Theory and application of quasi-elastic equations in terrain-following coordinates based on the full pressure field

by

Francois Alwyn Engelbrecht

Submitted in partial fulfilment of the requirements for the degree of

PHILISOPHIAE DOCTOR

in the
Faculty of Natural and Agricultural Sciences
University of Pretoria

May 2006
Theory and application of quasi-elastic equations in
terrain-following coordinates based on the full pressure
field

Francois Alwyn Engelbrecht

Promoter: Prof. C.J. deW. Rautenbach
Co-promoter: Dr. J.L. McGregor
Department: Department of Geography, Geoinformatics and Meteorology
Faculty: Faculty of Natural and Agricultural Sciences
University: University of Pretoria
Degree: Philosophiae Doctor

Summary

The thesis reports on the development of a new quasi-elastic nonhydrostatic
model, cast in a terrain-following coordinate based on the full pressure field.
The equations used are the $\sigma$ coordinate analogue of the nonhydrostatic
pressure coordinate equations formulated by White (1989). The equations are fil-
tered of vertically propagating acoustic waves. However, since Lamb waves
are present, the equations may be termed quasi-elastic. In contrast to similar
quasi-elastic pressure-based models, the equations and the numerical solution
procedure presented here are formulated independent of the use of a reference
state thermodynamic profile. Thus, it is possible that the equations may be used
to simulate atmospheric motion at spatial scales larger than the meso-scale.

A novel split semi-Lagrangian procedure is formulated to solve the quasi-elastic
equations on a grid that is nonstaggered in both the horizontal and vertical. A
nonstaggered grid is appealing to use in semi-Lagrangian discretizations of the
atmospheric equations, since only one set of trajectories needs to be calculated
during each advection time step. However, it is well known that the nonstag-
gerated grid has poor gravity wave dispersion properties. In this study, this prob-
lem is alleviated by using high-order centered spatial differencing, and by apply-
ing a spatial filter to remove two-grid-interval waves from the grid. It is shown
that large time steps (large Courant numbers) are allowed during the semi-
Lagrangian advection step. This makes the method computationally attractive
compared to explicit or split-explicit procedures that use an Eulerian approach
to treat the advection terms. For situations where the fast moving gravity waves
carry a non-negligible amount of the energy, the split semi-Lagrangian approach
may even be computationally more efficient than the widely used semi-implicit
semi-Lagrangian solution procedures. The thesis reports on a large set of bubble
convection tests performed with the new kernel. It is concluded that the new
model is worth developing further.
Teorie en toepassing van kwasi-elastiese vergelykings in terrein-volgende koordinate gebasseer op die volle drukveld

Francois Alwyn Engelbrecht

Promotor: Prof. C.J. deW. Rautenbach
Mede-promotor: Dr. J.L. McGregor
Departement: Departement Geografie, Geoinformatika en Meteorologie
Fakulteit: Fakulteit Natuur- en Landbouwetenskappe
Universiteit: Universiteit van Pretoria
Graad: Philosophiae Doctor

Samenvatting

Die proefschrift handel oor die ontwikkeling van ‘n nuwe kwasi-elastiese nie-hidrostatiese model, in ‘n terrein-volgende koordinate gebasseer op die volle drukveld. Die vergelykings wat gebruik word is die $\sigma$-koordinate analoog van die nie-hidrostatiese drukkoordinate vergelykings geformuleer deur White (1989). Die vergelykings is gefilter van vertikaal voortplantende klankgolwe. Lamb-golwe is egter teenwoordig en daarom kan die vergelykings kwasi-elasties genoem word. In kontras met soortgelyke kwasi-elastiese drukgebasseerde modelle, is die vergelykings wat hier gebruik word onafhanklik van die gebruik van ‘n termodynamiese verwysingsprofiel. Dit is dus moontlik dat die vergelykings gebruik kan word om atmosferiese sirkulasie op ruimtelike skale groter as die meso-skaal te simuleer.

‘n Oorspronlike split semi-Lagrange prosedure is geformuleer om die kwasi-elastiese vergelykings op te los op ‘n rooster wat in die horisontaal en vertikaal nie-verspringend is. So ‘n rooster is aankliklik om te gebruik in die semi-Lagrangian diskretisering van die atmosferiese vergelykings, aangesien dit nodig is om net ‘n enkele stel trajecte te bereken gedurende elke adveksie tydspan. Dit is egter welbekend dat die nie-verspringende rooster swak gravitasiegolf disper- sie eienkappe het. In die studie word hierdie probleem hanteer deur hoe orde differensiasie te gebruik en deur ‘n ruimtelike filter toe te pas wat twee-rooster-interval golwe van die rooster verwyder. Dit word aangetoon dat groot tydstape (groot Courant getalle) toegedaan word gedurende die semi-Lagrange adveksie stap. Dit maak die metode berekeningsgewys aantreklik in vergelyking met eksplisiete en split-eksplisiete prosedures wat ‘n Euler benadering gebruik vir die adveksie terme. Vir situasies waar die vinnigbewegende gravitasie golwe ‘n nie-weglaatbare hoeveelheid van die energie dra, kan die split semi-Lagrange benadering selfs meer berekeningseffektief wees as die gewilde semi-implisiete semi-Lagrange prosedures. ‘n Groot roeks borrel konveksie eksperimente is uitgevoer met die nuwe kern en dit blyk die moeite werd te wees om die nuwe model verder te ontwikkeld.
Acknowledgements

The author wishes to express his appreciation to the following persons and organisations for their assistance and contribution to make this dissertation possible:

- **Prof. C.J. de W. Rautenbach** (Head of the Department of Geography, Geoinformatics and Meteorology at the University of Pretoria) for his appreciation of my interest in numerical atmospheric modelling, and for supporting this theoretical study during times where research becomes increasingly application-driven.

- **Dr. J.L. McGregor** (Specialist Scientist) from the Commonwealth Scientific and Industrial Research Organisation (CSIRO), section Marine and Atmospheric Research in Australia, for his continuous encouragement, guidance and expert advice during the course of the study.

- **Dr. G. Green** (retired director of the Water Research Commission (WRC) in South Africa) for the interest that he took in the research and my career as an atmospheric scientist.

- **Dr. JD. Gertenbach** (South African Weather Service), **Me. H. Riphagen** (retired), **Mr Gusti van Zyl** (University of Pretoria) and **Me C.J. Potgieter** (Agricultural Research Council) for many helpful discussions during the course of the study.

- Two external examiners, whose comments helped to improve the thesis.

- **CSIRO Marine and Atmospheric Research** in Australia for inviting me to visit Dr. J.L. McGregor in January 2002 and 2004, for the purpose of collaborative research into nonhydrostatic atmospheric model development.

- The **WRC** for financially supporting the research into atmospheric model development in South Africa.

- The friendly librarians of the South African Weather Service, Karin and Anastasia, for assisting me with finding most of the references listed at the end of this thesis.

- My colleges in the Department of Geography, Geoinformatics and Meteorology for their encouragement and interest in my research.

- My family, dear friends and Duimpie, for their encouragement and support.

- My girlfriend Christien, who became my wife during the course of the study despite of all the hours I spent behind a computer.

- **Most of all, I would like to thank God for giving me the strength to undertake this study, and for the privilege of being able to study the atmosphere.**
Contents

1 Introduction ................................................................. 1
  1.1 Background to the research ........................................ 1
      1.1.1 Hydrostatic and nonhydrostatic atmospheric models .... 1
        1.1.1.1 Unapproximated and fully-elastic equations ......... 1
        1.1.1.2 The hydrostatic approximation and hydrostatic
          models ......................................................... 3
        1.1.1.3 The anelastic approximation and nonhydrostatic
          models ......................................................... 4
  1.1.2 Numerical atmospheric modelling in South Africa ......... 7
  1.1.3 Atmospheric modelling activities at the University of
          Pretoria ....................................................... 9
  1.2 Motivation for the research ........................................ 10
      1.2.1 Recent developments in nonhydrostatic atmospheric
          modelling ..................................................... 10
      1.2.2 Nonhydrostatic circulation systems over South Africa .. 12
        1.2.2.1 Convective rainfall over South Africa ............... 12
        1.2.2.2 Thunderstorms in South Africa ....................... 13
        1.2.2.3 Mountain waves ....................................... 15
        1.2.2.4 Modelling nonhydrostatic circulation systems oc-
          curring over South Africa .................................. 17
  1.3 Objectives of the research ......................................... 17
  1.4 Organisation of the report ......................................... 18
  1.5 New aspects of the research ....................................... 20

2 Nonhydrostatic models in pressure-based coordinates .......... 21
  2.1 Introduction .......................................................... 21
  2.2 Fully elastic equations in pressure-based vertical coordi-
          nates ......................................................... 24
      2.2.1 The fully-elastic equations with the full pressure field
          as vertical coordinate ....................................... 24
      2.2.2 The fully-elastic equations in \( \sigma \) coordinates based on
          the full pressure field ....................................... 25
      2.2.3 The fully-elastic equations in \( \sigma \) coordinates based on the
          hydrostatic pressure field .................................. 26
2.3 Approximated nonhydrostatic equation sets based on the full pressure field .......................... 27
2.3.1 The Miller-Pearce model ........................................ 28
2.3.2 Anelastic terrain-following equations ...................... 32
2.3.3 White's extension of the MP Model ......................... 34
2.4 Discussion .......................................................... 35

3 Derivation and properties of the quasi-elastic equations in terrain-following coordinates based on the full pressure field 37
3.1 Introduction .......................................................... 37
3.2 The Miller-Pearce model .......................................... 39
    3.2.1 Basic concepts .................................................. 39
    3.2.2 The Miller-Pearce model in pressure coordinates ....... 40
    3.2.3 The Miller-Pearce model in sigma coordinates ......... 43
3.3 White's extension of the MP model in pressure coordinates .. 44
    3.3.1 The momentum, continuity and thermodynamic energy equations ........................................ 44
    3.3.2 A diagnostic equation for \( \phi \) in pressure coordinates .......................................................... 45
    3.3.3 Two-dimensional equations in pressure coordinates .... 46
3.4 Derivation of White's equations in \( \sigma \) coordinates by a coordinate transformation ............................. 47
    3.4.1 Transformation relations ....................................... 47
    3.4.2 The horizontal momentum equations ....................... 48
    3.4.3 The vertical momentum equation .......................... 49
    3.4.4 The continuity equation ...................................... 49
    3.4.5 The thermodynamic energy equation ........................ 50
    3.4.6 The extended nonhydrostatic equation set .............. 50
    3.4.7 A diagnostic equation for \( \phi \) in \( \sigma \) coordinates .................. 51
    3.4.8 Two-dimensional version of White's equations in \( \sigma \) coordinates .............................................. 53
3.5 Properties of the nonhydrostatic \( \sigma \) coordinate equations based on the full pressure field .......................... 54
    3.5.1 Physical implications of the approximated vertical momentum equation .................................. 54
    3.5.2 Energetics of the \( \sigma \) coordinate equations .............. 55
    3.5.3 Linearized equations ......................................... 56
    3.5.4 Towards wave-like solutions of the linearized equations .... 57
    3.5.5 Solutions of (3.116) with exponential variation in height ...................................................... 59
        3.5.5.1 Form of the sound wave solutions ................... 59
        3.5.5.2 Finding an expression for \( \hat{\phi} \) at \( \sigma = 1 \) ........... 60
        3.5.5.3 Applying the linearized continuity equation ....... 60
        3.5.5.4 Utilizing the upper boundary condition on \( d\hat{\phi} / d\sigma \) 61
        3.5.5.5 A second relationship between \( \mu \) and \( c \) ............ 61
        3.5.5.6 The influence of the height of the model top on the phase speed of the Lamb waves .......... 62
    3.5.6 Solutions with sinusoidal variation in height .............. 66
4 The split semi-Lagrangian solution procedure

4.1 Introduction .................................................. 71
4.2 The semi-Lagrangian advection scheme ..................... 74
  4.2.1 McGregor’s method for the calculation of the departure
        points .................................................. 74
  4.2.2 Bicubic Lagrange spatial interpolation .................... 77
4.3 Finite differencing on the nonstaggered grid ................ 83
  4.3.1 Centered differencing for first derivatives ............... 83
  4.3.2 Centered differencing for second derivatives ............ 84
  4.3.3 Application to one-dimensional gravity waves .......... 85
    4.3.3.1 Second order spatial differencing .................. 85
    4.3.3.2 Fourth order spatial differencing .................. 86
    4.3.3.3 Sixth order spatial differencing .................... 88
4.4 Spatial filtering .............................................. 91
4.5 The split semi-Lagrangian solution procedure .............. 92
  4.5.1 Splitting off the advective part ....................... 92
  4.5.2 The adjustment step ................................... 93
  4.5.3 Spatial filtering ...................................... 95
  4.5.4 Explicit diffusion .................................... 96
4.6 Frequency response of the quasi-elastic equations to the forward-
    backward time discretization ................................ 97
4.7 Frequency response to spatial discretization on the nonstaggered
    grid ......................................................... 102
  4.7.1 Frequency response to horizontal discretization .......... 102
  4.7.2 Frequency response to vertical discretization .......... 104
    4.7.2.1 Second order vertical differencing ................. 106
    4.7.2.2 Fourth order vertical differencing ............... 108
    4.7.2.3 Sixth order vertical differencing ................. 109
4.8 Elliptic solvers for the diagnostic equation in the geopotential .. 112
  4.8.1 Spatial discretization ................................ 113
  4.8.2 Convergence of iterations ................................ 114
4.9 Boundary conditions ......................................... 114
  4.9.1 Lateral boundary conditions ............................ 114
  4.9.2 Lower and upper boundary conditions .................... 116
    4.9.2.1 Temperature field ................................ 116
    4.9.2.2 Geopotential field .............................. 116
    4.9.2.3 Velocity field .................................... 117
6.3.1 Marginally resolved flow .......................... 205  
6.3.2 A quasi-elastic universal model? ................ 205  
6.3.3 The study of nonhydrostatic circulation systems and 
        continued model development .................... 206  
6.3.4 Implementation of the quasi-elastic equations in C-CAM . 207  
6.4 The new Nonhydrostatic Sigma coordinate Model (NSM) .... 207

A Derivation of the elliptic equation directly from the \( \sigma \) coordinate quasi-elastic equations 209
B Alternative derivation of the linearized elliptic equation 215
C The linearized elliptic equation under transformations \( Z \) and \( F \) 217
D Alternative derivation of the Lamb wave frequency equation 219
E Applying the continuity equation for the case of solutions with 
       sinusoidal variation in height 221
List of Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{a}_x )</td>
<td>( x ) component of the estimated acceleration</td>
</tr>
<tr>
<td>( \dot{a}_y )</td>
<td>( y ) component of the estimated acceleration</td>
</tr>
<tr>
<td>( \dot{a}_z )</td>
<td>( \sigma ) component of the estimated acceleration</td>
</tr>
<tr>
<td>( c )</td>
<td>phase speed</td>
</tr>
<tr>
<td>( c_s )</td>
<td>speed of sound</td>
</tr>
<tr>
<td>( c_p )</td>
<td>specific heat at constant air pressure</td>
</tr>
<tr>
<td>( c_v )</td>
<td>specific heat at constant air volume</td>
</tr>
<tr>
<td>( f )</td>
<td>Coriolis parameter</td>
</tr>
<tr>
<td>( g )</td>
<td>acceleration of gravity</td>
</tr>
<tr>
<td>( h )</td>
<td>surface elevation</td>
</tr>
<tr>
<td>( H )</td>
<td>depth of fluid in the shallow-water equations (section 4.3.3)</td>
</tr>
<tr>
<td>( \bar{H} )</td>
<td>mean depth of fluid in the shallow-water equations</td>
</tr>
<tr>
<td>( H' )</td>
<td>scale of the height perturbation</td>
</tr>
<tr>
<td>( H_0 )</td>
<td>( RT_0/g )</td>
</tr>
<tr>
<td>( k )</td>
<td>wave number in ( x ) direction</td>
</tr>
<tr>
<td>( K_s )</td>
<td>horizontal diffusion coefficient applied to wind field</td>
</tr>
<tr>
<td>( K_{Ts} )</td>
<td>horizontal diffusion coefficient applied to temperature field</td>
</tr>
<tr>
<td>( K_\sigma )</td>
<td>vertical diffusion coefficient applied to wind field</td>
</tr>
<tr>
<td>( K_{T\sigma} )</td>
<td>vertical diffusion coefficient applied to temperature field</td>
</tr>
<tr>
<td>( l )</td>
<td>wave number in ( y ) direction</td>
</tr>
<tr>
<td>( L )</td>
<td>horizontal length scale</td>
</tr>
<tr>
<td>( L_x )</td>
<td>wave length in ( x ) direction</td>
</tr>
<tr>
<td>( L_y )</td>
<td>wave length in ( y ) direction</td>
</tr>
<tr>
<td>( L_z )</td>
<td>wave length in ( z ) direction</td>
</tr>
<tr>
<td>( m )</td>
<td>wave number in ( z ) direction</td>
</tr>
<tr>
<td>( N )</td>
<td>( \equiv \sqrt{g\kappa H_0} )</td>
</tr>
</tbody>
</table>
\( p \) pressure
\( p_{surf} \) surface pressure
\( p_{surf-ref} \) reference surface pressure
\( p_{surf-ave} \) mean sea-level pressure
\( p_0 \) \( \equiv p_{surf-ref} - p_T \)
\( p_T \) constant pressure at top of model
\( p_s \) \( \equiv p_{surf} - p_T \)
\( \dot{p}_s \) amplitude of wave-like solution for \( p_s \)
\( p_0(x) \) pressure at lower boundary that is independent of time but may depend on horizontal position
\( p_{sr} \) \( \equiv p_0(x) - p_T \)
\( p_{STAN} \) standard pressure level
\( P \) pressure scale
\( r \) \( \equiv gp/RT \)
\( r_{ref} \) \( \equiv gp/RT_{ref} \)
\( r_l \) relaxation coefficient
\( r \) vector moving with fluid
\( R \) gas constant
\( R_A \) relative phase speed
\( s \) \( \equiv (p/p_s)(g/RT) \)
\( S_{ref} \) \( \equiv -dT_{ref}/dp + \kappa T_{ref}/p \), reference state static stability function
\( t \) time
\( \tau \) time
\( T \) temperature
\( T' \) temperature perturbation
\( T'' \) amplitude of wave-like solution for the temperature perturbation
\( T_0 \) temperature of isothermal atmosphere
\( T_{ref} \) reference state temperature
\( T_{\text{ref-ave}} \) mean reference state temperature
\( u \) wind speed in \( x \) direction
\( \dot{u} \) amplitude of wave-like solution for \( u \) (Chapter 3);
\( \ddot{u} \) estimated wind speed in \( x \) direction at time-level \( \tau + \Delta t/2 \) (Chapter 4)
\( \dot{u} \) horizontal velocity scale
\( U \) constant wind speed in \( x \) direction
\( \mathbf{u} \) three-dimensional velocity vector
\( \dot{u} \) estimated velocity at time-level \( \tau + \Delta t/2 \)
\( v \) wind speed in \( y \) direction
\( \dot{v} \) estimated wind speed in \( y \) direction at time-level \( \tau + \Delta t/2 \)
\( V \) constant wind speed in \( y \) direction
\( \mathbf{v} \equiv (u, v) \), horizontal velocity.
\( w \) wind speed in \( z \) direction
\( \dot{w}_{\text{ref}} \equiv -R\omega T_{\text{ref}}/g_{\text{p}}, \) approximated vertical velocity
\( \dot{\mathbf{w}} \equiv -R\omega T/g_{\text{p}}, \) approximated vertical velocity
\( x^* \) \( x \) coordinate of departure point
\( y^* \) \( y \) coordinate of departure point
\( z \) geometric height
\( z' \) geometric height perturbation
\( z_{\text{ref}} \) reference state geometric height
\( \Delta x \) constant grid increment along \( x \) axis
\( \Delta y \) constant grid increment along \( y \) axis
\( \Delta t \) constant time-step
\( \Delta t_a \) advection time-step
\( \Delta t_a \) adjustment time-step
\( \Delta \sigma \) constant grid increment along \( \sigma \) axis
\( \alpha \) specific volume (Chapter 1);
\[ \equiv u\Delta t/\Delta x \text{ (Chapter 4 and 5)} \]
\[ \alpha^* \equiv - \left( p_0/\theta_{ref} \right) d\theta_{ref}/dp \]
\[ \beta \equiv v\Delta t/\Delta y \]
\[ \gamma \quad c_p/c_v \]
\[ \epsilon \equiv (1/g) DW/Dt \text{, measure of the vertical acceleration} \]
\[ \zeta \quad \text{vertical component of the vorticity} \]
\[ \theta \quad \text{potential temperature} \]
\[ \theta' \quad \text{potential temperature perturbation} \]
\[ \theta_0 \quad \text{homogeneous reference state potential temperature} \]
\[ \theta_{ref} \quad \text{reference state potential temperature} \]
\[ \vartheta \quad \text{numerical value of the local frequency} \]
\[ \vartheta_T \quad \text{analytic local frequency} \]
\[ \kappa \equiv R/c_p, \text{ ratio of gas constant to specific heat at constant pressure} \]
\[ \lambda \quad \text{latitude (Chapter 1);} \]
\[ \quad \text{amplification factor (Chapter 5)} \]
\[ \mu \quad \text{wave number in } z \text{ direction} \]
\[ \nu \quad \text{frequency of oscillation} \]
\[ \pi \quad \text{hydrostatic pressure (Chapter 2);} \]
\[ \quad \equiv \arccos(-1) \text{ (Chapter 3 to 5)} \]
\[ \pi_{surf} \quad \text{hydrostatic pressure at the surface} \]
\[ \pi_T \quad \text{hydrostatic pressure at model top} \]
\[ \bar{\pi} \equiv \bar{p}_s/p_0 \]
\[ \rho \quad \text{density} \]
\[ \rho_0 \quad \text{constant basic state density} \]
\[ \rho_{ref} \quad \text{reference state density} \]
\[ \sigma \quad \text{pressure-scaled vertical coordinate} \]
\[ \sigma^* \quad \sigma \text{ coordinate of departure point} \]
\[ \hat{\sigma} \equiv D\sigma/Dt, \text{ vertical velocity in } \sigma \text{ coordinates} \]
\( \hat{\sigma} \) \hspace{1cm} \text{amplitude of wave-like solution for} \ \dot{\sigma} \ (\text{Chapter 3}); \\
\text{estimated vertical velocity in} \ \sigma \ \text{coordinates at time-level} \ \tau + \Delta t/2 \ \text{ (Chapter 4)} \\
\phi \hspace{1cm} \text{geopotential} \\
\phi' \hspace{1cm} \text{geopotential perturbation} \\
\hat{\phi}' \hspace{1cm} \text{amplitude of wave-like solution for geopotential perturbation} \\
\phi_{\text{ref}} \hspace{1cm} \text{reference state geopotential} \\
\chi \equiv [(p/RT)(\partial \phi/\partial p)]^{-1} \\
\omega \equiv Dp/Dt, \ \text{vertical velocity in isobaric coordinates} \\
\tilde{\omega} \hspace{1cm} \omega \ \text{scale} \\
\omega_T \hspace{1cm} \text{gravity wave frequency} \\
\Omega \hspace{1cm} \omega/p \\
\Omega_T \hspace{1cm} \text{true frequency} \\
\Omega_N \hspace{1cm} \text{frequency of waves in the numerical solution}
List of Figures

1.1 A Meteosat 7 colour enhanced infrared satellite image showing a severe thunderstorm over Swaziland and the Lowveld of South Africa. Storm splitting may have occured, since two overshooting tops are indicated by the light blue regions (coolest cloud top temperatures). .......................................................... 13

1.2 A Meteosat 8 visible satellite image showing the formation of mountain waves downstream of the Drakensberg region of South Africa and Lesotho. .......................................................... 16

3.1 Lamb wave phase speed as a function of the normalised wave number, for various choices of the height of the model top: $p_T = 0 \text{ hPa}$ (yellow line); $p_T = 135 \text{ hPa}$ (green line); $p_T = 442 \text{ hPa}$ (black line). The true sound wave speed is depicted by the red line. 64

3.2 Lamb wave phase speed as a function of horizontal wave length, for various choices of the height of the model top: $p_T = 0 \text{ hPa}$ (yellow line); $p_T = 135 \text{ hPa}$ (green line); $p_T = 442 \text{ hPa}$ (black line). The true sound wave speed is depicted by the red line. ... 65

4.1 Isolines of the amplification factor for bicubic spatial interpolation, as a function of $\alpha$ and $k\Delta x/\pi$ (following McDonald, 1984). 80

4.2 Normalised phase speed isolines for bicubic spatial interpolation, as a function of $\alpha$ and $k\Delta x/\pi$ (following McDonald, 1984). ... 82

4.3 The relative frequency of pure gravity waves as a function of wave number, for second order (black line), fourth order (green line) and sixth order (yellow line) spatial differencing on the nonstaggered grid. .......................................................... 87

4.4 The relative frequency of pure gravity waves as a function of wave length, for second order (black line), fourth order (green line) and sixth order (yellow line) spatial differencing on the nonstaggered grid with $\Delta x = 100 \text{ m}$. The red line represents the relative frequency of pure gravity waves for second order differencing on the nonstaggered grid with $\Delta x = 50 \text{ m}$. ................................................. 90
4.5 Relative frequency of the gravity waves in response to the forward-backward time discretization, as a function of the wave number. The red, yellow, green and black lines represent Courant numbers of 0.2, 0.3, 0.4 and 0.5, respectively. .................. 101

4.6 Relative frequency of the gravity waves described by the quasi-elastic equations, in response to centered finite differencing in the vertical on the nonstaggered grid, as a function of the vertical wave number. The black, green and yellow lines represent second, fourth and sixth order differencing, respectively. .............. 107

4.7 Relative frequency of the gravity waves described by the quasi-elastic equations, in response to centered finite differencing in the vertical on the nonstaggered grid, as a function of the vertical wave length. The black, green and yellow lines represent second, fourth and sixth order differencing, respectively, with \( \Delta Z = 100 \text{ m} \). The red line was obtained using second order differencing with \( \Delta Z = 50 \text{ m} \). .................. 111

5.1 Initialization procedure for the two-dimensional cold bubble test. Perturbation from the geopotential distribution corresponding to the hydrostatic, isentropic environmental state, for \( 0 \leq \sigma \leq 1 \): using as condition of convergence (a) \( \epsilon = 10^{-5} \); (b) \( \epsilon = 10^{-6} \); (c) \( \epsilon = 10^{-6}/5 \); (d) \( 10^{-7} \). The contour interval is 50 gpm. ......... 128

5.2 Reference solution for the cold bubble test. Potential temperature perturbation in the right-hand part of the integration domain for \( 0 \leq \sigma \leq 1 \): (a) at 0 s; (b) after 300 s; (c) after 600 s; (d) after 900 s. The contour interval is 1 K. Note the displacement of the horizontal scale in (d). .................. 130

5.3 Reference solution for the cold bubble test. The \( \omega \) component of the wind (top panel) and the \( \dot{\omega} \) component of the wind (bottom panel) after 900 s in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \). The contour interval is 2 ms\(^{-1}\). ......... 131

5.4 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) \( K_s = 75 \text{ ms}^{-2} \); (b) \( K_s = 50 \text{ ms}^{-2} \); (c) \( K_s = 25 \text{ ms}^{-2} \); (d) \( K_s = 0 \text{ ms}^{-2} \). The contour interval is 1K. ... 135

5.5 The \( \dot{\omega} \) component of the wind for the cold bubble test after 900 s, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) \( K_s = 75 \text{ ms}^{-2} \); (b) \( K_s = 50 \text{ ms}^{-2} \); (c) \( K_s = 25 \text{ ms}^{-2} \); (d) \( K_s = 0 \text{ ms}^{-2} \). The contour interval is 2 ms\(^{-1}\). ............. 137

5.6 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) \( K_s = 75 \text{ ms}^{-2} \); (b) \( K_s = 50 \text{ ms}^{-2} \); (c) \( K_s = 25 \text{ ms}^{-2} \); (d) \( K_s = 0 \text{ ms}^{-2} \). The Shapiro filter is applied with \( p = 4 \). The contour interval is 1K. ............. 139
5.7 The \( \dot{w} \) component of the wind for the cold bubble test after 900 s, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( K_s = 75 \text{ms}^{-2} \); (b) \( K_s = 50 \text{ms}^{-2} \); (c) \( K_s = 25 \text{ms}^{-2} \); (d) \( K_s = 0 \text{ms}^{-2} \). The Shapiro filter is applied with \( p = 4 \). The contour interval is \( 2 \text{ms}^{-1} \).

5.8 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( K_s = 75 \text{ms}^{-2} \); (b) \( K_s = 50 \text{ms}^{-2} \); (c) \( K_s = 25 \text{ms}^{-2} \); (d) \( K_s = 0 \text{ms}^{-2} \). The fourth order discretization of spatial derivatives in the adjustment step equations and the Shapiro filter with \( p = 4 \) were used. The contour interval is 1K.

5.9 The \( \dot{w} \) component of the wind for the cold bubble test after 900 s, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( K_s = 75 \text{ms}^{-2} \); (b) \( K_s = 50 \text{ms}^{-2} \); (c) \( K_s = 25 \text{ms}^{-2} \); (d) \( K_s = 0 \text{ms}^{-2} \). The fourth order discretization of spatial derivatives in the adjustment step equations and the Shapiro filter with \( p = 4 \) were used. The contour interval is \( 2 \text{ms}^{-1} \).

5.10 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( D_0 \) scheme; (b) \( D_1 \) scheme; (c) \( D_2 \) scheme; (d) \( D_3 \) scheme with fourth order differencing applied to the departure point formula and the term \( A_p^* \). The fourth order discretization of spatial derivatives in the adjustment step equations and the Shapiro filter with \( p = 4 \) are used. \( K_s = 25 \text{m}^2\text{s}^{-1} \). The contour interval is 1K.

5.11 The \( \dot{w} \) component of the wind after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( D_0 \) scheme; (b) \( D_1 \) scheme; (c) \( D_2 \) scheme (d) \( D_3 \) scheme with fourth order differencing applied to the departure point formula and the term \( A_p^* \). The fourth order discretization of spatial derivatives in the adjustment step equations and the Shapiro filter with \( p = 4 \) are used. \( K_s = 25 \text{m}^2\text{s}^{-1} \). The contour interval is \( 2 \text{ms}^{-1} \).

5.12 Marginally and poorly resolved flow in the cold bubble test. The potential temperature deviation after 900 s in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \):
(a) \( \Delta z \approx \Delta x = 200 \text{m} \) with second order differencing; (b) \( \Delta z \approx \Delta x = 200 \text{m} \) with fourth order differencing; (c) \( \Delta z \approx \Delta x = 400 \text{m} \) with fourth order differencing; (d) \( \Delta z \approx 100 \text{m}, \Delta x = 500 \text{m} \) with fourth order differencing. The \( D_3 \) scheme with second order discretization of spatial derivatives was used in the advection step. The Shapiro filter with \( p = 4 \) was used. \( K_s = 50 \text{m}^2\text{s}^{-1} \). The contour interval is 1 K.
5.13 Marginally and poorly resolved flow in the cold bubble test. The \( \dot{w} \) component of the wind after 900 s in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) \( \Delta z \approx \Delta x = 200 \, m \) with second order differencing; (b) \( \Delta z \approx \Delta x = 200 \, m \) with fourth order differencing; (c) \( \Delta z \approx \Delta x = 400 \, m \) with fourth order differencing; (d) \( \Delta z \approx 100 \, m \), \( \Delta x = 500 \, m \) with fourth order differencing. The \( D_3 \) scheme with second order discretization of spatial derivatives was used in the advection step. The Shapiro filter with \( p = 4 \) was used. \( K_s = 50 \, m^2 s^{-1} \). The contour interval is 2 ms\(^{-1} \).

5.14 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) SH simulation with \( \Delta t_s = \Delta t_a = 0.5 \, s \); (b) SH simulation with \( \Delta t_s = \Delta t_a = 1 \, s \); (c) SH simulation with \( \Delta t_s = \Delta t_a = 1.5 \, s \); (d) FH simulation with \( \Delta t_s = \Delta t_a = 1 \, s \).

The Shapiro filter with \( p = 4 \) was used, with \( K_s = 50 \, m^2 s^{-1} \). The contour interval is 1K.

5.15 The potential temperature deviation after 900 s for the cold bubble test, in the right-hand part of the integration domain, for \( 0 \leq \sigma \leq 1 \): (a) SH simulation with \( \Delta t_s = 2 \, s \), \( \Delta t_a = 0.5 \, s \) and \( K_s = 50 \, m^2 s^{-1} \); (b) SH simulation with \( \Delta t_s = 3 \, s \), \( \Delta t_a = 0.5 \, s \) and \( K_s = 50 \, m^2 s^{-1} \); (c) FH simulation with \( \Delta t_s = 2 \, s \), \( \Delta t_a = 0.5 \, s \) and \( K_s = 50 \, m^2 s^{-1} \); (d) FH simulation with \( \Delta t_s = 2 \, s \), \( \Delta t_a = 0.5 \, s \) and \( K_s = 25 \, m^2 s^{-1} \). The Shapiro filter with \( p = 4 \) was used. The contour interval is 1K.

5.16 Reference solution for the warm bubble test. Potential temperature perturbation for \(-8000 \, m \leq x \leq 8000 \, m \) and \( 0 \leq \sigma \leq 1 \): (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is 1 K.

5.17 Reference solution for the warm bubble test. Vertical velocity \( \dot{w} \) for \(-8000 \, m \leq x \leq 8000 \, m \) and \( 0 \leq \sigma \leq 1 \): (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is 2 ms\(^{-1} \).

5.18 Marginally and poorly resolved flow in the warm bubble test. The potential temperature deviation after 900 s, for \(-8000 \, m \leq x \leq 8000 \, m \) and \( 0 \leq \sigma \leq 1 \): (a) \( \Delta z \approx \Delta x = 200 \, m \) with \( K_s = 300 \, m^2 s^{-1} \) and \( K_{T_s} = 50 \, m^2 s^{-1} \); (b) \( \Delta z \approx \Delta x = 200 \, m \) with \( K_s = 600 \, m^2 s^{-1} \) and \( K_{T_s} = 100 \, m^2 s^{-1} \); (c) \( \Delta z \approx \Delta x = 400 \, m \) with \( K_s = 1200 \, m^2 s^{-1} \) and \( K_{T_s} = 200 \, m^2 s^{-1} \); (d) \( \Delta z \approx 100 \, m \), \( \Delta x = 500 \, m \) with \( K_s = 300 \, m^2 s^{-1} \) and \( K_{T_s} = 50 \, m^2 s^{-1} \). The contour interval is 1 K.
5.19 Marginally and poorly resolved flow in the warm bubble test. The $\dot{w}$ component of the wind after 900 s, for $-8000 m \leq x \leq 8000 m$ and $0 \leq \sigma \leq 1$: (a) $\Delta z \approx \Delta x = 200 m$ with $K_s = 300 m^2s^{-1}$ and $K_{Ts} = 50 m^2s^{-1}$; (b) $\Delta z \approx \Delta x = 200 m$ with $K_s = 600 m^2s^{-1}$ and $K_{Ts} = 100 m^2s^{-1}$; (c) $\Delta z \approx \Delta x = 400 m$ with $K_s = 1200 m^2s^{-1}$ and $K_{Ts} = 200 m^2s^{-1}$; (d) $\Delta z \approx 100 m$, $\Delta x = 500 m$ with $K_s = 300 m^2s^{-1}$ and $K_{Ts} = 50 m^2s^{-1}$. The contour interval is $2 ms^{-1}$.

5.20 The potential temperature deviation after 900 s for the warm bubble test, for $-8000 m \leq x \leq 8000 m$ and $0 \leq \sigma \leq 1$: (a) $\Delta t_s = \Delta t_a = 1.5 s$; (b) $\Delta t_s = 1.5 s$, $\Delta t_a = 0.5 s$; (c) $\Delta t_s = 2.5 s$, $\Delta t_a = 0.5 s$; (d) $\Delta t_s = 5 s$, $\Delta t_a = 0.5 s$. The contour interval is $1 K$.

5.21 The vertical component of the velocity field $\dot{w}$ after 900 s for the warm bubble test, for $-8000 m \leq x \leq 8000 m$ and $0 \leq \sigma \leq 1$: (a) $\Delta t_s = 1.5 s$; (b) $\Delta t_s = 2.5 s$, $\Delta t_a = 0.5 s$; (c) $\Delta t_s = 5 s$, $\Delta t_a = 0.5 s$. The contour interval is $2 ms^{-1}$.

5.22 The three-dimensional cold bubble test. Vertical cross section of the potential temperature perturbation at $y = 0$, for $0 m \leq x \leq 12000 m$ and $0.75 \leq \sigma \leq 1$: (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is $1 K$.

5.23 The three-dimensional cold bubble test. Horizontal cross section of the potential temperature perturbation at $\sigma = 0$, for: (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The full horizontal domain $-20000 m \leq x \leq 20000 m$, $-20000 m \leq y \leq 20000 m$ is shown. The contour interval is $1 K$.

5.24 The three-dimensional cold bubble test. Vertical cross section of the vertical velocity $\dot{w}$ field at $y = 0$, for $0 \leq \sigma \leq 1$: (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is $1 ms^{-1}$. Note the displacement of the horizontal scale in (d).

5.25 The warm bubble test in three spatial dimensions. Vertical cross section of the potential temperature perturbation at $y = 0$, for $-8000 m \leq x \leq 8000 m$ and $0 \leq \sigma \leq 1$: (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is $0.5 K$.

5.26 The warm bubble test in three spatial dimensions. Vertical cross section of the vertical velocity $\dot{w}$ at $y = 0$, for $-8000 m \leq x \leq 8000 m$ and $0 \leq \sigma \leq 1$: (a) after 360 s; (b) after 520 s; (c) after 720 s; (d) after 900 s. The contour interval is $2 ms^{-1}$.
5.27 The three-dimensional warm bubble in an environment with strong unidirectional vertical wind shear. Vertical cross section of the potential temperature perturbation at \( y = 25\,000\,m \) and \( 0 \leq \sigma \leq 1 \): (a) after 360 s; (b) after 540 s; (c) after 720 s; (d) after 900 s. The contour interval is 0.5 \( K \). ........................................... 191

5.28 The three-dimensional warm bubble in an environment with strong unidirectional vertical wind shear. Vertical cross section of the vertical component of the wind \( \dot{w} \) at \( y = 25\,000\,m \) and \( 0 \leq \sigma \leq 1 \): (a) after 360 s; (b) after 540 s; (c) after 720 s; (d) after 900 s. The contour interval is 1 \( ms^{-1} \). ........................................... 192

5.29 The three-dimensional warm bubble in an environment with strong unidirectional vertical wind shear. Horizontal cross section of the potential temperature perturbation for: (a) after 360 s at \( \sigma = 0.44 \); (b) after 540 s at \( \sigma = 0.37 \); (c) after 720 s at \( \sigma = 0.29 \); (d) after 900 s at \( \sigma = 0.22 \). The contour interval is 0.5 \( K \). The \( \sigma \) level used for each time-step correspond to the height of maximum vertical velocity along \( y = 25\,000\,m \). Note that \( 20\,000\,m \leq y \leq 30\,000\,m \), with a displacement of the \( x \) direction scale in the Panels. ........................................... 193

5.30 The vertical component of the wind \( \dot{w} \) (shaded, \( ms^{-1} \)) and the vertical component of the vorticity \( \zeta \) (contours, \( s^{-1} \)) at \( \sigma = 0.48 \) and \( t = 900\,s \). ........................................... 195
List of Tables

2.1 Scale analysis of the horizontal momentum equation ............ 29
2.2 Scale analysis of the continuity equation .......................... 30
2.3 Scale analysis of the vertical momentum equation ............... 30

5.1 Comparison of minimum and maximum values of $\theta$, $u$ and $\dot{w}$ for the reference solution REFC, and simulations obtained using different values of explicit diffusion (see section 5.2.4). The values of the diffusion coefficients used are $K_s = 75\, m^2 s^{-1}$ (REFC and FA), $K_s = 50\, m^2 s^{-1}$ (FB), $K_s = 25\, m^2 s^{-1}$ (FC) and $K_s = 0\, m^2 s^{-1}$ (FD), for diffusion of the $u$ field along the $x$ axis. The diffusion applied along the $\sigma$ axis, and the $T$ field diffusion, is as specified in the text. Note that diffusion of double the magnitude is applied along the $\sigma$ axis for $T$ in solution REFC, compared to solution FA. ................................................................. 132

5.2 Comparison of minimum and maximum values of $\theta$, $u$ and $\dot{w}$ obtained for the various values of explicit diffusion. The values of the diffusion coefficients used are $K_s = 75\, m^2 s^{-1}$ (FA), $K_s = 50\, m^2 s^{-1}$ (FB), $K_s = 25\, m^2 s^{-1}$ (FC) and $K_s = 0\, m^2 s^{-1}$ (FD). The Shapiro filter is applied, with $p = 4$ .............. 143

5.3 Comparison of minimum and maximum values of $\theta$, $u$ and $\dot{w}$ obtained when fourth order discretization of spatial derivatives is applied. The Shapiro filter with $p = 4$ is used. The values of the diffusion coefficients used are $K_s = 75\, m^2 s^{-1}$ (FA), $K_s = 50\, m^2 s^{-1}$ (FB), $K_s = 25\, m^2 s^{-1}$ (FC) and $K_s = 0\, m^2 s^{-1}$ (FD). 146

5.4 Comparison of minimum and maximum values of $\theta$, $u$ and $\dot{w}$ obtained for the various departure point schemes. The fourth order discretization of spatial derivatives in the adjustment step equations and the Shapiro filter with $p = 4$ are used. $K_s = 25\, m^2 s^{-1}$. ................................................................. 152
5.5 Comparison of minimum and maximum values of $\theta'$, $u$ and $\dot{w}$
for the cases of marginally and poorly resolved flow. The spatial
resolutions corresponding to the listed values are $\Delta z \approx \Delta x = 200 \text{ m}$ (M-2 and M-4), $\Delta z \approx \Delta x = 400 \text{ m}$ (P) and $\Delta z \approx 100 \text{ m}$, $\Delta x = 500 \text{ m}$ (PM). Fourth order differencing was used to dis-
cretize the adjustment step equations, except for simulation M-2,
where second order differencing was used. ........................ 158
5.6 Stability experiments $\Delta t_s = \Delta t_a$ for various simulations as de-
scribed in the text. ................................................. 159
5.7 Advection time-step stability experiments, with $\Delta t_a = 0.5$, for
various simulations as described in the text. ...................... 163
5.8 Efficiency of the second and fourth order elliptic solvers, giving
the amount of iterations required for convergence per second of
integration time, for various simulations as described in the text. 166
5.9 Experimental design, maximum horizontal (HC) and vertical (VC)
advection Courant numbers, criterion of convergence $\epsilon$ and av-
verage number of iterations per second of integration time, for
various of the simulations as described in the text. .............. 181
List of Abbreviations

AGCM    Atmospheric general circulation model
ALADIN  Aire Limitee Adaptation Dynamique Dyveloppement International
CAT     Clear air turbulence
C-CAM   Conformal-cubic atmospheric model
CFL     Courant-Friedrichs-Lewy
CSIR    Center for Scientific and Industrial Research
CSIRO   Commonwealth Scientific and Industrial Research Organisation
DARLAM  Division of Atmospheric Research Limited Area Model
HC      Horizontal advection Courant number
VC      Vertical advection Courant number
MM5     Fifth-generation Pennsylvania State University-National Center for Atmospheric Research Meso-scale Model
MP      Miller-Pearce
NCAR    National Center for Atmospheric Research
NCEP    National Centers for Environmental Prediction
NWP     Numerical weather prediction
PC      Personal Computer
RAMS    Regional Atmospheric Modelling System
SAWB    South African Weather Bureau
SAWS    South African Weather Service
SAST    South African Standard Time
SOR     Successive Over-Relaxation
UKMO    United Kingdom Meteorological Office
UCT     University of Cape Town
UP      University of Pretoria
WITS    University of the Witwatersrand
WRC     Water Research Commission