IFS DOCUMENTATION – Cy47r1
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PART III: DYNAMICS AND NUMERICAL PROCEDURES

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REVISION HISTORY

Changes since Cy43r3

- Section 3.7.3 extended by paragraph describing the actual code implementation.

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 were 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.

1.2 STRUCTURE OF DOCUMENT

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.

Chapter 2
Basic equations and discretisation

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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 $\zeta - D$ (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 $\eta(p, p_s)$ is a monotonic function of the pressure p, and also depends on the surface pressure p_s in such a way that

$$\eta(0, p_s) = 0 \quad \text{and} \quad \eta(p_s, p_s) = 1$$

The momentum equations are

$$\frac{\partial U}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial U}{\partial \lambda} + V\cos\theta\frac{\partial U}{\partial \theta}\right\} + \dot{\eta}\frac{\partial U}{\partial \eta} - fV + \frac{1}{a}\left\{\frac{\partial \phi}{\partial \lambda} + R_{\text{dry}}T_v\frac{\partial}{\partial \lambda}(\ln p)\right\} = P_U + K_U \qquad (2.1)$$

$$\frac{\partial V}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial V}{\partial \lambda} + V\cos\theta\frac{\partial V}{\partial \theta} + \sin\theta(U^2 + V^2)\right\} + \dot{\eta}\frac{\partial V}{\partial \eta} + fU + \frac{\cos\theta}{a}\left\{\frac{\partial \phi}{\partial \theta} + R_{\text{dry}}T_v\frac{\partial}{\partial \theta}(\ln p)\right\} = P_V + K_V \qquad (2.2)$$

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

$$T_v = T[1 + \{(R_{\text{vap}}/R_{\text{dry}}) - 1\}q]$$

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

The thermodynamic equation is

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

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

The moisture equation is

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

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

The continuity equation is

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

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

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

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

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

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

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 $\eta=1$

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

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

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

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

2.2 DISCRETISATION

2.2.1 Original vertical discretisation

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 Simmons and Strufing (1983)

$$p_{k+1/2}=A_{k+1/2}+B_{k+1/2}p_{\rm s} \tag{2.11}$$

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

The values of the $A_{k+1/2}$ and $B_{k+1/2}$ for all $0 \leq k \leq NLEV$ 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 $p_k = \frac{1}{2}(p_{k-1/2} + p_{k+1/2})$ with $1 \leq k \leq NLEV$ 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

$$\frac{\partial}{\partial t}(\ln p_s) = -\frac{1}{p_s}\sum_{k=1}^{NLEV} \nabla \cdot (\mathbf{v}_k \Delta p_k) \tag{2.12}$$

where

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

From (2.11) we obtain

$$\frac{\partial}{\partial t}(\ln p_s) = -\sum_{k=1}^{NLEV} \left\{ \frac{1}{p_s} D_k \Delta p_k + (\mathbf{v}_k \cdot \nabla \ln p_s) \Delta B_k \right\} \tag{2.14}$$

where D_k is the divergence at level k given by

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

and

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

The discrete analogue of (2.9) is

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

and from (2.11) we obtain

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

where $\partial/\partial t(\ln p_s)$ 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

$$\phi_{k+1/2} - \phi_{k-1/2} = -R_{\mathrm{dry}} (T_v)_k \ln\left(\frac{p_{k+1/2}}{p_{k-1/2}} \right) \tag{2.20}$$

which gives

$$\phi_{k+1/2} = \phi_s + \sum_{j=k+1}^{NLEV} R_{\mathrm{dry}} (T_v)_j \ln\left(\frac{p_{j+1/2}}{p_{j-1/2}} \right) \tag{2.21}$$

where ϕ_s 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

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

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

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

with α_k given by (2.23) for all k.

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

$$\left(\frac{\kappa T_v \omega}{(1+(\delta-1)q)p}\right)_k = \frac{\kappa(T_v)_k}{1+(\delta-1)q_k}\left\{-\frac{1}{\Delta p_k}\left[\ln\left(\frac{p_{k+1/2}}{p_{k-1/2}}\right)\sum_{j=1}^{k-1}(D_j \Delta p_j + p_s(\mathbf{v}_j \cdot \nabla \ln p_s)\Delta B_j)\right.\right.$$
$$\left.\left. + \alpha_k(D_k \Delta p_k + p_s(\mathbf{v}_k \cdot \nabla \ln p_s)\Delta B_k)\right] + \frac{p_s}{\Delta p_k}\left[\Delta B_k + \frac{C_k}{\Delta p_k}\ln\left(\frac{p_{k+1/2}}{p_{k-1/2}}\right)\right](\mathbf{v}_k \cdot \nabla \ln p_s)\right\} \tag{2.25}$$

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 discretisation 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 discretisation

In Cy24r3 the vertical discretisation was changed in the operational model from the finite-difference discretisation in Lorenz staggering described in the previous subsection to a finite-element discretisation using cubic B-splines as basis functions.

For the finite-element (FE) discretisation, 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 $\partial p/\partial\eta = (\mathrm{d}A/\mathrm{d}\eta) + (\mathrm{d}B/\mathrm{d}\eta)p_s$. 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

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

The two conditions of (2.28) 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 (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 that have to be evaluated 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 (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 $A\tilde{C} = B\tilde{c} \Rightarrow \tilde{C} = A^{-1}B\tilde{c}$.

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 (2004).

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 discretisation).

2.2.3 Time discretisation

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

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

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 Chapter 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, (2.1) to (2.4) become:

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

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

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

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

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 linearised versions of the pressure gradient terms in (2.1) and (2.2) and the energy conversion term in (2.3). Thus $T^{\rm ref}$ is a reference temperature (here chosen to be independent of vertical level), while $[\gamma]$ and $[\tau]$ are matrices such that

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

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

where the half-level pressures appearing in (2.35) and (2.36) are reference values obtained from (2.11) by choosing a reference value $p_{\rm s}^{\rm ref}$ of $p_{\rm s}$, and the coefficients $\alpha_k^{\rm ref}$ are based on these reference values. The reference values adopted for the semi-implicit scheme are $T^{\rm ref} = 300$ K and $p_{\rm s}^{\rm ref} = 800$ hPa.

The integrated surface pressure tendency equation (2.14) becomes

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

where

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

2.2.4 The fast spectral transform method in IFS

The spectral transform method has been successfully applied at ECMWF for more than thirty years, with the first spectral model introduced into operations in April 1983. The spectral transform method was introduced to numerical weather prediction following the work of Eliasen *et al.* (1970)) and Orszag (1970) who achieved high efficiency by alternating the computations between a grid-point and a spectral representation at every time step.

In IFS, the horizontal wind, the virtual temperature and the surface pressure are transformed to spectral space and back to grid-point space at every time-step. All the water variables and the passive tracers, e.g. specific humidity and prognostic cloud and precipitation are kept in grid-point space because they are not needed for any of the computations in spectral space and because the spectral transforms can violate positiveness of the transformed field, in particular for non-smooth fields.

A direct spherical harmonics transformation of a field $X(\lambda, \mu)$ where λ is the longitude and μ the sinus of the latitude θ, is a Fourier transformation in longitude

$$X_m(\mu) = \frac{1}{2\pi} \int_0^{2\pi} X(\lambda, \mu) e^{-im\lambda} d\lambda \tag{2.39}$$

followed by a Legendre transformation in latitude of each Fourier coefficients at zonal wavenumber m $X_m(\mu)$ as

$$X_n^m = \frac{1}{2} \int_{-1}^{1} X_m(\mu) \overline{P}_n^m(\mu) d\mu. \tag{2.40}$$

where $\overline{P}_n^m(\mu)$ is the normalised associated Legendre polynomial for the zonal wavenumber m and the total wavenumber n. The discrete Fourier transform is computed numerically very efficiently by using a fast Fourier transform (FFT). The discrete Legendre transforms require the accurate discrete computation of the integral in (2.40) which is accomplished by a Gaussian quadrature

$$X_n^m = \sum_{k=1}^{N_{\text{lat}}} w_k X_m(\mu_k) \overline{P}_n^m(\mu_k) \tag{2.41}$$

at N_{lat} special quadrature points. Mathematically, the μ_k are the roots of the ordinary Legendre polynomials, which, in the context of IFS, are used to compute the N_{lat} latitudes of the Gaussian grid between the two poles.

The inverse discrete Legendre and Fourier transforms using a triangular spectral truncation N (i.e. $0 \le n \le N$ and $-n \le m \le n$) return a field in grid-point space

$$\tilde{X}(\lambda, \mu) = \sum_{n=0}^{N} \sum_{-n \le m \le n} X_n^m \overline{P}_n^m(\mu) e^{im\lambda}$$

The maximum truncation for a given N_{lat} is $N = N_{\text{lat}} - 1$, i.e. the smallest wavenumber has to be described by a minimum of 2 grid points (linear discretisation), so as not to be misinterpreted as a larger wavenumber by aliasing. $\tilde{X}(\lambda, \mu) \simeq X(\lambda, \mu)$ if $N = N_{\text{lat}} - 1$, otherwise the spectral transforms eliminate any inadequate variance corresponding to wavenumbers $N < n \le N_{\text{lat}} - 1$ outside the spectral truncation as, for example, for the cubic discretisation, where $N = N_{\text{lat}}/2 - 1$.

Recent concerns about the computational cost of the Legendre transform have been mitigated by a fast Legendre transform which exploits similarities of the associated Legendre polynomials to simplify the computations (Wedi *et al.*, 2013). Further computational acceleration can be expected from using modern hardware accelerator technologies. However, the parallel communications involved in the data transfer within transpositions from grid-point space to spectral space and back, at every time-step of the model, remain a concern on future computing architectures (Wedi *et al.*, 2015).

2.2.5 Horizontal grid

The accuracy of the transformation from grid-point space to spectral space and back is assured if the grid is a Gaussian grid, i.e. characterised by N specially determined quadrature points along a meridian between the pole and the equator (the 'Gaussian latitudes'), and their associated 'Gaussian quadrature weights' used to compute the spectral coefficients (section 2.2.4).

The choice for the number of grid points in the zonal direction at each latitude circle is more flexible. If the same number of points is used for each latitude circle in a full Gaussian grid, the zonal resolution near the poles is substantially higher than the zonal resolution at the equator. Such a configuration generates a strong anisotropy of the discrete horizontal representation of the fields, potentially risks numerical instabilities, and carries a significant computational cost due to the large number of points near the poles. Since 1991, ECMWF has used a reduced grid (Hortal and Simmons, 1991), in which the number of points on each latitude circle is reduced towards the poles, keeping the relative grid-point distances approximately constant. This reduction lowers the number of points by approximately 30% without significant loss of meteorological accuracy in the spectral transforms. A new method to reduce

the number of grid points towards the poles was explored for the horizontal resolution upgrade of the IFS which took place in March 2016, both to optimize the total number of points around the globe and to introduce a regular reduction of the number of points per latitude circle towards the poles. The design of this grid is inspired by a regular triangular mapping onto an octahedron, which corresponds to a reduction of 4 points per latitude circle (one per face of the octahedron) starting from the equator and progressing towards the poles. The resulting grid is called the octahedral reduced Gaussian grid. The nominal resolution of the grid in the zonal direction is not as uniform around the globe as in the original reduced Gaussian grid, but the number of points per latitude circle is significantly lower (for the N = 1280 grid, the original reduced grid has about 8.5 million points against 6.5 million for the newer octahedral grid). In practice, this saves another 22% of total computation time. With the original reduced Gaussian grid, the number of points per latitude circle was constrained to be a multiple of 2, 3 and 5 by the FFT algorithm FFT992 originally developed at ECMWF (Temperton, 1983). The octahedral reduced Gaussian grid is used in the IFS together with the FFT package FFTW (`http://www.fftw.org/`), which efficiently allows any number of points per latitude circle.

2.2.6 Pairing an horizontal grid with a spectral truncation

Several choices can be made to pair the maximum wavenumber of the spectral truncation, N , with the number of latitude circles between the pole and equator, $N_{\rm lat}$, which characterises the Gaussian grid. In the so-called linear grid, $N_{\rm lat} = 2N - 1$. A spectral transform using a linear grid represents the smallest wavelength $2\pi a/N_{\rm lat}$ (a is the radius of the Earth) by 2 grid points. Two other choices are the quadratic grid and the cubic grid, which represent the smallest wavelength by 3 and 4 points, respectively. The names linear, quadratic and cubic stem from the ability of the different grids to accurately represent linear, quadratic and cubic products in the equations.

Until 1998, a quadratic grid was used in the IFS to avoid the aliasing resulting from the computation of the Eulerian advection. With the implementation of the semi-Lagrangian advection scheme, a linear grid was introduced to enable finer scales in the spectral representation for a given grid resolution. However, recent experience suggests that the importance of non-linear processes increases with increasing resolution, thus exacerbating the problem of aliasing and requiring computationally expensive de-aliasing filters to suppress poorly resolved or misrepresented motions (Wedi, 2014).

The resolution of the IFS is indicated by specifying the spectral truncation N prefixed by the acronym TL (for truncation-linear), TQ (for truncation-quadratic), TC (for truncation-cubic) or TCo (for truncation-cubic-octahedral). For example, the resolution of the high resolution forecast, HRES, in operation before March 2016 was TL1279 , a linear original reduced Gaussian grid truncated at $N = 1279$. After the resolution upgrade of March 2016, it became TCo1279 , a cubic octrahedral reduced Gaussian grid truncated at $N = 1279$.

2.2.7 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 $\ln p_{\rm s}$ 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

$$P = [\gamma]T + R_{\rm dry}T^{\rm ref}\ln p_{\rm s} \tag{2.42}$$

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

$$\cos\theta\frac{\partial V}{\partial\theta} = aD\cos^2\theta - \frac{\partial U}{\partial\lambda}$$
$$\cos\theta\frac{\partial U}{\partial\theta} = \frac{\partial V}{\partial\lambda} - a\zeta\cos^2\theta$$

All the information is then available to evaluate the terms at time t on the left-hand sides of (2.31) to (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 parameterisation 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) to (2.34) and (2.37) can be written in the form

$$U^+ + \frac{\beta\Delta t}{a}\frac{\partial P^+}{\partial\lambda} = R_1 \tag{2.43}$$

$$V^+ + \frac{\beta\Delta t}{a}\cos\theta\frac{\partial P^+}{\partial\theta} = R_2 \tag{2.44}$$

$$T^+ + \beta\Delta t[\tau]D^+ = R_3 \tag{2.45}$$

$$q^+ = R_4 \tag{2.46}$$

$$(\ln p_s)^+ + \beta\Delta t[\nu]D^+ = R_5 \tag{2.47}$$

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 (2.43) and (2.44) are then computed in spectral space, leading to

$$\zeta^+ = \mathrm{curl}(R_1, R_2) \tag{2.48}$$

$$D^+ + \beta\Delta t\nabla^2 P^+ = \mathrm{div}(R_1, R_2) \tag{2.49}$$

Equations (2.45), (2.47) and (2.49) can then be combined with the aid of (2.42) to obtain an equation of the form

$$\left([I] + \frac{n(n+1)}{a^2}[\Gamma]\right)(D_n^m)^+ = (\tilde{D})_n^m \tag{2.50}$$

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

$$[\Gamma] = \beta^2(\Delta t)^2([\gamma][\tau] + R_{\mathrm{dry}}T^{\mathrm{ref}}[\nu]) \tag{2.51}$$

couples all the $NLEV$ values of $(D_n^m)^+$ in a vertical column. Once D^+ has been found, the calculation of T^+ and $(\ln p_s)^+$ can be completed, while q^+ and ζ^+ have already been obtained from (2.46) and (2.48).

2.2.8 Time filtering

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

$$X_f = X + \varepsilon(X_f^- - 2X + X^+) \tag{2.52}$$

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 (2.52) into two parts:

$$\tilde{X}_f = X + \varepsilon(X_f^- - 2X) \tag{2.53}$$

$$X_f = \tilde{X}_f + \varepsilon X^+ \tag{2.54}$$

The 'partially filtered' values computed by (2.53) 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 (2.54), which after shifting by one timestep becomes:

$$X_f^- = \tilde{X}_f^- + \varepsilon X \tag{2.55}$$

The computations described in Subsection 2.2.7 are performed using these fully filtered values at time $(t-\Delta t)$ and the unfiltered values at time t. Once (2.55) has been implemented, values of X_f^- are also available to implement (2.53) for the partially filtered values to be passed on to the next timestep.

2.2.9 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 discretisation 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 $\ln p_s$), 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.

2.2.10 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, $\partial T_v/\partial\mu$ and $\partial T_v/\partial\lambda$ 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 parameterisation routines, the 'provisional' value of $T(t+\Delta t)$ is combined with $q(t+\Delta t)$ to compute a provisional value of $T_v(t+\Delta t)$. The semi-implicit correction terms evaluated at time-levels $(t-\Delta t)$ and t are then added to the provisional value of $T_v(t+\Delta t)$, just before the transform back to spectral space.

There are corresponding slight changes in the semi-implicit correction terms. The linearised hydrostatic matrix $[\gamma]$ in (2.31) and (2.32) and (2.42) 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

$$\delta_t T_v = \ldots - \frac{\beta}{2}\Delta_{tt}([\tau]D) \tag{2.56}$$

although as explained above it is not necessary to formulate or compute the missing terms explicitly. Hence, (2.45) is replaced by

$$T_v^+ + \beta\Delta t[\tau]D^+ = R_3' \tag{2.57}$$

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 Chapter 3.

2.2.11 Numerical filters

In the IFS, all the prognostic variables which are part of the semi-implicit solver are transformed to spectral space at the end of the time step. For linear, quadratic and cubic grids (see section 2.2.6 for definitions), the spectral truncation corresponds respectively to a $2\Delta x$, $3\Delta x$ or $4\Delta x$ spectral filter.

Additional numerical filters may be necessary, firstly to sufficiently dampen the accumulation of kinetic energy and enstrophy at the smallest resolved scales, secondly, to use as an effective absorber for vertically propagating gravity waves at the top of the model ("sponge"), and thirdly in the spirit of an eddy viscosity term to represent unresolved sub-gridscale mixing.

(*a*) *Implicit diffusion operators in spectral space*

A simple linear diffusion of order $2r$

$$\frac{[X]_{\text{after diff}} - [X]_{\text{before diff}}}{\Delta t} = -(-1)^r K \nabla^{2r} X \tag{2.58}$$

can be applied along the hybrid coordinate surfaces to any of the prognostic variables transformed to spectral space.

Equation (2.58) is solved fully implicitly in spectral space

$$[X_n^m]_{\text{after diff}} = \left\{ 1 + \Delta t K \left(\frac{n(n+1)}{a^2} \right)^r \right\}^{-1} X_n^m \tag{2.59}$$

where X_n^m is the spectral coefficient for the zonal wavenumber m and the total wavenumber n of variable X before the numerical diffusion operator is applied. Outside the sponge layer, the K coefficients are independent of the vertical.

A modified form of (2.59) is used for the temperature, T, to approximate diffusion on surfaces of constant pressure rather than on the sloping hybrid coordinate surfaces (Simmons, 1987).

With a linear grid, the IFS default configuration uses a fourth-order horizontal diffusion ($r = 2$) with the diffusion coefficient defined as

$$K = \tau^{-1} \left(\frac{a^2}{N(N+1)} \right)^r \tag{2.60}$$

and timescale $\tau = 6\Delta t$.

With a cubic grid, the IFS default configuration uses a diffusion operator with properties mimicking spectral viscosity after Gelb and Gleeson (2001). In this case, the diffusion coefficient K is a function of the total wavenumber n:

$$\frac{[X]_{\text{after diff}} - [X]_{\text{before diff}}}{\Delta t} = -K(n) \nabla^4 X \tag{2.61}$$

with $K(n) = 0$ for $n < N_{cutoff}$ ($N_{cutoff} = N/2$ in the current implementation) and

$$K(n) = \frac{1}{2 * N * \Delta t} \left(\frac{a^2}{N(N+1)} \right)^2 * exp(-\frac{1}{2}(n-N)^2/(n-N_{cutoff})^2) \tag{2.62}$$

for $n > N_{cutoff}$.

For all the prognostic variables which remains in grid point space (all the water variables, chemical species and tracers), there is no diffusion other than the intrinsic diffusion from the semi-Lagrangian advection.

(*b*) *Sponge at model top*

Inside the sponge layer the K-coefficients of the diffusion (see section above) are augmented by an additional function $F(n, k)$ where n is the total wavenumber and k is the level index. The specification of the function $F(n, k)$ depends of the number of levels and of the pressure at the last full level. For the 91 and 137 levels which are used in operation, the stratospheric sponge starts at 10 hPa. Then an extra mesospheric sponge of order 1 acts on the divergence from 1 hPa to the model top. An extra sponge of order 4 has been introduced with the resolution upgrade to TCo1279 for the vorticity at the 3 top levels in order to avoid the development of vorticity "solitons" in the non-divergent layers near the model top.

(*c*) *De-aliasing*

On a cubic grid, there is almost no aliasing at all. But with a linear grid, aliasing will show up as "spectral blocking", a build up of energy at the smallest scales that may ultimately lead to instability. For example, quadratic terms (i.e. products of prognostic variables such as the pressure gradient term in the momentum equation) cannot be represented accurately beyond $2/3N$, as quadratic interactions will alias onto waves beyond $2/3N$. East-west aliasing is mostly eliminated on the *reduced* linear grid due to the choices made in the grid creation. The number of grid points used at each "reduced" latitude is chosen to be $3N_r + 1$ for N_r waves, see Courtier and Naughton (1994) for details. The term most responsible for the aliasing noise is the pressure gradient term in the momentum equation, although (higher-order) aliasing also exists due to the right-hand-side of the thermodynamic equation. In the IFS a de-aliasing procedure is applied where the difference between a filtered pressure gradient term and the unfiltered pressure gradient term is subtracted at every timestep from the right-hand-side of the momentum equation. The filtered term is obtained by computing the rotational and divergent components of the pressure gradient term in spectral space, smoothly truncate only the rotational component at approximately 2/3 of the maximum truncation wavenumber N and transforming the result back to grid-point space.

Chapter 3
Semi-Lagrangian formulation

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3.1 GENERAL DESCRIPTION

The general form of the model equations is

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

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 $(\underset{\sim}{x}-\alpha, t)$, and the departure point $(\underset{\sim}{x}-2\alpha, t-\Delta t)$. 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

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

since only a single interpolation (of the combined field $X(t-\Delta t) + \Delta t R(t)$ at the point $(\underset{\sim}{x}-2\alpha)$) is then required in order to determine X^+. At ECMWF the three-time-level semi-Lagrangian scheme uses (3.3)

but the interpolation of R to the departure point is done with the tri-linear interpolation while the interpolation of X is of a higher order.

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

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

and again the terms to be evaluated at the departure point $(\underset{\sim}{x} - 2\alpha)$ can be added to other right-hand side terms before interpolation. Notice that the evaluation of $\widetilde{\Delta}_{tt} X$, 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 right-hand side of the equations, but that cubic interpolation is essential for the advected field 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.

It was found that a further increase in the order of the vertical interpolation of temperature, results in a reduction of the resolution dependent systematic cold bias in the lower tropical stratosphere which intensifies in high resolution model simulations. This cold bias is significantly reduced (Polichtchouk *et al.* (2019)) when replacing the default 32-point stencil quasi-cubic interpolation by a 56-point stencil quintic interpolation in the vertical (5^{th} order accurate), involving two additional vertical layers each with 12 horizontal points. To maintain the consistency with the closely related moisture field, the same quintic interpolation operator is applied to the specific humidity prognostic variable as well. The vertical quintic interpolation is evaluated as a weighted sum of three cubic interpolations computed from shifted and overlapping four point stencils. Although at first glance this complicates implementation, it enables to design the quintic interpolation from the existing code for the cubic interpolation method. In addition, it allows to control the smoothness and the non-oscillatory behavior of the resulting interpolation formula by adopting the WENO (weighted essentially non-oscillatory) reconstruction (described for example in Carlini *et al.* (2005)). This way of smooth and targeted interpolation was found beneficial for layers near the model top. The remaining atmospheric layers are interpolated with a different coefficient set up that results in quintic Lagrangian method.

For the reduced Gaussian grid described in Subsection 2.2.5, 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 than 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 $(\underset{\sim}{x} - \alpha)$ and the departure point $(\underset{\sim}{x} - 2\alpha)$ of the trajectory for each arrival point $\underset{\sim}{x}$ are found by iteratively solving the equation

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

where $\underset{\sim}{\mathbf{v}}$ 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 (2.18) and (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 $\eta = 1$ 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 in the finite-difference version of the model 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

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

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):

$$\eta_{k+1/2} = A_{k+1/2}/p_0 + B_{k+1/2} \tag{3.8}$$

where p_0 is a constant pressure (chosen to be 1013.25 hPa).

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

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

The horizontal components of (3.9) are found taking into account the spherical geometry following Ritchie (1987,1988). The first guess is given by

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

The calculations can 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), only two further iterations were found to be adequate.

Once the midpoint $(\underset{\sim}{x} - \alpha)$ of the trajectory has been found, the departure point $(\underset{\sim}{x} - 2\alpha)$ 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 SEMI-LAGRANGIAN DISCRETIZATION

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) and (2.32) is

$$\frac{\mathbf{v}_{\mathrm{H}}^{+} - \mathbf{v}_{\mathrm{H}}^{-}}{2\Delta t} + [f\mathbf{k} \times \mathbf{v}_{\mathrm{H}} + \nabla\phi + R_{\mathrm{dry}}T_{\mathrm{v}}\nabla \ln p]^{0} = \mathbf{P}_{\mathbf{v}} + \mathbf{K}_{\mathbf{v}} - \frac{\beta}{2}\Delta_{tt}\nabla\{[\gamma]T + R_{\mathrm{dry}}T_{\mathrm{v}} \ln p_{\mathrm{s}}\} \tag{3.11}$$

where $\mathbf{k}$ is the vertically directed unit vector and ∇ is the horizontal gradient operator in spherical coordinates. On the right-hand side of (3.11), $\mathbf{P}_{\mathbf{v}}$, and $\mathbf{K}_{\mathbf{v}}$ respectively denote the contributions of the physical parametrization schemes and horizontal diffusion, to be discussed in Section 3.5, 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 (3.11) 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) and (2.34) become

$$\frac{T^{+} - T^{-}}{2\Delta t} - \left\{\frac{\kappa T_v \omega}{(1 + (\delta - 1)q)p}\right\}^{0} = P_T + K_T - \frac{\beta}{2}\Delta_{tt}([\tau]D) \tag{3.12}$$

$$\frac{q^{+} - q^{-}}{2\Delta t} = P_q + K_q \tag{3.13}$$

In (3.12), 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

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial p}{\partial \eta}\right) + \frac{\partial p}{\partial \eta}\left(D + \frac{\partial \dot{\eta}}{\partial \eta}\right) = 0 \tag{3.14}$$

Setting

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

and noting that

$$\frac{\partial}{\partial t}\left(\frac{\partial A}{\partial \eta}\right) = \nabla \cdot \left(\frac{\partial A}{\partial \eta}\right) = \frac{\partial p_{\mathrm{s}}}{\partial \eta} = 0$$

we also have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial p}{\partial \eta}\right) = \frac{\partial B}{\partial \eta}\frac{\mathrm{d}p_{\mathrm{s}}}{\mathrm{d}t} + \dot{\eta}\frac{\partial}{\partial \eta}\left(\frac{\partial p}{\partial \eta}\right) \tag{3.15}$$

Combining (3.14) and (3.15)

$$\frac{\partial B}{\partial \eta}\frac{\mathrm{d}p_{\mathrm{s}}}{\mathrm{d}t}+\frac{\partial p}{\partial \eta}D+\frac{\partial}{\partial \eta}\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)=0 \tag{3.16}$$

Now introducing the vertical discretization, (3.16) becomes

$$\Delta B_k\frac{\mathrm{d}p_{\mathrm{s}}}{\mathrm{d}t}+\Delta p_k D_k+\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}}-\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k-\frac{1}{2}}=0 \tag{3.17}$$

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

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

$$\Delta B_k\frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{s}})+\frac{1}{p_{\mathrm{s}}}\left\{\Delta p_k D_k+\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k+\frac{1}{2}}-\left(\dot{\eta}\frac{\partial p}{\partial \eta}\right)_{k-\frac{1}{2}}\right\}=0 \tag{3.18}$$

Combining (3.18) with the discrete definition of $\dot{\eta}\partial p/\partial\eta$ given by (2.18) leads to

$$\Delta B_k\frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{s}})-\Delta B_k\left\{\frac{\partial(\ln p_{\mathrm{s}})}{\partial t}+\mathbf{v}_k\cdot\nabla(\ln p_{\mathrm{s}})\right\}=0 \tag{3.19}$$

where $\partial(\ln p_{\mathrm{s}})/\partial t$ 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

$$(\ln p_{\mathrm{s}})^{+}=\sum_{k=1}^{NLEV}\Delta B_k\left[(\ln p_{\mathrm{s}})^{-}+2\Delta t\left\{\frac{\partial(\ln p_{\mathrm{s}})}{\partial t}+\mathbf{v}_k\cdot\nabla\ln p_{\mathrm{s}}\right\}^{0}-\frac{\beta\Delta t}{p_{\mathrm{s}}^{\mathrm{ref}}}\Delta_{tt}\left\{\sum_{j=1}^{NLEV}(\Delta p_j^{\mathrm{ref}}D_j)\right\}\right] \tag{3.20}$$

(Since there is no vertical advection term in (3.20), 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 (3.20) involves a different trajectory. The interpolations for $(\ln p_{\mathrm{s}})^{-}$ 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 (3.11) to (3.13) together with (3.20).

3.4 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 (3.12), and of the right-hand side of the continuity equation (3.20). Both involve terms of the form $\mathbf{v}\cdot\nabla\ln p_{\mathrm{s}}$, 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 $\mathbf{v}\cdot\nabla$ 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 $\mathbf{v}\cdot\nabla\ln p_{\mathrm{s}}$ 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 σ. A possible disadvantage of such an approach is that $\dot{\eta}\partial p/\partial\eta$ (or σ) then follows an independent evolution, no longer satisfying a diagnostic relationship of the form (2.18). Our 'Eulerian' treatment of the $\mathbf{v}\cdot\nabla\ln p_{\mathrm{s}}$, 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, (3.16), 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 $\partial p_s/\partial\eta$ is zero). However the vertically discretized form, (3.17), is well-defined only at discrete model levels, implying that for consistency the semi-Lagrangian discretization (3.20) 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.

3.5 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 2.2.7. 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 $\ln p_s$, on the Gaussian grid. To complete the semi-implicit corrections, the $(t-\Delta t)$ values of D, $\partial P/\partial\mu$ 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 $\ln p_s$. Legendre transforms followed by Fourier transforms are then used to compute $D, U, V, T, \partial T/\partial\mu, q, \partial q/\partial\mu, \ln p_s$, and $\partial(\ln p_s)/\partial\mu$ 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 $\partial(\ln p_s)/\partial\lambda$. 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 (3.13), 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 (3.11)). If T_v is chosen as the spectral variable as in Subsection 2.2.10, 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

$$X^+(\underset{\sim}{x}) = X^-(\underset{\sim}{x}-2\alpha) + \Delta t\{R^0(\underset{\sim}{x}-2\alpha) + R^0(\underset{\sim}{x})\} + S^-(\underset{\sim}{x}-2\alpha) + S^+(\underset{\sim}{x}) \tag{3.21}$$

or

$$X^+(\underset{\sim}{x}) = X^-(\underset{\sim}{x}-2\alpha) + 2\Delta t R^0(\underset{\sim}{x}-\alpha) + S^-(\underset{\sim}{x}-2\alpha) + S^+(\underset{\sim}{x}) \tag{3.22}$$

depending on whether the R^0 terms are averaged between the end points of the trajectory or evaluated at the midpoints. In (3.21) and (3.22), 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 (3.21), the combined field $X^+ + \Delta t R^0 + S^-$ is computed, and the value of this combined field at each departure point $(\underset{\sim}{x}-2\alpha)$ is then found by interpolation. Adding the (uninterpolated) value $\Delta t R^0$ results in a provisional value X^+ at each grid point, incorporating all the terms in (3.21) except for S^+. The calculation for equations of the form (3.22)

proceeds similarly, except that two interpolations are required, one for $X^- + S^-$ at $(\underset{\sim}{x} - 2\alpha)$, and one for $2\Delta t R^0$ at $(\underset{\sim}{x} - \alpha)$.

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

$$U^+ + \frac{\beta\Delta t}{a}\frac{\partial P^+}{\partial \lambda} = Q_1 \tag{3.23}$$

$$V^+ + \frac{\beta\Delta t}{a}\cos\theta\frac{\partial P^+}{\partial \theta} = Q_2 \tag{3.24}$$

$$T^+ + \beta\Delta t[\tau]D^+ = Q_3 \tag{3.25}$$

$$q^+ = Q_4 \tag{3.26}$$

$$(\ln p_s)^+ + \beta\Delta t[v]D^+ = Q_5 \tag{3.27}$$

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 (3.23) to (3.27) have exactly the same form as (2.43) to (2.47) 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 2.2.8.

3.6 MODIFIED SEMI-LAGRANGIAN EQUATIONS

3.6.1 Momentum equations

The momentum equations are treated in vector form (see (3.11)). Following Rochas (1990) and Temperton (1997), the Coriolis terms can be incorporated in the semi-Lagrangian advection. Thus, the advected variable becomes $\underset{\sim}{\mathbf{v}}_H + 2\underset{\sim}{\Omega} \times \underset{\sim}{\mathbf{r}}$ where Ω is the earth's rotation and $\underset{\sim}{\mathbf{r}}$ 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 (3.1) is then

$$\mathbf{X} = \underset{\sim}{\mathbf{v}}_H + 2\underset{\sim}{\Omega} \times \underset{\sim}{\mathbf{r}} \tag{3.28}$$

$$\mathbf{L} = \underset{\sim}{\nabla}([\gamma]T_v + R_{dry}T_{ref}\ln p_s) \tag{3.29}$$

$$\mathbf{N} = -(\underset{\sim}{\nabla}\phi + R_{dry}T_v\underset{\sim}{\nabla}\ln p_s) - L \tag{3.30}$$

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

In component form, $2\Omega \times \underset{\sim}{\mathbf{r}}$ 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 $2\Omega \times \underset{\sim}{\mathbf{r}}$ 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).

3.6.2 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

$$\frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{s}}) = [RHS] \tag{3.31}$$

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:

$$\ln p_{\mathrm{s}} = l^* + l' \tag{3.32}$$

where the time-independent part l^* depends on the underlying orography ϕ_{s} such that

$$l^* = (-\phi_{\mathrm{s}})/(R_{\mathrm{dry}}\bar{T}) \tag{3.33}$$

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

$$\nabla\phi_{\mathrm{s}} + R_{\mathrm{dry}}\bar{T}\nabla l^* = 0 \tag{3.34}$$

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

Using (3.32) and (3.33) gives

$$\frac{\mathrm{d}}{\mathrm{d}t}(\ln p_{\mathrm{s}}) = \frac{\mathrm{d}l'}{\mathrm{d}t} - \left(\frac{1}{R_{\mathrm{dry}}\bar{T}}\underset{\sim}{\mathbf{v}}_{\mathrm{H}} \cdot \underset{\sim}{\nabla}\phi_{\mathrm{s}}\right) \tag{3.35}$$

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 (3.31), which becomes

$$\frac{\mathrm{d}l'}{\mathrm{d}t} = [RHS] + \frac{1}{R_{\mathrm{dry}}\bar{T}}\underset{\sim}{\mathbf{v}}_{\mathrm{H}} \cdot \underset{\sim}{\nabla}\phi_{\mathrm{s}} \tag{3.36}$$

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

3.6.3 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

$$T_{\mathrm{c}} = \left(p_{\mathrm{s}}\frac{\partial p}{\partial p_{\mathrm{s}}}\frac{\partial T}{\partial p}\right)_{\mathrm{ref}} \ln p_{\mathrm{s}} \tag{3.37}$$

where the subscript 'ref' denotes a reference value which is a function only of model level. For the purposes of the semi-Lagrangian advection $\ln p_{\mathrm{s}}$ is replaced by a time-independent value as in (3.33), to define a "temperature" T_{b} which depends only on the model level and the underlying orography:

$$T_{\mathrm{b}} = -\left(p_{\mathrm{s}}\frac{\partial p}{\partial p_{\mathrm{s}}}\frac{\partial T}{\partial p}\right)_{\mathrm{ref}} \cdot \phi_{\mathrm{s}}/(R_{\mathrm{dry}}\bar{T}) \tag{3.38}$$

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

$$- \underset{\sim}{\mathbf{v}}_{\rm H} \cdot \nabla T_{\rm b} - \dot{\eta} \frac{\partial T_{\rm b}}{\partial \eta} \tag{3.39}$$

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).

3.7 TWO-TIME-LEVEL SEMI-LAGRANGIAN SCHEME

3.7.1 Formal two-time-level scheme

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

$$\frac{X_{\rm A}^{+} - X_{\rm D}^{-}}{\Delta t} = \frac{1}{2}(L_{\rm D}^{-} + L_{\rm A}^{+}) + \frac{1}{2}(N_{\rm D}^{*} + N_{\rm A}^{*}) \tag{3.40}$$

where

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

$X_{\rm D}^{-} = X(\underset{\sim}{x} - \alpha, t)$ is the value interpolated at the "departure" point at time t

$L_{\rm A}^{+}$ and $L_{\rm D}^{-}$ are the linear terms defined similarly

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

$$N^{*} = \frac{3}{2}N(t) - \frac{1}{2}N(t - \Delta t) \tag{3.41}$$

The displacement equation becomes

$$\alpha = \Delta t - \underset{\sim}{V}^{*}\left(\underset{\sim}{x} - \frac{1}{2}\alpha, t + \frac{1}{2}\Delta t\right) \tag{3.42}$$

where the three-dimensional wind field V^{*} is also extrapolated in time so that

$$\underset{\sim}{V}^{*} = \frac{3}{2}\underset{\sim}{V}(t) - \frac{1}{2}\underset{\sim}{V}(t - \Delta t) \tag{3.43}$$

The iterative scheme and first-guess for solving (3.42) 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.

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

An alternative second-order accurate scheme to solving (3.42) 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 so that

$$\vec{R}_{\rm A}^{t+\Delta t} \approx \vec{R}_{\rm D}^{t} + \Delta t \cdot \left[\frac{\mathrm{d}}{\mathrm{d}t}\vec{R}\right]_{\rm D}^{t} + \frac{\Delta t^2}{2} \cdot \left[\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\vec{R})\right]_{\rm AV} \tag{3.44}$$

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

$$\vec{R}_{\rm A}^{t+\Delta t} \approx \vec{R}_{\rm D}^{t} + \Delta t \cdot \vec{V}_{\rm D}^{t} + \frac{\Delta t^2}{2} \cdot \left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]_{\rm AV} \tag{3.45}$$

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

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(\vec{V})\right]_{\mathrm{AV}} \tag{3.46}$$

To estimate (3.46) 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 (3.46) and the expression

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}(W)\right]_{\mathrm{AV}} \approx \frac{W_{\mathrm{A}}^{t} - W_{\mathrm{D}}^{t-\Delta t}}{\Delta t} \tag{3.47}$$

for the vertical part.

After exploring many other possibilities, the estimate adopted was

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

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 $t + \Delta t$.

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 (3.48) into (3.45) we obtain

$$\vec{R}_{\mathrm{A}}^{t+\Delta t} = \vec{R}_{\mathrm{D}}^{t} + \frac{\Delta t}{2} \cdot ([2\vec{V}^{t} - \vec{V}^{t-\Delta t}]_{\mathrm{D}} + \vec{V}_{\mathrm{A}}^{t}) \tag{3.49}$$

which is solved for $\vec{R}_{\mathrm{D}}^{t}$ iteratively. A similar expression can be used in every evolution equation to treat the non-linear terms of the r.h.s.

More detail about SETTLS can be found in Hortal (2002).

3.7.3 A limiter for the SETTLS trajectory scheme in the stratosphere

Temperature and wind fields can become very noisy in the stratosphere when the winter stratospheric polar vortex is disrupted. This noise is not extensive enough to threaten overall model stability but can result in incorrect temperature forecasts in noisy regions. Such flow regimes changes typically occur during sudden stratospheric warmings where the westerly night stratospheric polar jet migrates south and in some cases breaks down completely to be replaced by easterlies.

The noise is strongly linked with the vertical part of SETTLS procedure and specifically with the extrapolatory term used in (3.49). In the vertical this is: $2\dot{\eta}^{t} - \dot{\eta}^{t-\Delta t}$. Removing this extrapolation by using the following formula for the vertical part of (3.49):

$$\eta_{A}^{t+\Delta t} = \eta_{D}^{t} + \frac{\Delta t}{2}(\dot{\eta}_{D}^{t} + \dot{\eta}_{A}^{t}) \tag{3.50}$$

eliminates the noise problem. However, it also reduces the formal order of accuracy of the SETTLS trajectory scheme from 2 to 1. To avoid any loss of accuracy a modification of SETTLS has been

implemented for the stratosphere in which grid-points prone to develop noise are identified and the lower order non-extrapolatory scheme (3.50) is applied on them. The standard method (3.49) is applied on the remaining grid points. The new formula in the vertical is

$$\eta_A^{t+\Delta t} = \begin{cases} \eta_D^t + \dfrac{\Delta t}{2}\left(\left[2\dot{\eta}^t - \dot{\eta}^{t-\Delta t}\right]_D + \dot{\eta}_A^t\right), & \left|\dot{\eta}_A^t - \dot{\eta}_A^{t-\Delta t}\right| \le \frac{\beta}{2}\left(\left|\dot{\eta}_A^t\right| + \left|\dot{\eta}_A^{t-\Delta t}\right|\right) \\ \eta_D^t + \dfrac{\Delta t}{2}\left(\dot{\eta}_D^t + \dot{\eta}_A^t\right), & \left|\dot{\eta}_A^t - \dot{\eta}_A^{t-\Delta t}\right| > \frac{\beta}{2}\left(\left|\dot{\eta}_A^t\right| + \left|\dot{\eta}_A^{t-\Delta t}\right|\right) \end{cases} \tag{3.51}$$

where, $0 \le \beta/2 \le 1$. In effect this is a 1st order "limiter", applied to the 2nd order scheme for computing the vertical coordinate of the semi-Lagrangian trajectory departure point, analogous to spatial 1st order limiters used in cubic interpolation to avoid overshootings and undershootings. In this modified formula, at each grid point, the magnitude of the $\dot{\eta}_A$ jump during two consecutive timesteps is compared with the average of the $\dot{\eta}_A$ magnitude. This is the criterion which determines if the 1st or 2nd order scheme will be used. For grid points with large velocity jumps the formula switches to 1st order. The parameter β controls how frequently this happens: for $\beta = 0$ the 1st order scheme will be activated everywhere while for $\beta = 2$ the standard 2nd order SETTLS will be applied on all grid-points. Testing has shown that large values of β close to the upper limit 2 are sufficient to yield satisfactory results i.e. to inhibit noise growth and to provide accurate prediction of sudden stratospheric warming events without reducing overall accuracy of forecasts.

In order to comply with the temporal and spatial continuity requirements (which is the prerequisite for convergence of the TL/AD models) the previous formulae (3.51) to determine $\eta_A^{t+\Delta t}$ needs to be further adapted to a quasi-equivalent but smoother form. This is achieved by unifying the two alternative options into following general expression

$$\eta_A^{t+\Delta t} = \eta_D^t + \frac{\Delta t}{2}\left[\left(\dot{\eta}_D^t + \dot{\eta}_A^t\right) + \alpha\left(\dot{\eta}_D^t - \dot{\eta}_D^{t-\Delta t}\right)\right] \tag{3.52}$$

with parameter $\alpha \in \langle 0, 1\rangle$ representing a transition from the first order to the second order approximation defined by its bounding values. The smooth transition between the two regimes is ensured by following definition of α

$$\alpha = \frac{1}{2}\left[1 + \tanh\left(\tau_1(\dot{\eta}_A^{t-\Delta t}\dot{\eta}_A^t + \tau_2)\right)\right] \tag{3.53}$$

which is easily incrementable. In the previous the tunable parameter τ_1 stands for steepness of the transition and τ_2 represents a threshold offset shifting the transition zone off the weighted center between the two bounding regimes. To maintain any smooth transition between the two original regimes the first parameter is limited by machine precision. For example in the case 64 bits representation of reals (double precision) $\tau_1 < 10^{15}$. The second parameter τ_2 is affecting model accuracy. As a sensible compromise between efficiency of the whole modification and the model accuracy default values are set to be $\tau_1 = 10^{14}$, $\tau_2 = 10^{-14}$. (Note the setting of $\tau_1 > 10^{15}$ and $\tau_2 = 0$ results in situation very close to the one described by (3.51).)

3.8 NUMERICAL COUPLING OF THE PHYSICAL PARAMETRIZATIONS TO THE "DYNAMICAL" EQUATIONS (SLAVEPP)

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

3.8.1 SLAVEPP scheme

In (3.11) to (3.13) the contribution of the physical parametrizations are denoted as P indicating an evaluation of the parametrizations at the arrival point only. In the two time level scheme as described

in section 3.7 this is replaced by a partly second order accurate coupling of the parametrizations 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 parametrized processes the contributions of radiation, convection and cloud parametrization are averaged "along" the semi-Lagrangian trajectory while the contributions of vertical diffusion and parametrized gravity waves are taken at the arrival point only. Equation (3.40) then becomes

$$\frac{X_{\rm A}^{+}-X_{\rm D}^{-}}{\Delta t}=\frac{1}{2}(L_{\rm D}^{-}+L_{\rm A}^{+})+\frac{1}{2}(N_{\rm D}^{*}+N_{\rm A}^{*})+\frac{1}{2}(P_{\rm D,rad+conv+cloud}^{-}+P_{\rm A,rad+conv+cloud}^{+})+P_{\rm A,vdif+gwdrag}^{+} \tag{3.54}$$

Part of the implicit calculations of the physical parametrizations use the tendency in the form

$$\tilde{D}_{\rm A}=\frac{\tilde{X}_{\rm A,Dyn}^{+}-X_{\rm A}^{-}}{\Delta t}, \tag{3.55}$$

with (3.40) modified to yield

$$\frac{\tilde{X}_{\rm A,Dyn}^{+}-X_{\rm D}^{-}}{\Delta t}=\frac{1}{2}(L_{\rm D}^{-}+\tilde{L}_{\rm A}^{+})+\frac{1}{2}(N_{\rm D}^{*}+N_{\rm A}^{*}) \tag{3.56}$$

The "$\sim$" denotes that only provisional values of the dynamic fields are available because semi-implicit correction terms are still to be computed (see Section 3.5). Therefore $L_{\rm A}^{+}\approx\tilde{L}_{\rm A}^{+}=L_{\rm A}^{-}$ is used for the linear terms. Equation (3.55) describes local tendencies, which are computed subtracting the new provisional explicit values $\tilde{X}_{\rm A,Dyn}^{+}$ of the dynamic fields (at the arrival point) from their values $X_{\rm A}^{-}$ at the previous time step. The parametrizations at the time step $t+\Delta t$ are computed at the arrival point as shown by

$$\begin{aligned}P_{\rm A}^{+}=&P_{\rm A,rad}^{+}(X_{\rm A}^{-})\\&+P_{\rm A,vdif}^{+}(X_{\rm A}^{-},\tilde{D}_{\rm A},P_{\rm A,rad}^{+})\\&+P_{\rm A,gwdrag}^{+}(X_{\rm A}^{-},\tilde{D}_{\rm A})\\&+P_{\rm A,conv}^{+}(X_{\rm A,predict}^{+},(output)F_{\rm conv})\\&+P_{\rm A,cloud}^{+}(X_{\rm A,predict}^{+},(input)F_{\rm conv})\end{aligned} \tag{3.57}$$

where the "first guess" predictor $X_{\rm A,predict}^{+}$ 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 parametrizations of radiation, convection and clouds at the previous time-step t and the tendency of vertical diffusion and gravity waves at $t+\Delta t$:

$$X_{\rm A,predict}^{+}=\tilde{X}_{\rm A,Dyn}^{+}+\alpha P_{\rm D,rad+conv+cloud}^{-}\Delta t+P_{\rm A,vdif+gwdrag}^{+}\Delta t. \tag{3.58}$$

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

3.8.2 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.

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