The Karlsruhe Simulation Model of the Middle Atmosphere (KASIMA)
Version 1

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Abstract

The first version of the Karlsruhe Simulation Model of the Middle Atmosphere (KASIMA) is described that is designed to simulate dynamical szenarios of the atmosphere between 10 and 100 km Altitude on the global scale. Idealized transport processes based on these scenarios can also be investigated.

This model provides the fundamentals of an entire modelsystem that is currently in development at the research centre Karlsruhe. This purpose of this modelsystem is the interpretation of measurements of trace gas distributions in the middle atmosphere.

The development of the numerical scheme based on the meteorological set of the primitive equations is described in detail. The physical parameterizations applied to force the model are described briefly. The appendix repeats some general mathematical relations used in the body of the manual and a cross reference of the most important modules of the model.

Das Karlsruher Simulationsmodell der mittleren Atmosphäre KASIMA, Version 1

Zusammenfassung

Die erste Version des Karlsruher Simulationsmodells der mittleren Atmosphäre (KASIMA) ist beschrieben, das entwickelt ist, dynamische Szenarien der Atmosphäre auf globaler Skala zwischen 10 und 100 km Höhe zu simulieren. In idealisierter Weise können auch damit verbundene Transportprozesse studiert werden.

Dieses Modell bildet die Basis für ein am Forschungszentrum Karlsruhe in Entwicklung befindliches Modellsystem, mit dem Interpretationen von Spurengasmessungen in der mittleren Atmosphäre durchgeführt werden sollen.

Die Ableitung der numerischen Methoden zur Integration des meteorologischen Grundgleichungssystems ist detailliert beschrieben. Die angewandten physikalischen Parameterisierungen sind nur in ihrer numerischen Implementierung wiedergegeben. Im Anhang werden allgemeine mathematische Relationen wiederholt, die im Textteil wichtig sind. Außerdem wird eine Liste der wichtigsten Module des Modells bereitgestellt.

Contents

1 Introduction

This manual contains a technical description of the 3-dimensional global spectral primitive equation model KASIMA (KArlsruher SImulationsmodell der Mittleren Atmosphäre, KArlsruhe SImulation model of the Middle Atmosphere) of the Institut für Meteorologie und Klimaforschung, Forschungszentrum Karlsruhe. Its use is primarily for scientists who intend to work with the model either by application or by development.

Section 2 develops the meteorological equations from the set of partial differential equations to the finite difference scheme used in the model. Section 3 describes the algorithm used to transport a set of idealized tracers by the model atmosphere. Section 4 describes the physical parameterizations used to drive the model.

2 The Meteorology

2.1 Introduction

This section develops the set of primitive equations as used in the model. Section 2.2 introduces to the differential equations. Section 2.3 develops the differential equations as a series of coefficients of spherical harmonics. Section 2.4 describes the finite difference scheme used in the model and develops the finite difference equations.

2.2 The Differential Equations

The model is based on the full set of the primitive equations with a logarithmic pressure z as vertical coordinate. Following the notation of *Holton* [1975] the horizontal momentum equation, the thermodynamic equation, the hydrostatic equation and the continuity equation are:

$$\frac{D\vec{v}_p}{Dt} + f\vec{k} \times \vec{v}_p + \vec{\nabla}_p \Phi - \vec{F} = 0 \tag{2.1}$$

$$\frac{DT}{Dt} + wT\frac{\kappa}{H} - Q = 0 \tag{2.2}$$

$$\frac{\partial \Phi}{\partial z} = \frac{RT}{H} \tag{2.3}$$

$$\vec{\nabla}_p \cdot \vec{v}_p + \frac{1}{\rho_0}\frac{\partial \rho_0 w}{\partial z} = 0 \tag{2.4}$$

Equation 2.1 can be decomposed into its zonal and meridional component yielding:

$$\frac{Du}{Dt} - \left(f + \frac{u\tan\varphi}{a}\right)v + \frac{1}{a\cos\varphi}\frac{\partial \Phi}{\partial \lambda} - F_\lambda = 0 \tag{2.5}$$

$$\frac{Dv}{Dt} + \left(f + \frac{u\tan\varphi}{a}\right)u + \frac{1}{a}\frac{\partial \Phi}{\partial \varphi} - F_\varphi = 0 \tag{2.6}$$

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Instead of having two prognostic equations for the horizontal velocity vector components (equations 2.5, 2.6) two equivalent equations for the scalar quantities $\zeta = \vec{k} \cdot \vec{\nabla}_p \times \vec{v}_p$ (the relative vorticity) and $D = \vec{\nabla}_p \cdot \vec{v}_p$ (horizontal divergence) can be obtained by applying $\vec{k} \cdot \vec{\nabla}_p \times$ and $\vec{\nabla}_p \cdot$ on equation 2.1 From the horizontal momentum equation 2.1 in advection and flux form the following alternative sets of equations are derived:

1. For the advection form it is convenient to rewrite the advection term in equation 2.1 using equation A.22 or A.25:

$$\vec{v}_p \cdot \vec{\nabla}_p \vec{v}_p = \vec{\nabla}_p \left(\frac{\vec{v}_p^2}{2} \right) - \vec{v}_p \times (\vec{\nabla}_p \times \vec{v}_p) = \vec{\nabla}_p \left(\frac{\vec{v}_p^2}{2} \right) + \zeta \vec{k} \times \vec{v}_p \qquad (2.7)$$

The vorticity- and divergence equation thus become in advection form:

$$\frac{\partial \zeta}{\partial t} + \vec{\nabla}_p \cdot (\zeta + f) \vec{v}_p + \vec{k} \cdot \vec{\nabla}_p \times \left[w \frac{\partial \vec{v}_p}{\partial z} - \vec{F} \right] = 0 \qquad (2.8)$$

and

$$\frac{\partial D}{\partial t} - \vec{k} \cdot \vec{\nabla}_p \times (\zeta + f) \vec{v}_p + \vec{\nabla}_p \cdot \left[w \frac{\partial \vec{v}_p}{\partial z} - \vec{F} \right] + \vec{\nabla}_p^2 \left[\Phi + \left(\frac{\vec{v}_p^2}{2} \right) \right] = 0 \qquad (2.9)$$

2. Equation 2.7 becomes for the momentum flux:

$$\vec{\nabla}_p \cdot \vec{v}_p \vec{v}_p = \vec{v}_p \cdot \vec{\nabla}_p \vec{v}_p + \vec{v}_p \vec{\nabla}_p \cdot \vec{v}_p \overset{(2.7)}{=} \vec{\nabla}_p \left(\frac{\vec{v}_p^2}{2} \right) + \zeta \vec{k} \times \vec{v}_p + D \vec{v}_p \qquad (2.10)$$

so that the vorticity and divergence equations become in flux form

$$\frac{\partial \zeta}{\partial t} + \vec{\nabla}_p \cdot (\zeta + f) \vec{v}_p + \vec{k} \cdot \vec{\nabla}_p \times \left[\frac{1}{\rho_0} \frac{\partial \rho_0 w \vec{v}_p}{\partial z} + D \vec{v}_p - \vec{F} \right] = 0 \qquad (2.11)$$

and

$$\frac{\partial D}{\partial t} - \vec{k} \cdot \vec{\nabla}_p \times (\zeta + f) \vec{v}_p + \vec{\nabla}_p \cdot \left[\frac{1}{\rho_0} \frac{\partial \rho_0 w \vec{v}_p}{\partial z} + D \vec{v}_p - \vec{F} \right] + \vec{\nabla}_p^2 \left[\Phi + \left(\frac{\vec{v}_p^2}{2} \right) \right] = 0 \qquad (2.12)$$

2.3 The Spectral Representation

The model is based on the vorticity equation 2.11 and the divergence equation 2.12 in flux form, the thermodynamic equation 2.2 in flux form, the hydrostatic equation 2.3, and the continuity equation 2.4. Equations for the spherical harmonic coefficients are obtained by multiplying the equations 2.11, 2.12, 2.2, 2.3, and 2.4 with $P_n^m(\mu)e^{-\imath m\lambda}$ and integrating over the sphere (see equation A.44):

$$\frac{\partial \zeta_n^m}{\partial t} = \frac{1}{4\pi a} \int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} \left[-\frac{1}{(1-\mu^2)}\frac{\partial K_V}{\partial \lambda} + \frac{\partial K_U}{\partial \mu} \right] P_n^m(\mu)e^{-\imath m\lambda}d\lambda d\mu + (F_\zeta)_n^m \tag{2.13}$$

$$\begin{aligned}
\frac{\partial D_n^m}{\partial t} = {}&{} -\frac{1}{4\pi a} \int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} \left[\frac{1}{(1-\mu^2)}\frac{\partial K_U}{\partial \lambda} + \frac{\partial K_V}{\partial \mu} \right] P_n^m(\mu)e^{-\imath m\lambda}d\lambda d\mu \\
&{} -\frac{1}{4\pi} \int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} \vec{\nabla}_p^2 \left[\Phi + \frac{\vec{v}_p^2}{2} \right] P_n^m(\mu)e^{-\imath m\lambda}d\lambda d\mu + (F_D)_n^m
\end{aligned} \tag{2.14}$$

$$\frac{\partial T_n^m}{\partial t} = \frac{1}{4\pi} \int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} -K_T P_n^m(\mu)e^{-\imath m\lambda}d\lambda d\mu + Q_n^m \tag{2.15}$$

$$\frac{\partial \Phi_n^m}{\partial z} = \frac{RT_n^m}{H} \tag{2.16}$$

$$D_n^m + \frac{1}{\rho_0}\frac{\partial W_n^m}{\partial z} = 0 \tag{2.17}$$

where

$$K_U = -(\zeta + f)V + DU + \frac{1}{\rho_0}\frac{\partial WU}{\partial z} \tag{2.18}$$

$$K_V = +(\zeta + f)U + DV + \frac{1}{\rho_0}\frac{\partial WV}{\partial z} \tag{2.19}$$

$$K_T = \frac{1}{a(1-\mu^2)}\frac{\partial UT}{\partial \lambda} + \frac{1}{a}\frac{\partial VT}{\partial \mu} + \frac{1}{\rho_0}\frac{\partial WT}{\partial z} + wT\frac{\kappa}{H}$$

$$= \frac{1}{a(1-\mu^2)}\frac{\partial UT}{\partial \lambda} + \frac{1}{a}\frac{\partial VT}{\partial \mu} + \frac{1}{\gamma\rho_0}\frac{\partial \gamma WT}{\partial z} \tag{2.20}$$

In equation 2.20, γ is the conversion factor between the temperature and the potential temperature and is defined by equation A.12.

Using equations A.41, A.45 and A.46 the vorticity equation 2.13 and the divergence equation 2.14 may be written:

$$\frac{\partial \zeta_n^m}{\partial t} = \frac{1}{4\pi a}\int_{-1}^{+1}\int_0^{2\pi}\frac{-imK_V P_n^m(\mu) + K_U H_n^m(\mu)}{(1-\mu^2)}e^{-im\lambda}d\lambda d\mu + (F_\zeta)_n^m \tag{2.21}$$

$$\frac{\partial D_n^m}{\partial t} = -\frac{1}{4\pi a}\int_{-1}^{+1}\int_0^{2\pi}\frac{imK_U P_n^m(\mu) + K_V H_n^m(\mu)}{(1-\mu^2)}e^{-im\lambda}d\lambda d\mu$$

$$+\frac{n(n+1)}{4\pi a^2}\int_{-1}^{+1}\int_0^{2\pi}\left[\Phi + \frac{\vec{v}_p^2}{2}\right]P_n^m(\mu)e^{-im\lambda}d\lambda d\mu + (F_D)_n^m \tag{2.22}$$

The equations 2.21, 2.22, 2.15, 2.16, and 2.17 are a complete set of equations for the model variables $\zeta_n^m(t,z)$, $D_n^m(t,z)$, $T_n^m(t,z)$, $\Phi_n^m(t,z)$, and $W_n^m(t,z)$,

In order to compute $K_U(\lambda,\mu,z)$, $K_V(\lambda,\mu,z)$, and $K_T(\lambda,\mu,z)$ in equations 2.21, 2.22, and 2.15 the values for $\zeta(\lambda,\mu,z)$, $D(\lambda,\mu,z)$, and $T(\lambda,\mu,z)$ can immediately be obtained from the transformation equation A.43. $U(\lambda,\mu,z)$ and $V(\lambda,\mu,z)$ can be computed from equations A.7 and A.9 by means of A.39, A.41, and A.44 yielding:

$$U = a\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{1}{n(n+1)}\left[-imD_n^m P_n^m(\mu) - \zeta_n^m H_n^m(\mu)\right]e^{im\lambda} \tag{2.23}$$

$$V = a\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{1}{n(n+1)}\left[D_n^m H_n^m(\mu) - im\zeta_n^m P_n^m(\mu)\right]e^{im\lambda} \tag{2.24}$$

The spherical harmonic coefficients of the horizontal flux terms in equation 2.20 are computed using equations A.45 and A.46:

$$\int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} \frac{1}{(1-\mu^2)} \left(\frac{\partial UT(\lambda,\mu)}{\partial \lambda} + \left(1-\mu^2\right)\frac{\partial VT}{\partial \mu} \right) P_n^m(\mu)e^{-im\lambda}d\lambda d\mu$$

$$= \int\limits_{-1}^{+1}\int\limits_{0}^{2\pi} \frac{1}{(1-\mu^2)} \left(imUTP_n^m(\mu) + VTH_n^m(\mu) \right) e^{-im\lambda}d\lambda d\mu \qquad (2.25)$$

The first integral of the solution of equation A.46 vanishes because all the terms K_U, K_V, and VT in the equations 2.21, 2.22, and 2.25 vanish for $\mu = \pm 1$.

2.4 The Numerical Methods

2.4.1 The Horizontal Truncation

A fully triangular truncation scheme is used in the model: All series are truncated after the degree $n = N_{max}$, such that $0 \leq n \leq N_{max}$ and $-n \leq m \leq n$.

The integration with respect to λ is done on an equally spaced grid with at least $I_{grid} = 3N_{max} + 1$ gridpoints [e.g. *Machenhauer and Rasmussen, 1972*].

The integrals with respect to μ are computed using Gaussian quadrature. The Gaussian grids are obtained from the zeros of the Legendre polynomial $P_{N_{grid}}^0$, where N_{grid} is the number of gridpoints in meridional direction. The Gaussian weights $\Delta\mu_i$ at gridpoint i are obtained from equation A.14 [e.g. *Korn and Korn, 1968*]). The integrals with respect to μ are therefore approximated by:

$$\int\limits_{-1}^{+1} X(\mu)d\mu = \sum_{i=1}^{J_{grid}} X(\mu_i)\Delta\mu_i \qquad (2.26)$$

2.4.2 The Vertical Discretization

The hydrostatic equation 2.16 is integrated vertically from the bottom to the upper boundary in order to compute the geopotential. If subscript k denotes the actual model layer, Φ_k is computed by:

$$\frac{\Phi_k - \Phi_{k-1}}{\Delta z} = \frac{R}{H}0.5\left(T_k + T_{k-1}\right) \qquad (2.27)$$

At the bottom boundary the actual temperature and geopotential field is taken from the ECMWF consolidated dataset. These fields are interpolated linearly in time in order to be applied for the actual timestep.

The continuity equation 2.17 is integrated downward from the upper boundary to the bottom boundary in order to compute $\rho_0 w$. At the upper boundary it is assumed that $w = 0$:

$$\frac{1}{\rho_{0k}} \frac{W_{k+0.5} - W_{k-0.5}}{\Delta z} = -D_k \tag{2.28}$$

The vertical flux terms in 2.18, 2.19, and 2.20 are approximated by:

$$\frac{\partial \rho_0 w \alpha}{\partial z} \approx \frac{W_{k+0.5}(\alpha_{k+1} + \alpha_k) - W_{k-0.5}(\alpha_k + \alpha_{k-1})}{2\rho_{0k}\Delta z} \tag{2.29}$$

where $\alpha = \{U, V, \gamma T\}$.

2.4.3 The Semi-implicit Time Integration Scheme

The time integration scheme is adapted from the semi implicit scheme developed by *Haltiner and Williams* [1980]. All the terms that describe fast propagating internal gravity waves are treated implicitly, whereas for the other terms an explicit leapfrog scheme is applied. The terms being treated implicitely are the Laplacian of the geopotential in the divergence equation 2.22 and the vertical heat flux terms in the thermodynamic equation 2.15. Consequently, the continuity equation and the hydrostatic equation have to be treated implicetely. One entire column of model layers has to be computed simultaneously, because the continuity equation and the hydrostatic equation are integrated from the top to the bottom boundary and vise versa, respectively. Therefore the equations have to be written in matrix form. Since the vertical velocity defined between two model layers, the vertical grid is now defined as being twice as large as the vertical model layers, where the vertical velocity is defined on odd gridpoints and the other variables are defined on even gridpoints.

Because the Laplacian of the Geopotential is involved in the semi-implicit formulations, all derivations shown in this section have to be done in terms of the spherical harmonics of the variables, which is straight foreward because of the linearity of the equations discussed

here. As long as subscripts in the equations describe the vertical model layer considered, their meaning is changed for convenience in this section: even subscripts denote the variable is defined on the model layer and odd subscripts denote their definition between the model layer.

The hydrostatic 2.27 and the continuity equation 2.28 can be written in matrix form with these conventions:

$$\Phi_{2k} = A_{2k,2l}T_{2l} + \Phi_k^s \tag{2.30}$$

$$W_{2k-1} = B_{2k-1,2l}D_{2l} \tag{2.31}$$

In equations 2.30 and 2.31 the subscripts k and l denote the vertical model grid with $1 \leq k,l \leq k_{grid}$, where k_{grid} is the number of model layers and Φ_k^s is specified from the lower boundary condition.

From equations 2.27 and 2.28 the matrix equations 2.30 and 2.31 are explicitely:

$$
\begin{bmatrix} \Phi_2 \\ \Phi_4 \\ \Phi_6 \\ \cdots \\ \Phi_{2k_{grid}-2} \\ \Phi_{2k_{grid}} \end{bmatrix}
= \frac{R\Delta z}{2H}
\begin{bmatrix}
1 & 0 & 0 & \cdots & 0 & 0 \\
2 & 1 & 0 & \cdots & 0 & 0 \\
2 & 2 & 1 & \cdots & 0 & 0 \\
\cdots & & & & & \\
2 & 2 & 2 & \cdots & 1 & 0 \\
2 & 2 & 2 & \cdots & 2 & 1
\end{bmatrix}
\begin{bmatrix} T_2 \\ T_4 \\ T_6 \\ \cdots \\ T_{2k_{grid}-2} \\ T_{2k_{grid}} \end{bmatrix}
+
\begin{bmatrix} \Phi^s \\ \Phi^s \\ \Phi^s \\ \cdots \\ \Phi^s \\ \Phi^s \end{bmatrix}
\tag{2.32}
$$

$$
\begin{bmatrix} W_1 \\ W_3 \\ W_5 \\ \cdots \\ W_{2k_{grid}-3} \\ W_{2k_{grid}-1} \end{bmatrix}
= \Delta z
\begin{bmatrix}
\rho_{02} & \rho_{04} & \rho_{06} & \cdots & \rho_{02k_{grid}-2} & \rho_{02k_{grid}} \\
0 & \rho_{04} & \rho_{06} & \cdots & \rho_{02k_{grid}-2} & \rho_{02k_{grid}} \\
0 & 0 & \rho_{06} & \cdots & \rho_{02k_{grid}-2} & \rho_{02k_{grid}} \\
\cdots & & & & & \\
0 & 0 & 0 & \cdots & \rho_{02k_{grid}-2} & \rho_{02k_{grid}} \\
0 & 0 & 0 & \cdots & 0 & \rho_{02k_{grid}}
\end{bmatrix}
\begin{bmatrix} D_2 \\ D_4 \\ D_6 \\ \cdots \\ D_{2k_{grid}-2} \\ D_{2k_{grid}} \end{bmatrix}
\tag{2.33}
$$

Φ^s is specified from the lower boundary condition as:

$$\Phi^s = \frac{R\Delta z}{2H}T_0 + \Phi_0 \tag{2.34}$$

where T_0 and Φ_0 are the lower boundary temperature and Geopotential, defined one model layer below the lower boundary.

The vertical heat flux terms are linearized for the purpose of the semi-implicit treatment by separating the temperature:

$$T(\lambda, \mu, z, t) = T^*(z) + T'(\lambda, \mu, z, t) \qquad (2.35)$$

The linearized part of the vertical heat flux K_T^*

$$K_T^* = -\frac{1}{\gamma \rho_0} \frac{\partial \gamma W T^*}{\partial z} - DT^* \qquad (2.36)$$

is treated implicitly, whereas the nonlinear part is treated explicitly. Using equations 2.29 equation 2.36 can be written in matrix form:

$$
\begin{aligned}
K_{T2k}^* &= Y_{2k,2l-1} W_{2l-1} + T^*_{2k,2k} D_{2k} \\
&= +W_{2k+1} \left[-\frac{\gamma_{2k+2} T^*_{2k+2} + \gamma_{2k} T^*_{2k}}{2\gamma_{2k} \rho_{02k} \Delta z} \right] \\
&\quad +W_{2k-1} \left[+\frac{\gamma_{2k} T^*_{2k} + \gamma_{2k-2} T^*_{2k-2}}{2\gamma_{2k} \rho_{02k} \Delta z} \right] \\
&\quad -T^*_{2k,2k} D_{2k}
\end{aligned}
\qquad (2.37)
$$

For $k = k_{grid}$, $W_{2k+1} = 0$ and for $k = 1$, T_0^* is taken from the reference temperature.

The Laplacian of the geopotential can immediately be obtained in spherical harmonic coefficients from equation 2.22:

$$\left[\vec{\nabla}_p^2 \Phi_{2k} \right]_n^m = \frac{n(n+1)}{a^2} \left[\Phi_{2k} \right]_n^m \qquad (2.38)$$

The semi-implicit Formulation of the divergence equation 2.22 and the thermodynamic equation 2.15 can be derived with the matrix equations derived in this section. If the superscripts denote the timestep and the subscripts the vertical gridpoint, one obtains for the relevant terms of the divergence and thermodynamic equation:

$$\frac{D_k^{n+1} - D_k^{n-1}}{2\Delta t} \overset{(2.38)}{=} \vec{\nabla}_p^2 \left(\Phi_k^{n+1}\right) + \text{explicit terms}$$

$$\overset{(2.30)}{=} \vec{\nabla}_p^2 \left(A_{k,m}T_m^{n+1} + \Phi_l^{s,n+1}\right) + \overset{(2.39)}{\cdots} \tag{2.39}$$

$$\frac{T_k^{n+1} - T_k^{n-1}}{2\Delta t} \overset{(2.37)}{=} Y_{k,l}\left(W_l^{n+1}\right) - T_{k,l}^*\left(D_l^{n+1}\right) + \text{explicit terms}$$

$$\overset{(2.31)}{=} \left(Y_{k,l}B_{l,m} - T_{k,m}^*\right)\left(D_m^{n+1}\right) + \overset{(2.40)}{\cdots} \tag{2.40}$$

In equation 2.39 the values for Φ_k^s are taken from the lower boundary condition using equation 2.34. Solving equation 2.40 for T_k^{n+1} and inserting the result into 2.39 gives an equation for D_k^{n+1}:

$$
\begin{aligned}
\left(I_{k,l} - X_{k,l}\right) D_l^{n+1} = \ & + \left(I_{k,l} + X_{k,l}\right) D_l^{n-1} \\
& + (2\Delta t)\vec{\nabla}_p^2 A_{k,m}\left(T_m^{n-1} + (2\Delta t)\overset{(2.40)}{\cdots}\right) \\
& + (2\Delta t)\vec{\nabla}_p^2\left(\Phi_k^{s,n+1}\right) \\
& + (2\Delta t)\overset{(2.39)}{\cdots}
\end{aligned}
\tag{2.41}
$$

where

$$X_{l,o} = (2\Delta t)^2 \left(\vec{\nabla}_p^2 I_{l,k}\right) A_{k,m}\left(Y_{m,n}B_{n,o} - T_{m,o}^*\right) \tag{2.42}$$

and $I_{k,l}$ is the identity matrix.

2.4.4 The Finite Difference Equations

A computational overview for the computation of one timestep is presented together with the finite difference equations in the following list:

1. The spherical harmonics of the vorticity and the temperature of the the deviation from the reference temperature T' (see equation 2.35) of the actual timestep is

transformed on gridpoints using equation A.43:

$$\zeta(\lambda,\mu) = \sum_{n=0}^{N_{max}} \sum_{m=-n}^{n} \zeta_n^m P_n^m(\mu) e^{im\lambda} \tag{2.43}$$

$$D(\lambda,\mu) = \sum_{n=0}^{N_{max}} \sum_{m=-n}^{n} D_n^m P_n^m(\mu) e^{im\lambda} \tag{2.44}$$

$$T'(\lambda,\mu) = \sum_{n=0}^{N_{max}} \sum_{m=-n}^{n} T'^m_n P_n^m(\mu) e^{im\lambda} \tag{2.45}$$

2. The values of U, V, and W are computed at the actual timestep on gridpoints by means of equations 2.23, 2.24, 2.28 using the transformation A.43:

$$U = a \sum_{n=0}^{N_{max}} \sum_{m=-n}^{n} \frac{1}{n(n+1)} \left[-im D_n^m P_n^m(\mu) - \zeta_n^m H_n^m(\mu) \right] e^{im\lambda} \tag{2.46}$$

$$V = a \sum_{n=0}^{N_{max}} \sum_{m=-n}^{n} \frac{1}{n(n+1)} \left[D_n^m H_n^m(\mu) - im \zeta_n^m P_n^m(\mu) \right] e^{im\lambda} \tag{2.47}$$

$$W_{k-0.5} = W_{k+0.5} + \rho_{0k} \Delta z D_k(\lambda,\mu) \tag{2.48}$$

3. The non-linear terms K_U and K_V used in the vorticity equation 2.21 and in the divergence equation 2.22 are computed for the actual timestep on gridpoints from equations 2.18 and 2.19 using 2.29:

$$K_U = -(\zeta + f)V + DU + \frac{W_{k+0.5}(U_{k+1} + U_k) - W_{k-0.5}(U_k + U_{k-1})}{2\rho_0 \Delta z} \tag{2.49}$$

$$K_V = +(\zeta + f)U + DV + \frac{W_{k+0.5}(V_{k+1} + V_k) - W_{k-0.5}(V_k + V_{k-1})}{2\rho_0 \Delta z} \tag{2.50}$$

4. With the separation of the temperature 2.35 and the implicit treatment of the vertical heat flux of associated with the reference temperature T^* (see Section 2.4.3) the explicitely treated non-linear terms of the thermodynamic equation 2.15 K_T are computed using T' only in equation 2.20. The spherical harmonic coefficients $(K_{T'})_n^m$ are then computed using 2.25 and A.6:

$$
\begin{aligned}
(K_{T'})_n^m = & +\frac{1}{4\pi a} \sum_{j=1}^{J_{grid}} \sum_{i=1}^{I_{grid}} \frac{im U T' P_n^m(\mu_j) + V T' H_n^m(\mu_j)}{(1 - \mu_j^2)} e^{-im\lambda_i} \Delta\lambda\Delta\mu_j \\
& +\frac{1}{4\pi} \sum_{j=1}^{J_{grid}} \sum_{i=1}^{I_{grid}} \frac{W_{k+0.5}(\gamma_{k+1} T'_{k+1} + \gamma_k T'_k)}{2\gamma_k \rho_{0k} \Delta z} P_n^m(\mu_j) e^{-im\lambda_i} \Delta\lambda\Delta\mu_j \\
& -\frac{1}{4\pi} \sum_{j=1}^{J_{grid}} \sum_{i=1}^{I_{grid}} \frac{W_{k-0.5}(\gamma_k T'_k + \gamma_{k-1} T'_{k-1})}{2\gamma_k \rho_{0k} \Delta z} P_n^m(\mu_j) e^{-im\lambda_i} \Delta\lambda\Delta\mu_j
\end{aligned}
\tag{2.51}
$$

5. The vorticity equation 2.21 is solved explicitely. Using a leap-frog scheme and let the superscript t denote the timestep, one obtaines from equation 2.21:

$$
\begin{aligned}
\left(\zeta^{t+\Delta t}\right)_n^m \;=\; & +\left(\zeta^{t-\Delta t}\right)_n^m \\
& -\frac{2\Delta t}{4\pi a}\sum_{j=1}^{J_{grid}}\sum_{i=1}^{I_{grid}}\frac{imK_V^t P_n^m(\mu_j)}{(1-\mu_j^2)}e^{-im\lambda_i}\Delta\lambda\Delta\mu_j \\
& +\frac{2\Delta t}{4\pi a}\sum_{j=1}^{J_{grid}}\sum_{i=1}^{I_{grid}}\frac{K_U^t H_n^m(\mu_j)}{(1-\mu_j^2)}e^{-im\lambda_i}\Delta\lambda\Delta\mu_j \\
& +2\Delta t\left(F_\zeta^t\right)_n^m
\end{aligned}
\tag{2.52}
$$

6. The divergence- and thermodynamic equation are already discussed in Section 2.4.3. The explicitely computed terms marked by $\cdots$ in equations 2.40 and 2.41 now become:

$$
\begin{aligned}
\overset{(2.39)}{\cdots} \;=\; & -\frac{1}{4\pi a}\sum_{j=1}^{J_{grid}}\sum_{i=1}^{I_{grid}}\frac{imK_U P_n^m(\mu_j)+K_V H_n^m(\mu_j)}{1-\mu_j^2}e^{-im\lambda_i}\Delta\lambda\Delta\mu_j \\
& +\frac{n(n+1)}{4\pi a^2}\sum_{j=1}^{J_{grid}}\sum_{i=1}^{I_{grid}}\frac{U^2+V^2}{2(1-\mu_j^2)}P_n^m(\mu_j)e^{-im\lambda_i}\Delta\lambda\Delta\mu_j \\
& +\left(F_D\right)_n^m
\end{aligned}
\tag{2.53}
$$

$$
\overset{(2.40)}{\cdots} = -\left(K_{T'}\right)_n^m + Q_n^m
\tag{2.54}
$$

3 Transport of idealized Tracers

3.1 Introduction

The behavor of middle atmospheric trace constituents is simulated entirely on the Gaussian grid introduced in Section 2.4.

Section 3.2 describes the algorithm that computes the flux divergencies of the prognostic chemical variables. In this model, the transport algorithm is applied to a set of idealized tracers only that is described in section 3.3. In future versions of the model this algorithm will be applied to transport chemical active middle atmospheric trace constituents. Their chemical sources and sinks will be simulated by a detailled chemical module.

3.2 The Transport Algorithm

The behavor of atmospheric trace constituents is simulated by integrating balance equations for their mixing ratios in time of the form:

$$\frac{\partial q}{\partial t} = -\vec{\nabla}_p \cdot (\vec{v}_p q) - \frac{1}{\rho_0} \frac{\partial \rho_0 w q}{\partial z} + S \tag{3.1}$$

where q and S denote the mixing ratio and the sources and sinks, respectively.

The first two terms on the right hand side of equation 3.1 describe the horizontal and vertical flux divergence. When reduced to a one dimensional problem, the flux divergence is computed by

$$\frac{\partial u q}{\partial x} \approx \frac{f_{i+0.5} - f_{i-0.5}}{\Delta x} \tag{3.2}$$

where $f = uq$ is the flux of q, the subscript i is the actual gridpoint and Δx is the distance between the gridpoints. The flux f is computed using a two step flux corrected transport (FCT) algorithm introduced by *Zalesak* [1979]:

1. An 1. order upwind scheme from *Courant et al.* [1952]:

$$f_{i+0.5}^{UP} = 0.5 \left(u_{i+0.5} + |u_{i+0.5}| \right) q_i + 0.5 \left(u_{i+0.5} - |u_{i+0.5}| \right) q_{i+1} \tag{3.3}$$

2. An antidiffusive step based on the difference between the Lax-Wendrof [*Lax and Wendroff*, 1960] and the 1. order upwind scheme multiplied by a limiter function $\Phi(r)$:

$$
\begin{aligned}
f_{i+0.5}^{FC} = & +0.5 \left(u_{i+0.5} + |u_{i+0.5}| \right) q_i + 0.5 \left(u_{i+0.5} - |u_{i+0.5}| \right) q_{i+1} \\
& +\Phi(r_{i+0.5}) 0.5 |u_{i+0.5}| \left(1 - \frac{\Delta t}{\Delta x} |u_{i+0.5}| \right) (q_{i+1} - q_i)
\end{aligned}
\tag{3.4}
$$

where the limiter function $\Phi(r)$ is given by *Roe and Baines* [1982]:

$$\Phi(r) = \max\left(0, \min(2r, 1), \min(r, 2)\right) \tag{3.5}$$

with

$$
r_{i+0.5} = \begin{cases} \frac{q_i - q_{i-1}}{q_{i+1} - q_i} & \text{for} \quad u_{i+1} \geq 0 \\ \frac{q_{i+2} - q_{i+1}}{q_{i+1} - q_i} & \text{for} \quad u_{i+1} < 0 \end{cases}
\tag{3.6}
$$

The total flux is given by

$$f_{i+0.5} = f_{i+0.5}^{UP} + f_{i+0.5}^{FC} \tag{3.7}$$

3.3 Transport of idealized Tracers

With this version the transport of 4 idealized tracers is possible. The difference between these tracers is the initial condition, that is defined as follows:

- The sine of geographic latitude

- The pressure altitude in km

- Ertel's potential vorticity of the initialization timestep

- The potential temperature of the initialization timestep

The tracers have no chemical sources or sinks.

4 Physical Parameterizations

4.1 Introduction

The model is driven by the competetive action of the net heating rate and the effects of breaking gravity waves on the model atmosphere. A detailled description of their algorithms is given in Sections 4.2 and 4.3.

4.2 The Radiation

The net heating rate Q is obtained from the balance of the absorption of ultraviolet solar radiation by ozone in the stratosphere and molecular oxygene in the thermosphere and the infrared cooling.

The absorption of ultraviolet radiation is parameterized by the scheme of *Strobel* [1978]. It takes into account the radiative heating by ozone absorption in the Hartley region (200-300 nm), Huggins bands (300-350 nm), and Chappius bands (450-750 nm). Above the mesopause, O_2 absorption in the Schumann-Runge bands (175-205 nm) and the Schumann-Runge continuum (125-175 nm) is included.

The parameterization is based on the computation of either constant or exponentially functions dependent on the wavenumber of the absorption cross sections and the solar fluxes. Some Parameters are modifies according to *Apruzese et al.* [1982]. The single absorption bands are parameterized by the following formulars:

- The Chapius Bands:

$$\frac{Q_C}{[O_3]} = F_C \sigma_C \exp(-\sigma_C N_3) \tag{4.1}$$

with $F_C = 3.7 \times 10^5 \; ergs \; cm^{-2} \; s^{-1}$ and $\sigma_C = 2.85 \times 10^{-21} \; cm^2$.

- The Hartley Region:

$$\frac{Q_{Ha}}{[O_3]} = F_{Ha} \sigma_{Ha} \exp(-\sigma_{Ha} N_3) \tag{4.2}$$

with $F_{Ha} = 4600 \ ergs \ cm^{-2} \ s^{-1}$ and $\sigma_{Ha} = 8.8 \times 10^{-18} \ cm^2$.

● The Huggins Bands:

$$\frac{Q_{Hu}}{[O_3]} = \frac{1}{MN_3}\{(I_1 + (I_2 - I_1)\exp(-\sigma_{Hu}N_3 e^{-M\lambda_{long}})$$

$$-I_2 \exp(-\sigma_{Hu}N_3 e^{-M\lambda_{short}})\} \qquad (4.3)$$

with $I_1 = 59.2 \ ergs \ cm^{-2} \ s^{-1} \ A^{-1}$, $I_2 = 40.0 \ ergs \ cm^{-2} \ s^{-1} \ A^{-1}$, $M = 0.0127A^{-1}$, $\lambda_{short} = 2805 \ A$, $\lambda_{long} = 3055 \ A$, and $\sigma_{Hu} = 0.0125 \ cm^2$.

● The Herzberg Continuum:

$$Q_{Hz} = F_{Hz}\{\sigma_{Hz}(O_2)[O_2] + \sigma_{Hz}(O_3)[O_3]\}$$

$$\exp[-\sigma_{Hz}(O_2)N_2 - \sigma_{Hz}(O_3)NO_3] \qquad (4.4)$$

with $F_{Hz} = 1.2 \times 10^3 \ ergs \ cm^{-2} \ s^{-1}$, $\sigma_{Hz}(O_2) = 6.6 \times 10^{-24}cm^2$, and $\sigma_{Hz}(O_3) = 4.9 \times 10^{-18}cm^2$.

● The Schumann-Runge Continuum is computed in two terms:

$$\frac{Q_{SRC}}{[O_2]} = F_{SRC}\sigma_{SRC}\exp\{-\sigma_{SRC}N_2\}$$

$$+ \frac{1}{N_2}\left\{\frac{I_l}{M}e^{-\sigma_l N_2} + \frac{I_s - I_l}{M}e^{-\sigma_m N_2} - \frac{I_s}{M}e^{-\sigma_s N_2}\right\} \qquad (4.5)$$

with $F_{SRC} = 1.1 \ ergs \ cm^{-2} \ s^{-1}$, $\sigma_{SRC} = 10^{-17}cm^2$, $\frac{I_l}{M} = 3.43 \ ergs \ cm^{-2} \ s^{-1}$, $\frac{I_s}{M} = 1.35 \ ergs \ cm^{-2} \ s^{-1}$, $\sigma_l = 2.9 \times 10^{-19}cm^2$, $\sigma_m = 1.7 \times 10^{-18}cm^2$, and $\sigma_s = 1.1 \times 10^{-17}cm^2$.

● The Schumann-Runge Bands:

$$\frac{Q_{SRB}}{[O_2]} = \begin{cases} 1/(aN_2 + bN_2^{0.5}) & \text{for} \quad N_2 \geq 10^{18} \ cm^{-2} \\ 2.43 \times 10^{-19}ergs \ s^{-1} & \text{for} \quad N_2 < 10^{18} \ cm^{-2} \end{cases} \qquad (4.6)$$

with $a = 0.67$, and $b = 3.44 \times 10^{-19}$ (in cgs units).

In the equations 4.1-4.6 N_2, N_3, $[O_2]$, and $[O_3]$ denote the colmumn densities and concentratopns of O_2 and O_3, respectively. The heating rate due to the absorption of UV radiation Q_{UV} is then computed by the sum of equations 4.1-4.6:

$$Q_{UV} = Q_C + Q_{Ha} + Q_{Hu} + Q_{Hz} + Q_{SRC} + Q_{SRB} \qquad (4.7)$$

The cooling rates due to infrared radiation are parameterized in two steps:

1. An only vertical and time dependent term being equal to the global mean value of Q_{UV}:

$$Q_{IR_1}(z,t) = -\frac{1}{4\pi} \int_{-1}^{+1} \int_{0}^{2\pi} Q_{UV}(\lambda, \mu, z, t) d\lambda d\mu \tag{4.8}$$

2. A Newtonian Cooling Term of the form:

$$Q_{IR_2}(z,t) = -\alpha(z)\{T(\lambda, \mu, z, t) - T^*(z)\} \tag{4.9}$$

where the Newtonian cooling coefficient $\alpha(z)$ is taken from *Wehrbein and Leovy* [1982].

4.3   The Effects of Breaking Gravity Waves

The effects of gravity waves are implemented according to the theory of breaking gravity waves of *Lindzen* [1981]. Lindzen applied the theory of internal gravity waves on a basic flow with weak vertical shear compared to the vertical component of the gravity wavenumber vector in an atmosphere with constant static stability. With these assumptions a simplified set of the primitive equations 2.1-2.4 describing internal gravity waves can be solved analytically. From the solution the following quantities relevant for the parameterization scheme can be derived [*Holton*, 1982]:

- The breaking level z_b is computed from the assumption of momentum and energy conservation of an undamped gravity wave leading to an increase of wave amplitude with height due to the decrease of density. Assuming a non-zero vertical momentum flux of the gravity wave, the static becomes locally unstable at some altitude resulting in convection. This breaking level is computed by:

$$z_b = 3H \ln \left(\frac{|\bar{u} - c|}{\tilde{u}} \right), \tag{4.10}$$

where

$$\tilde{u} = \left(2 \, \overline{u'w'} \, \frac{N}{k} \right)^{1/3} \tag{4.11}$$

is a measure of wave amplitude, $\bar{u}$ is the component of the horizontal basic flow parallel to the horizontal wavenumber vector, $\overline{u'w'}$ is the vertical momentum flux devided by the basic state density ρ_0, k is the absolute value of the horizontal wave number vector and c is the phase velocity of the gravity wave.

- The critical level is the level where the component of the basic flow parallel to the wavenumber vector is equal to the phase velocity of the gravity wave.

- Between the breaking and the critical level the convection processes are parameterized by vertical diffusion D and an force per unit mass F parallel to the horizontal wavenumber vector:

$$D = \frac{k(\bar{u} - c)^4}{N^3} \left[\frac{1}{2H} - \frac{3}{2} \frac{\partial \bar{u}/\partial z}{\bar{u} - c} \right], \tag{4.12}$$

$$F = \frac{N^2 D}{\bar{u} - c}, \tag{4.13}$$

where k is the absolute value of the horizontal wavenumber vector.

The parameterization scheme described above is actually implemented as follows:

- The vertical momentum flux is an analytical function of the phase velocity and direction of the horizontal wavenumber vector:

$$\overline{u'w'} = \left(\overline{u'w'} \right)_0 \exp \left[-\frac{(c - c_0)^2}{\sigma^2} \right], \tag{4.14}$$

where $\left(\overline{u'w'} \right)_0 = 10^{-3} \ m^2/s^2$, $c_0 = 8 \ m/s \cos\theta$, and $\sigma = \sqrt{\sigma_x^2 + \sigma_y^2}$ with $\sigma_x = 25 \ m/s \cos\theta$, and $\sigma_y = 20 \ m/s \sin\theta$, is. θ is the angle towards east of the horizontal wavenumber vector.

- The absolut value of the horizontal wavenumber vector is constant:

$$k = \frac{2\pi}{120 \ km}. \tag{4.15}$$

- A spectrum of 12 independent gravity waves is implemented with three phasevelocities (8, 16, and 41 m/s) and four directions of the horizontal wavenumber vector pointing to the four cardinal points.

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A   Mathematical Symbols and Relations

A.1   List of Symbols

a Radius of the earth $(a = 6366\ km)$

c_p Specific heat of dry air at constant pressure $(c_p = 1005\ J\ kg^{-1}\ K^{-1})$

D Horizontal divergence

$$
\begin{aligned}
D &= \vec{\nabla}_p \cdot \vec{v}_p = \vec{\nabla}_p^2 \chi \\
&= \frac{1}{a\cos\varphi}\frac{\partial u}{\partial \lambda} + \frac{1}{a\cos\varphi}\frac{\partial v\cos\varphi}{\partial\varphi} \\
&= \frac{1}{a(1-\mu^2)}\frac{\partial U}{\partial\lambda} + \frac{1}{a}\frac{\partial V}{\partial\mu}
\end{aligned} \tag{A.1}
$$

$\dfrac{D\alpha}{Dt}$ time rate of change of α following the motion

    1.The advection form:

$$
\begin{aligned}
\frac{D\alpha}{Dt} &= \frac{\partial\alpha}{\partial t} + \vec{v}_p \cdot \vec{\nabla}_p\alpha + w\frac{\partial\alpha}{\partial z} \\
&= \frac{\partial\alpha}{\partial t} + \frac{u}{a\cos\varphi}\frac{\partial\alpha}{\partial\lambda} + \frac{v}{a}\frac{\partial\alpha}{\partial\varphi} + w\frac{\partial\alpha}{\partial z} \\
&= \frac{\partial\alpha}{\partial t} + \frac{U}{a(1-\mu^2)}\frac{\partial\alpha}{\partial\lambda} + \frac{V}{a}\frac{\partial\alpha}{\partial\mu} + w\frac{\partial\alpha}{\partial z}
\end{aligned} \tag{A.2}
$$

    2.The flux form is obtained using equation 2.4:

$$
\begin{aligned}
\frac{D\alpha}{Dt} &= \frac{\partial\alpha}{\partial t} + \vec{\nabla}_p \cdot (\vec{v}_p\alpha) + \frac{1}{\rho_0}\frac{\partial\rho_0 w\alpha}{\partial z} \\
&= \frac{\partial\alpha}{\partial t} + \frac{1}{a\cos\varphi}\left(\frac{\partial u\alpha}{\partial\lambda} + \frac{\partial v\alpha\cos\varphi}{\partial\varphi}\right) \\
&\quad + \frac{1}{\rho_0}\frac{\partial\rho_0 w\alpha}{\partial z} \\
&= \frac{\partial\alpha}{\partial t} + \frac{1}{a(1-\mu^2)}\frac{\partial U\alpha}{\partial\lambda} + \frac{1}{a}\frac{\partial V\alpha}{\partial\mu} + \frac{1}{\rho_0}\frac{\partial\rho_0 w\alpha}{\partial z}
\end{aligned} \tag{A.3}
$$

f Coriolis Parameter $(f = 2\Omega\sin\varphi = 2\Omega\mu)$

$\vec{F}$, F_λ, F_φ Additional forces in zonal and meridional direction, respectively

F_ζ

$$F_\zeta = \vec{k} \cdot \vec{\nabla}_p \times \vec{F} \tag{A.4}$$

F_D

$$F_D = \vec{\nabla}_p \cdot \vec{F} \tag{A.5}$$

H Atmospheric Scale Height ($H = 7\ km$)

I_{grid} No. of zonal

J_{grid} No. of meridional gridpoints

k_{grid} No. of model layers

$\vec{i}$ Zonal unit vector

$\vec{j}$ Meridional unit vector

$\vec{k}$ Vertical unit vector

p Pressure

p_0 Constant reference pressure ($p_0 = 1013\ hPa$)

T Temperature

$T^*(z)$ Reference temperature (US-Standard Atmosphere)

Q Net Heating Rate

R Gas constant of dry air ($R = 287.04\ J\ kg^{-1}\ K^{-1}$)

u Zonal component of velocity

$$u = \frac{1}{a\cos\varphi}\frac{\partial\chi}{\partial\lambda} - \frac{1}{a}\frac{\partial\Psi}{\partial\varphi} = \frac{1}{a\sqrt{1-\mu^2}}\frac{\partial\chi}{\partial\lambda} - \frac{\sqrt{1-\mu^2}}{a}\frac{\partial\Psi}{\partial\mu} \tag{A.6}$$

U

$$\begin{aligned}
U &= u\cos\varphi \\
&= \frac{1}{a}\frac{\partial\chi}{\partial\lambda} - \frac{\cos\varphi}{a}\frac{\partial\Psi}{\partial\varphi} \\
&= \frac{1}{a}\frac{\partial\chi}{\partial\lambda} - \frac{(1-\mu^2)}{a}\frac{\partial\Psi}{\partial\mu} \tag{A.7}
\end{aligned}$$

v Meridional component of velocity

$$v = \frac{1}{a}\frac{\partial \chi}{\partial \varphi} + \frac{1}{a\cos\varphi}\frac{\partial \Psi}{\partial \lambda} = \frac{\sqrt{1-\mu^2}}{a}\frac{\partial \chi}{\partial \mu} + \frac{1}{a\sqrt{1-\mu^2}}\frac{\partial \Psi}{\partial \lambda} \qquad (A.8)$$

V

$$
\begin{aligned}
V &= v\cos\varphi \\
&= \frac{\cos\varphi}{a}\frac{\partial \chi}{\partial \varphi} + \frac{1}{a}\frac{\partial \Psi}{\partial \lambda} \\
&= \frac{(1-\mu^2)}{a}\frac{\partial \chi}{\partial \mu} + \frac{1}{a}\frac{\partial \Psi}{\partial \lambda} \qquad (A.9)
\end{aligned}
$$

$\vec{v}$ Three dimensional velocity vector $(\vec{v} = u\vec{i} + v\vec{j} + w\vec{k})$

$\vec{v}_p$ Horizontal velocity vector on pressure surface

$$\vec{v}_p = u\vec{i} + v\vec{j} = \vec{\nabla}_p\chi + \vec{k} \times \vec{\nabla}_p\Psi \qquad (A.10)$$

w Vertical component of velocity

W

$$W = \rho_0 w \qquad (A.11)$$

z Vertical coordinate $(z = -H\ln(p/p_0))$

γ Conversion factor between temperature and potential temperature $\theta = \gamma(z)T$:

$$\gamma(z) = \exp\left(\frac{\kappa z}{H}\right) \qquad (A.12)$$

χ Horizontal velocity potential on pressure surface (see equation A.1)

Δt Timestep

Δz Distance between 2 model layers

$\Delta \lambda$ Distance between 2 zonal gridpoints

$$\Delta\lambda = \frac{2\pi}{I_{grid}} \qquad (A.13)$$

$\Delta\mu_i$ Gaussian weight at $\mu = \mu_i$

$$\Delta\mu_i = \frac{2}{(1-\mu_i^2)^2\,[P_n'(\mu_i)]^2} \qquad (A.14)$$

Φ Geopotential

φ Geographical latitude

κ Ratio of gas constant over specific heat at constant pressure of dry air
$(\kappa = R/c_p)$

λ Geographical longitude

μ Alternate meridional coordinate $\mu = \sin(\varphi)$

$$\mu = \sin \varphi \tag{A.15}$$

Ψ Vertical component of velocity stream function (see equation A.16)

ρ_0 Basic state density $(\rho_0 \sim \exp(-z/H))$

Ω Absolute value of angular velocity of the earth $\Omega = 2\pi day^{-1}$

$\vec{\Omega}$ Angular velocity of the earth

ζ Relative vorticity

$$
\begin{aligned}
\zeta &= \vec{k} \cdot \vec{\nabla}_p \times \vec{v}_p = \vec{\nabla}_p^2 \Psi \\
&= \frac{1}{a \cos \varphi} \frac{\partial v}{\partial \lambda} - \frac{1}{a \cos \varphi} \frac{\partial u \cos \varphi}{\partial \varphi} \\
&= \frac{1}{a(1 - \mu^2)} \frac{\partial V}{\partial \lambda} - \frac{1}{a} \frac{\partial U}{\partial \mu}
\end{aligned} \tag{A.16}
$$

ζ_a Absolute vorticity $(\zeta_a = \zeta + f)$

$\vec{\nabla}_p \alpha$ Gradient of α on constant pressure surface

$$
\begin{aligned}
\vec{\nabla}_p \alpha &= \frac{1}{a \cos \varphi} \frac{\partial \alpha}{\partial \lambda} \vec{i} + \frac{1}{a} \frac{\partial \alpha}{\partial \varphi} \vec{j} \\
&= \frac{1}{a\sqrt{1 - \mu^2}} \frac{\partial \alpha}{\partial \lambda} \vec{i} + \frac{\sqrt{1 - \mu^2}}{a} \frac{\partial \alpha}{\partial \mu} \vec{j}
\end{aligned} \tag{A.17}
$$

$\vec{\nabla}_p \cdot \vec{\alpha}$ Divergence of $\vec{\alpha} = \alpha_\lambda \vec{i} + \alpha_\varphi \vec{j}$ on pressure surface

$$
\begin{aligned}
\vec{\nabla}_p \cdot \vec{\alpha} &= \frac{1}{a \cos \varphi} \frac{\partial \alpha_\lambda}{\partial \lambda} + \frac{1}{a \cos \varphi} \frac{\partial \alpha_\varphi \cos \varphi}{\partial \varphi} \\
&= \frac{1}{a\sqrt{1 - \mu^2}} \frac{\partial \alpha_\lambda}{\partial \lambda} + \frac{1}{a} \frac{\partial \alpha_\varphi \sqrt{1 - \mu^2}}{\partial \mu}
\end{aligned} \tag{A.18}
$$

$\vec{\nabla}_p \times \vec{\alpha}$ Vertical component of $\vec{\nabla} \times \vec{\alpha}$, $\vec{\alpha} = \alpha_\lambda \vec{i} + \alpha_\varphi \vec{j}$ on pressure surface

$$
\begin{aligned}
\vec{\nabla}_p \times \vec{\alpha} &= \vec{k} \cdot \vec{\nabla} \times \vec{\alpha} \\
&= \frac{1}{a \cos\varphi} \frac{\partial \alpha_\varphi}{\partial \lambda} - \frac{1}{a \cos\varphi} \frac{\partial \alpha_\lambda \cos\varphi}{\partial \varphi} \\
&= \frac{1}{a\sqrt{1-\mu^2}} \frac{\partial \alpha_\varphi}{\partial \lambda} - \frac{1}{a} \frac{\partial \alpha_\lambda \sqrt{1-\mu^2}}{\partial \mu}
\end{aligned}
\tag{A.19}
$$

$\vec{\nabla}_p^2 \alpha$ Horizontal Laplacian of α on pressure surface

$$
\begin{aligned}
\vec{\nabla}_p^2 \alpha &= \vec{\nabla}_p \cdot \vec{\nabla}_p \alpha \\
&= \frac{1}{a^2 \cos^2\varphi} \frac{\partial^2 \alpha}{\partial \lambda^2} + \frac{1}{a^2 \cos\varphi} \frac{\partial}{\partial \varphi} \left[\cos\varphi \frac{\partial \alpha}{\partial \varphi} \right] \\
&= \frac{1}{a^2(1-\mu^2)} \frac{\partial^2 \alpha}{\partial \lambda^2} + \frac{1}{a^2} \frac{\partial}{\partial \mu} \left[(1-\mu^2) \frac{\partial \alpha}{\partial \mu} \right]
\end{aligned}
\tag{A.20}
$$

A.2   Vector Operations

If $\vec{A}$, $\vec{B}$, $\vec{C}$ denote arbitrary three-dimensional vectorfields and α denotes an arbitrary scalar field, the following vector operations apply (partly adapted from *Haltiner and Williams* [1980]).

$$
\begin{aligned}
\vec{A} \cdot (\vec{B} \times \vec{C}) &= (\vec{A} \times \vec{B}) \cdot \vec{C} \\
&= (\vec{C} \times \vec{A}) \cdot \vec{B}
\end{aligned}
\tag{A.21}
$$

$$
\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\vec{B} - (\vec{A} \cdot \vec{B})\vec{C}
\tag{A.22}
$$

$$\vec{\nabla} \times \vec{\nabla}\alpha = 0$$
$$\vec{\nabla} \cdot \vec{\nabla} \times \vec{A} = 0 \qquad \text{(A.23)}$$

$$\vec{\nabla} \cdot (\alpha\vec{A}) = \alpha\vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla}\alpha$$
$$\vec{\nabla} \times (\alpha\vec{A}) = \alpha\vec{\nabla} \times \vec{A} - \vec{A} \times \vec{\nabla}\alpha \qquad \text{(A.24)}$$

$$\vec{\nabla}(\vec{A} \cdot \vec{B}) = (\vec{A} \cdot \vec{\nabla})\vec{B} + (\vec{B} \cdot \vec{\nabla})\vec{A} + \vec{A} \times (\vec{\nabla} \times \vec{B}) + \vec{B} \times (\vec{\nabla} \times \vec{A}) \qquad \text{(A.25)}$$

$$\vec{\nabla} \cdot (\vec{A}\vec{B}) = \vec{B}\vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla}\vec{B} \qquad \text{(A.26)}$$

$$\vec{\nabla} \cdot (\vec{A} \times \vec{B}) = \vec{B} \cdot \vec{\nabla} \times \vec{A} - \vec{A} \cdot \vec{\nabla} \times \vec{B} \qquad \text{(A.27)}$$

$$\vec{\nabla} \times (\vec{A} \times \vec{B}) = \vec{A}\vec{\nabla} \cdot \vec{B} - \vec{B}\vec{\nabla} \cdot \vec{A} + (\vec{B} \cdot \vec{\nabla})\vec{A} - (\vec{A} \cdot \vec{\nabla})\vec{B} \qquad \text{(A.28)}$$

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{A}) = \vec{\nabla}(\vec{\nabla} \cdot \vec{A}) - \vec{\nabla}^2\vec{A} \qquad \text{(A.29)}$$

Let $\vec{A} = \vec{A}_\psi + \vec{A}_\chi$, where $\vec{\nabla} \times \vec{A}_\chi = 0$ and $\vec{\nabla} \cdot \vec{A}_\psi = 0$, then:

$$\vec{A}_\chi = \vec{\nabla}\chi \quad , \quad \vec{A}_\psi = -\vec{\nabla} \times \vec{\psi}$$
$$\vec{\nabla}^2\chi = \vec{\nabla} \cdot \vec{A}_\chi = \vec{\nabla} \cdot \vec{A} \quad , \quad \vec{\nabla}^2\vec{\psi} = \vec{\nabla} \times \vec{A}_\psi = \vec{\nabla} \times \vec{A} \qquad \text{(A.30)}$$

A.3 The Spherical Harmonics

The associated Legendre polynomials $Q_n^m(\mu)$ can be computed by:

$$
\begin{aligned}
Q_n^m(\mu) &= \frac{1}{2^m} \frac{(n+m)!}{(n-m)!m!} \left(1 - \mu^2\right)^{m/2} \cdot F\left(m-n, m+n+1; m+1; \frac{1-\mu}{2}\right) \\
&= \left(1 - \mu^2\right)^{m/2} \frac{d^m}{d\mu^m} Q_n(\mu) \\
&= \frac{(1 - \mu^2)^{m/2}}{2^n n!} \frac{d^{n+m}}{d\mu^{n+m}} (\mu^2 - 1)^n \\
&= (-1)^{n+m} Q_n^m(-\mu) \tag{A.31}
\end{aligned}
$$

for $(-1 < \mu < 1)$, $n = 0, 1, 2, \cdots \ldots$, and $-n \leq m \leq n$ [*Korn and Korn*, 1968]. F is the hypergeometric series defined by

$$
\begin{aligned}
F(\alpha, \beta, \gamma, \mu) &= 1 + \frac{\alpha \cdot \beta}{1 \cdot \gamma} \mu + \frac{\alpha(\alpha+1)\beta(\beta+1)}{1 \cdot 2 \cdot \gamma(\gamma+1)} \mu^2 + \cdots \\
&\quad + \frac{\alpha(\alpha+1)\cdots(\alpha+n)\beta(\beta+1)\cdots(\beta+n)}{1 \cdot 2 \cdots \cdots (n+1)\gamma(\gamma+1)\cdots(\gamma+n)} \mu^{n+1} + \cdots \tag{A.32}
\end{aligned}
$$

[e.g. *Bronstein and Semendjajew*, 1975]. The non-normalized $Q_n^m(\mu)$ defined by equation A.31 satisfy the following recurrence relations [*Korn and Korn*, 1968]:

$$
(2n+1)\mu Q_n^m(\mu) - (n-m+1)Q_{n+1}^m(\mu) - (n+m)Q_{n-1}^m(\mu) = 0 \tag{A.33}
$$

$$
-\left(1 - \mu^2\right)\frac{dQ_n^m(\mu)}{d\mu} - (n-m+1)Q_{n+1}^m(\mu) + (n+1)\mu Q_n^m(\mu) = 0 \tag{A.34}
$$

Combining A.33 and A.34 yields:

$$
\begin{aligned}
\left(1 - \mu^2\right)\frac{dQ_n^m(\mu)}{d\mu} &= -\frac{n(n-m+1)}{2n+1} Q_{n+1}^m(\mu) \\
&\quad + \frac{(n+1)(n+m)}{(2n+1)} Q_{n-1}^m(\mu) \tag{A.35}
\end{aligned}
$$

The norm Y_n^m of $Q_n^m(\mu)$ is obtained from the orthogonality relation:

$$
\int_0^{+1} Q_n^m(\mu) Q_l^m(\mu) d\mu = \frac{1}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_n^l \tag{A.36}
$$

$$Y_n^m = \sqrt{\frac{1}{2n+1}\frac{(n+m)!}{(n-m)!}} \tag{A.37}$$

Hereafter and throughout the text of this document $P_n^m(\mu)$ refers to the normalized associated Legendre polynomial:

$$P_n^m(\mu) = \frac{Q_n^m(\mu)}{Y_n^m} \tag{A.38}$$

Equation A.35 becomes for the normalized associated Legendre Polynomials $P_n^m(\mu)$ using equation A.37 and A.38:

$$\begin{aligned} H_n^m(\mu) &= -\left(1-\mu^2\right)\frac{dP_n^m(\mu)}{d\mu} \\ &= n\epsilon_{n+1}^m P_{n+1}^m(\mu) - (n+1)\epsilon_n^m P_{n-1}^m(\mu) \end{aligned} \tag{A.39}$$

where

$$\epsilon_n^m = \sqrt{\frac{n^2-m^2}{4n^2-1}} \tag{A.40}$$

The spherical harmonics of degree n and order m $P_n^m(\mu)e^{\imath m\lambda}$ are solutions of the differential equation:

$$\vec{\nabla}_p^2\left[P_n^m(\mu)e^{\imath m\lambda}\right] + \frac{n(n+1)}{a^2}P_n^m(\mu)e^{\imath m\lambda} = 0 \tag{A.41}$$

They obey the orthogonality relation (using A.36):

$$\frac{1}{4\pi}\int\limits_{-1}^{+1}\int\limits_0^{2\pi} P_n^m(\mu)e^{\imath m\lambda}P_l^k(\mu)e^{-\imath k\lambda}d\lambda d\mu = \delta_k^m\delta_l^n \tag{A.42}$$

Any steady and differentiable field on a sphere can be developped in an infinite series of spherical harmonics:

$$X(\lambda,\mu) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} X_n^m P_n^m(\mu)e^{\imath m\lambda} \tag{A.43}$$

where the complex coefficients X_n^m are given by:

$$X_n^m = \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} X(\lambda, \mu) P_n^m(\mu) e^{-im\lambda} d\lambda d\mu \qquad \text{(A.44)}$$

Some properties of spherical harmonics are derived below:

$$\left[\frac{\partial X(\lambda, \mu)}{\partial \lambda} \right]_l^k = \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} \frac{\partial X(\lambda, \mu)}{\partial \lambda} P_l^k(\mu) e^{-ik\lambda} d\lambda d\mu$$

$$\stackrel{(A.43)}{=} \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} \frac{\partial}{\partial \lambda} \left[\sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(X_n^m P_n^m(\mu) e^{im\lambda} \right) \right] P_l^k(\mu) e^{-ik\lambda} d\lambda d\mu$$

$$= \frac{1}{4\pi} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left[im X_n^m \int\limits_{-1}^{+1} \int\limits_0^{2\pi} P_n^m(\mu) P_l^k(\mu) e^{im\lambda} e^{-ik\lambda} d\lambda d\mu \right]$$

$$\stackrel{(A.42)}{=} ik X_l^k$$

$$\stackrel{(A.44)}{=} \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} ik X(\lambda, \mu) P_l^k(\mu) e^{-ik\lambda} d\lambda d\mu \qquad \text{(A.45)}$$

Integration by parts (i.e.: $\int f'(x)g(x)dx = f(x)g(x) - \int f(x)g'(x)dx$), with $f(\mu) = X(\lambda, \mu)$ and $g(\mu) = P_n^m(\mu)$ yields using A.39

$$\left[\frac{\partial X(\lambda, \mu)}{\partial \mu} \right]_n^m \stackrel{(A.44)}{=} \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} \frac{\partial X(\lambda, \mu)}{\partial \mu} P_n^m(\mu) e^{-im\lambda} d\lambda d\mu$$

$$\stackrel{(A.39)}{=} + \frac{1}{2\pi} \int\limits_0^{2\pi} [X(\lambda, \mu) P_n^m(\mu)]_{\mu=-1}^{\mu=+1} e^{-im\lambda} d\lambda$$

$$+ \frac{1}{4\pi} \int\limits_{-1}^{+1} \int\limits_0^{2\pi} \frac{X(\lambda, \mu)}{(1 - \mu^2)} H_n^m(\mu) e^{-im\lambda} d\lambda d\mu \qquad \text{(A.46)}$$

B   Module Overview

B.1   Naming Conventions

In order to obtain a quick overview on the specific task or a certain component a single subroutine of the model belongs to, the first two letters of a subroutine name are attempted to satisfy the following conventions:

ch... a chemical module

di... a diagnostic module

dy... a dynamical module

rd... a radiation module

pl... a plotprogram, interface to the commercial graphic software

The following sections provide an overview of the most importent modules of the model.

B.2   Internal Modules

Module CHEMIE   Main entry to compute chemistry (see section 3)

Module CHTRAC   computes the transport of idealized tracers (see section 3.3)

Module DFLUXX   computes the flux through the boundary on the merdional plane between the actual gridpoint and the adjacent westard gridpoint according to the algorithm described in section 3.2.

Table B.1: Parameter List of module dfluxx

Name	Type	Description
wert	real*8	3-D array on the model grid of the quantity to be transported (Input)
flux	real*8	3-D array on the model grid of the flux of the quantity through the boundary between the two gridpoints (Output)
ddt	real*8	Timestep used for the actual iteration (Input)

Module DFLUXY computes the flux through the boundary on the height-longitude plane between the actual gridpoint and the adjacent southward gridpoint according to the algorithm described in section 3.2.

Table B.2: Parameter List of module dfluxy

Name	Type	Description
wert	real*8	3-D array on the model grid of the quantity to be transported (Input)
flux	real*8	3-D array on the model grid of the flux of the quantity through the boundary between the two gridpoints (Output)
ddt	real*8	Timestep used for the actual iteration (Input)

Module DFLUXZ computes the flux through the boundary on the horzontal plane between the actual gridpoint and the adjacent downward gridpoint according to the algorithm described in section 3.2.

Table B.3: Parameter List of module `dfluxz`

Name	Type	Description
wert	real*8	3-D array on the model grid of the quantity to be transported (Input)
flux	real*8	3-D array on the model grid of the flux of the quantity through the boundary between the two gridpoints (Output)
ddt	real*8	Timestep used for the actual iteration (Input)

Module DIFEDD   computes the eddy diffusion due to breaking gravity waves

Table B.4: Parameter List of module `difedd`

Name	Type	Description
wert	real*8	3-D array on the model grid of the quantity to be diffused (Input)
diff	real*8	3-D array on the model grid of the effekts of eddy diffusion of wert (Output)
wabove	real*8	Upper boundary of wert (Input)

Module DIFMOL   computes molecular diffusion

Table B.5: Parameter List of module `difmol`

Name	Type	Description
wert	real*8	3-D array on the model grid of the quantity to be diffused (Input)
diff	real*8	3-D array on the model grid of the effekts of diffusion of wert (Output)
wabove	real*8	Upper boundary of wert (Input)

Module DY2HNM   computes the nonlinear terms of equations 2.51-2.54 due to the function $H_n^m(\mu)$ defined by equation A.39.

Module DY2PNM   computes the nonlinear terms of equations 2.51-2.54 due to the normalized associated Legendre polynomials $P_n^m(\mu)$ defined by equation A.38.

Module DYEXPL initegrates the divergence- and thermodynamic equation 2.14 and 2.15 using the explicit leapfrog scheme (numerics not documented). Can be used alternitatively to module `dyimpl`

Module DYGRAV Main entry to compute the gravity wave parameterization described in section 4.3.

Module DYH2G computes the transformation of the prognostic variables to gridpoints in equations 2.46 and 2.47 due to the function $H_n^m(\mu)$ defined by equation A.39.

Module DYIMPL integrates the divergence- and thermodynamic equation as described in section 2.4.3.

Module DYLOWB establishes the lower boundary condition for temperature and geoptential.

Module DYNMIK is the main entry for integration of the primitive equations.

Module DYS2G computes the transformation of the prognostic variables to gridpoints in equations 2.43-2.47 due to the normalized associated Legendre polynomials $P_n^m(\mu)$ defined by equation A.38.

Module DYVBEW integrates the contiunuity equation 2.48.

Module DYVORT integrates the vorticity equation 2.52.

Module DYWFLX computes the vertical flux divergences (equation 2.29).

Module GRAVTY computes the gravity wave parameterization (section 4.3).

Module STRATO Main entry of the entire model.

Module RADIA Main entry to compute the net heating rate.

Module RADSS Entry to compute the net heating rate as described in section 4.2.

Module RD0001 computes the heating rate due to UV absrorption as described in section 4.2.

Module RD0002 computes the IR cooling by the Newtonian cooling algorithm as described in section 4.2.

B.3 General Purpose and Diagnostic Modules

Module ALEGR8 computes the full triangle of function values of the associated Legendre polynomials $P_n^m(\mu)$, $0 \leq n \leq N_{max}$, and $-n \leq m \leq n$ based on the recurrence relation A.33 starting with

$$P_m^m(\mu) = (-1)^m (2m - 1)!! \left(1 - \mu^2\right)^{m/2}, \tag{B.1}$$

where the notation $n!!$ denotes the product of all odd integers less than or equal to n [*Press et al.*, 1988].

Table B.6: Parameter List of module `alegr8`

Name	Type	Description
nmax	integer	Maximum degree of the associated Legendre Polynomials (Input)
nvalue	integer	Number of independent Variables (Input)
xeval	real*8	Array of independent Variables of length nvalue (Input)
yeval	real*8	Array of normalized associated Legendre polynomials with the structure real*8 yeval(nvalue, 0:nmax, 0:nmax) (Output)
		continued on next page

Table B.6, continued from previous page		
Name	Type	Description
ynorm	real*8	Array of the log of the norm of the associated Legendre polynomials with the structure real*8 ynorm(nvalue, 0:nmax, 0:nmax) (Output)

Module DICURL computes the curl, the streamfunction, and the rotational component of a vectorfield on one horizontal model layer by means of the spectral transform technics.

Table B.7: Parameter List of module dicurl

Name	Type	Description
xinp	real*8	zonal component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Input)
xinp	real*8	meridional component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Input)
curl	complex*16	Curl of the input vectorfield in terms of spherical harmonics of one model layer (Output)
xsol	real*8	zonal component of the rotational component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Output)
ysol	real*8	meridional component of the rotational component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Output)
strm	complex*16	Stream funcion of the input vectorfield in terms of spherical harmonics of one model layer (Output)
		continued on next page

Table B.7, continued from previous page		
Name	Type	Description
furi	complex*16	Workspace in terms of Fourier coefficients of one model layer (Output)

Module DIDICK computes the thickness in geometric meters between the actual model layer and the layer below.

Table B.8: Parameter List of module didick

Name	Type	Description
gitter	real*8	thickness in geometric meters between the actual model gridpoint and the gridpoint below (Output)

Module DIDIVG computes the divergence, the scalar potential, and the divergent component of a vectorfield on one horizontal model layer by means of the spectral transform technics.

Table B.9: Parameter List of module didivg

Name	Type	Description
xinp	real*8	zonal component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Input)
xinp	real*8	meridional component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Input)
divg	complex*16	Horizontal divergence of the input vectorfield in terms of spherical harmonics of one model layer (Output)
xdiv	real*8	zonal component of the divergent component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Output)
		continued on next page

Table B.9, continued from previous page		
Name	**Type**	**Description**
ydiv	real*8	meridional component of the divergent component of the vectorfield times $\cos\varphi$ on the grid of one horizontal model layer (Output)
potf	complex*16	Scalar potential of the input vectorfield in terms of spherical harmonics of one model layer (Output)
furi	complex*16	Workspace in terms of Fourier coefficients of one model layer (Output)

Module DIERTL computes Ertel's potential vorticity on a 3-D model grid

Table B.10: Parameter List of module diertl

Name	**Type**	**Description**
ertel	real*8	Ertel's potential vorticity on model grid

Module DISTAG computes the geopotantial from the hydrostatic equation (2.3)

Table B.11: Parameter List of module distag

Name	**Type**	**Description**
spharm	real*8	3-D Geopotential on the model structure of spherical harmonics (Output)
furier	real*8	3-D Geopotential on the model structure Fourier coefficients (Output)
gitter	real*8	3-D Geopotential on the model grid (Output)

Module DTSEC computes the difference between two dates in seconds where the dates are given in year, day of the year, and seconds of the day

Table B.12: Parameter List of module dtsec

Name	Type	Description
dat1	integer	Array of length 3 containing the first date (year, day of the year, seconds of the day) (Input)
dat2	integer	Array of length 3 containing the second date (year, day of the year, seconds of the day) (Input)
delta	real*8	Difference between dat2 and dat1 in seconds (Output)

Module MATADJ computes the adjunct of a matrix

Table B.13: Parameter List of module matadj

Name	Type	Description
atrix	real*8	Input Matrix structured real*8 atrix(norder, norder) (Input)
adjrix	real*8	Matrix containing the log of values of the adjunct matrix structured real*8 adjrix(norder, norder) (Output)
adjsgn	real*8	Matrix containing the sign of values of the adjunct matrix structured real*8 adjsgn(norder, norder) (Output)
wrkrix	real*8	Workspace structured real*8 wrkrix(norder-1, norder-1) (Output)
norder	integer	Dimension of matrices (Input)
knr	integer	Identification of caller (Input)

Module MATDET computes the determinant of a matrix

Table B.14: Parameter List of module `matdet`

Name	Type	Description
atrix	real*8	Input Matrix structured `real*8 atrix(norder, norder)` (Input)
norder	integer	Dimension of matrices (Input)
detl	real*8	log of determinant of `atrix` (Output)
dets	real*8	sign of determinant of `atrix` (Output)
knr	integer	Identification of caller (Input)

Module MATINV computes the inverse of a matrix

Table B.15: Parameter List of module `matinv`

Name	Type	Description
atrix	real*8	Input matrix structured `real*8 atrix(norder, norder)` (Input)
invrix	real*8	Matrix containing the inverse of `atrix` structured `real*8 adjrix(norder, norder)` (Output)
vrkrix, wrkrix	real*8	Workspaces structured `real*8 ...rix(norder, norder)` (Output)
norder	integer	Dimension of matrices (Input)
knr	integer	Identification of caller (Input)

Module MATPRD computes the product of two matrices

Table B.16: Parameter List of module `matprd`

Name	Type	Description
amat	real*8	First factor of matrix product structured `real*8 amat(nd1, nd2)` (Input)
		continued on next page

Table B.16, continued from previous page		
Name	Type	Description
bmat	real*8	Second factor of matrix product structured real*8 bmat(nd2, nd3) (Input)
rmat	real*8	Matrix containing the product amat·bmat structured real*8 rmat(nd1, nd3) (Output)
nd1, nd2, nd3	integer	Dimension of matrices (Input)

B.4   I/O Modules

Module BUFIN   reads one record from a sequantial unformatted dataset

Table B.17: Parameter List of module bufin

Name	Type	Description
arr	real*8	Array of length ndim to which the data is read (Output)
ndim	integer	Number of 8 byte words to be read (Input)
nunit	integer	FORTRAN unit number of the dataset to be read (Input)
npos	integer	unused
ndump	integer	unused
knr	integer	Key to identify the call of bufin

Module BUFOUT   writes one record to a sequantial unformatted dataset

Table B.18: Parameter List of module bufout

Name	Type	Description
arr	real*8	Array of length ndim of which the data is written (Output)

Name	Type	Description
		Table B.18, continued from previous page
ndim	integer	Number of 8 byte words to be read (Input)
nunit	integer	FORTRAN unit number of the dataset to be read (Input)
npos	integer	unused
ndump	integer	unused
knr	integer	Key to identify the call of bufout

Module CLSBUF closes a dataset for sequential I/O

Table B.19: Parameter List of module clsbuf

Name	Type	Description
nunit	integer	FORTRAN unit number of the dataset to be closed (Input)

Module CLSDIR closes a dataset for direct access I/O

Table B.20: Parameter List of module clsdir

Name	Type	Description
nunit	integer	FORTRAN unit number of the dataset to be closed (Input)

Module READST reads one record from an unformatted direct access dataset

Table B.21: Parameter List of module readst

Name	Type	Description
arr	real*8	Array of length ndim to which the data record is read (Output)
ndim	integer	Number of 8 byte words to be read (Input)

Table B.21, continued from previous page		
Name	Type	Description
nunit	integer	FORTRAN unit number of the dataset to be read (Input)
npos	integer	Number of record in the dataset identified by nunit
ncon	integer	unused
knr	integer	Key to identify the call of readst

Module WRITST   writes one record to an unformatted direct access dataset

Table B.22: Parameter List of module writst

Name	Type	Description
arr	real*8	Array of length ndim of which the data is written (Output)
ndim	integer	Number of 8 byte words to be read (Input)
nunit	integer	FORTRAN unit number of the dataset to be read (Input)
npos	integer	Number of record in the dataset identified by nunit
ncon	integer	unused
knr	integer	Key to identify the call of writst

Acknowledgments