A}} = \frac{\tilde{X}_{\mathrm{A,\,Dyn}}^{+} - X_{\mathrm{A}}^{-}}{\Delta t}\,, \qquad (3.54)$$

with equation (3.43) modified to yield

$$\frac{\tilde{X}_{A,\,Dyn}^{+} - X_{D}^{-}}{\Delta t} = \frac{1}{2}(L_{D}^{-} + \tilde{L}_{A}^{+}) + \frac{1}{2}(N_{D}^{*} + N_{A}^{*}) \qquad (3.55)$$

The "~" denotes that only provisional values of the dynamic fields are available because semi-implicit correction terms are still to be computed (see section 3.6). Therefore $L_{A}^{+} \approx \tilde{L}_{A}^{+} = L_{A}^{-}$ is used for the linear terms. Equation (3.54) describes local tendencies, which are computed subtracting the new provisional explicit values $\tilde{X}_{A,\,Dyn}^{+}$ of the dynamic fields (at the arrival point) from their values X_{A}^{-} at the previous time step. The parameterizations at the time step $t + \Delta t$ are computed at the arrival point as shown in the following equation:

$$\begin{aligned} P_{A}^{+} = {} & P_{A,\,\mathrm{rad}}^{+}(X_{A}^{-}) \\ & + P_{\mathrm{A,\,vdif}}^{+}(X_{\mathrm{A}}^{-}, \tilde{D}_{\mathrm{A}}, P_{\mathrm{A,\,rad}}^{+}) \\ & + P_{\mathrm{A,\,gwdrag}}^{+}(X_{\mathrm{A}}^{-}, \tilde{D}_{\mathrm{A}}) \\ & + P_{\mathrm{A,\,conv}}^{+}(X_{\mathrm{A,\,predict}}^{+}, (output)F_{\mathrm{conv}}) \\ & + P_{\mathrm{A,\,cloud}}^{+}(X_{\mathrm{A,\,predict}}^{+}, (input)F_{\mathrm{conv}}) \end{aligned} \qquad (3.56)$$

where the “first guess” predictor $X^{+}_{\mathrm{A,\,predict}}$ of the model variables at the arrival point at time step $t + \Delta t$ is computed from the tendency of the “dynamics”, the tendency of the parameterizations of radiation, convection and clouds at the previous time-step t and the tendency of vertical diffusion and gravity waves at $t + \Delta t$:

$$X^{+}_{\mathrm{A,\,predict}} = \tilde{X}^{+}_{\mathrm{A,\,Dyn}} + \alpha \bar{P}_{\mathrm{D,\,rad}+conv+cloud}\Delta t + P^{+}_{\mathrm{A,\,vdif+gwdrag}}\Delta t \;. \qquad (3.57)$$

F_{conv} denotes an explicit interaction of the parameterizations of cloud and convection.The parameter $\alpha = 0.5$ has been introduced in order to achieve a better balance between the physical parameterizations when the “first guess” predictor is computed.

3.10.1 Moisture adjustment and first time-step treatment

The parametrizations of cloud and convection show a sensitivity to the initial profiles. Therefore, at the initial time-step of the model “first guess” predictors are generated by a two step iteration of the parametrizations of cloud and convection consistent with the provisional dynamic fields as described above.

The effective profiles of temperature and humidity (including all contributions from the departure as well as the arrival point) are computed after all physical processes have been accounted for. A final moist adjustment is performed on these effective profiles and any amount of surplus humidity is added to the rainfall or snow fluxes in the next time-step. Note, that after this adjustment the temperature profile may still be altered as a result of the semi-implicit solution procedure.

Part III: DYNAMICS AND NUMERICAL PROCEDURES

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