CHAPTER 1

INTRODUCTION

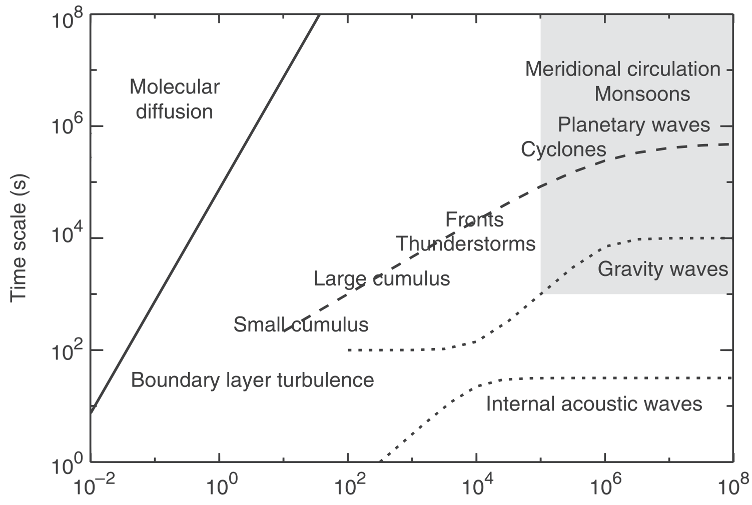
Extreme weather and climate conditions remain a threat to everyday human life. Understanding the atmospheric processes leading to extreme conditions which have devastating effects on human lives have become top priority for climate scientists and weather forecasters. Scientists and forecasters require the right tools to be able to reliably predict the extreme weather and climate events. The challenge in prediction of the extreme conditions lies in the fact that the evolution and movement in space of the atmospheric processes leading to these conditions need to be understood more at local and regional scales which are as small as about few hours in time and 1km in space. This therefore call for robust prediction tools which are able to resolve the processes across the scales of their occurrences. For a long time, grid point atmospheric prediction models have been used as a tool for both weather and climate predictions. Even though operational NWP is approaching fine enough temporal(Δt) and grid scales(Δx) resolution*, their effective† spatial resolutions are 4 to 8 times model's grid spacing Δx, and are thus inherently insufficient to explicitly resolve atmospheric processes up to scale of about 1km. Limited computational resources also limits model grid resolutions for long time simulations. For example, regional climate simulations are limited to spatial grid resolutions of approximately 10 times less than that of operational NWP due to much longer simulation periods of several years for the climate simulations. The complexity and multi-scale nature of the atmospheric processes is further making the design of the models very challenging. Figure 1.1‡ shows a schematic representation of the complexity and multi-scale nature of different important atmospheric phenomena, and the temporal and effective spatial resolution limit of the current climate models(the shaded region). The dashed line shows a representation of the observed horizontal kinetic energy spectra of Nastrom and Gage (1985) re-expressed in terms of length and time scales showing all phenomena important to weather and climate, and so need to be represented in the numerical models of weather and climate(Thuburn (2011b)). In the models, the unresolved processes(outside the shaded region) are usually represented as subgrid scale processes by parameterization of the resolved(grid scale) atmospheric variables, and this makes the representation of the interaction between the grid scale and sub-grid scale processes in the model quite challenging due to the fact that there is no significant spectral gap in the important atmospheric phenomena as shown by the dashed line in figure 1.1 (as figure 1.1 of Thuburn (2011b)). Intuitively, the best way to avoid such challenge is to increase the spatial resolution of the numerical model.

*High temporal resolution compared to the spatial resolution is partly attributed to the stability restrictions on the time steps for explicit solvers

†Effective resolution is used here in the context of the spatial scale at which the spectral characteristics of the simulated atmospheric variables compare to those of the observed, for example horizontal variance of wind and temperature. This is different from the resolution given by the model spatial grid spacing Δx

‡Reprinted from Thuburn (2011b) with permission from Springer Publishers.

Physical weather and climate models consist of governing nonlinear partial differential equations(PDEs) derived from physical conservation laws for mass, momentum, and energy describing atmospheric fluid flows. The numerical models are solving the closed system of equations referred to as dynamical cores of the model systems. For the development of dynamical cores , inviscid fluid flow regime described by the Euler equations is considered. For a complete weather and climate prediction model, additional terms for sub-grid scale parameterization[§] of unresolved physical and chemical processes are added to the dynamical core for a complete description of the humid state of the atmosphere. The equations are solved numerically to predict the state of the atmosphere for a given location at a given time. This is done by integrating the spatially discretized governing equations for a limited number of spatial grid points. It is natural to expect an error propagation due to discretization and/or sub-grid scale parameterization resulting in; limited predictability, and errors of the simulated climate variability. While sub-grid scale physical parameterization errors predominantly have a direct impact on the thermo-dynamical equilibrium state due to errors in forcing and or dissipation, errors in numerical methods applied in the model are considered to be relevant mainly with respect to stability. However, they can be artificial sources or sinks of the conserved quantities, and lead to errors in timing and or spatial distribution, e.g. of extreme weather phenomena.



source: (Thuburn,2011)

Figure 1.1: From Thuburn (2011b), show schematic representation of the complexity and multi-scale nature of different important atmospheric phenomena, and the temporal and spatial resolution limit of the current climate models(the shaded region). The dashed line shows a representation of the oberved horizontal kinetic energy spectra of Nastrom and Gage (1985) re-expressed in terms of length and time scales.

For the discretization of of the governing equations in space, finite difference(FD) discretization methods of different orders of accuracy are applied in many limited area models(LAM). However, with the increasing number of explicitly resolved phenomena as mentioned in the previous paragraph, improved numerical properties of the discretization methods and techniques used in the model systems become increasingly necessary in order to keep the signal to noise ratio for small scale phenomena large enough and to guarantee stable solution. For example, the discrete systems of equations which resolve more fast and very fast processes e.g. sound waves, may produce additional instabilities and have additional error sources. For the operational NWP, the model needs to correctly predict the structure and movements of weather phenomena, i.e. the numerical solution needs to correctly represent the speed, shape and propagation paths of important atmospheric features

[§]Sub-grid scale parameterization is based on approximations and simplifications of physical equations and generally do not completely represent the unresolved real physical processes. They aim at describing the mean effect of the processes at the scale of the model grid spacing.

relevant for weather forecasting. For climate projection, the equilibrium state(of the climate system) and its long term variability are most important. Thus, e.g. energy exchange among different components of climate system becomes important. For reliability of their results, climate models should be able to correctly represents the interaction between different components of the climate system across the scales. It is important that the model possesses the ability to correctly predict the amplitudes of different model parameters and to maintain the continuous statistical properties of the parameters. In the following paragraphs, we further look into three important properties of the FD methods used in state-of-the-art NWP models and RCMs, which should be considered for the numerical solutions obtained from the models to be confidently considered reliable.

For a useful application of FD methods for the numerical solution of the differential equations governing atmospheric flow, three fundamental properties of the numerical methods must be considered in the limit $\Delta x \rightarrow 0$, $\Delta t \rightarrow 0$. These are; consistency, stability and accuracy. They are described as follows:

- The *consistency* property demonstrates behaviour of the truncation error ϵ_{te}(the difference between the exact solution of the differential equations and the numerically approximated solution) with numerical grid refinement. A consistent numerical method for the differential equations is a method for which the truncation error becomes zero as the grid spacing Δx tend to zero. A number of texts, for example Ferziger and Perić (2002) have demonstrated the fact that truncation errors are usually proportional to a power of the grid spacing Δx which is called the order of convergence of the numerical method. A numerical method which is consistent is locally convergent, and it is expected that if a dominant term in a system of discrete equations is convergent in a certain order, then it is also globally convergent in that particular order. The higher the order of *convergence* the faster the truncation error approaches zero as grid spacing tend to zero, thus usually for the same truncation error, higher order methods can be applied with relatively coarser grid spacing than low order methods.

- Consistency of a numerical method however, does not guarantee convergence of the method. The numerical method will only converge if the solution is stable, therefore *stability* of the numerical solution is key for the convergence. Stability is measured in terms of the ability of the numerical error to remain bounded in time for problems whose exact solutions are bounded like atmospheric flow problems. For the NWP models and RCMs equations, the non-linearity and complexity of the systems make the stability analysis difficult. However, experience has shown that results obtained from stability analysis of the equations linearised and carefully reduced from the original model equations apply to the complete equations. Results from such linear stability analysis indicates that for the explicit time integration methods and spatial discretization methods(FD) applied in the models, time step is usually restricted by the Courant-Friedrichs-Lewy (CFL) stability condition. The complexity of the model system makes this condition necessary but not sufficient measure of the model's overall computational stability. Spectral analysis of the FD methods applied to the model's conservation equations can reveal that the discrete model can only resolve waves of wavelengths greater than twice the model's grid spacing(i.e. $>2\Delta x$). This is practically the limit at which the NWP models and RCMs are able to resolve any atmospheric feature. Due to the numerical resolution limit, waves smaller than $2\Delta x$

will be erroneously misrepresented as longer waves and the process is called *aliasing*[¶]. Observed spectra of atmospheric variables have been shown to decay at small scales through molecular diffusion. However, due to aliasing, fictitious variables' energy[‖] accumulates at smaller scales resulting to an increase in magnitude of the models dependent variables. Even if the linear stability criterion is met as mentioned before, the growth in magnitude of the model dependent variables due to aliasing can be unbounded resulting in another form of instability. Non-linear terms in the models system of equations can be shown to be the source of aliasing in the model's numerical solution. For example a numerical integration using the model can be started with an initial condition which do not contain any $2\Delta x$ feature. However, in the integration process the non-linear terms will cause non-linear interactions which result in $2\Delta x$ or even much smaller scales features which result to aliasing. The instability resulting from aliasing is thus referred to as non-linear instability. Both linear and non-linear instability thus contribute to the overall *instability* of the NWP models and RCMs.

- Absolute accuracy of the solution of the model's equations has different aspects. First, as mentioned in the previous paragraph, the order of convergence of a numerical method is the rate at which the truncation error approaches zero ($\epsilon_{te} \to 0$) in the limit of $\Delta x \to 0$. From this statement it can be deduced that the order of convergence of a numerical solution is a measure of how fast high accuracy of the numerical method can be achieved and is sometimes referred to as the order of accuracy of the numerical method in the literature. Second, it is apparent that the continuous systems of equations of the model systems are based on physical conservation laws for mass, momentum and energy. Thus, numerical methods which inherit the conservation properties of the continuous equations are considered accurate in the sense that the solution error[**] is minimized by the fact that no artificial sources and sinks are generated. In operational NWP and climate simulations, the degree of importance of the discrete conservation of any of the conserved quantities compared to dealing with other numerical model deficiencies might vary depending on the aim of the model user. For example non-conservative numerical schemes(methods) which are convergent and stable can be successfully applied to simulate synoptic scale atmospheric dynamics which are weakly dissipative over short time scales. For long time integration, particularly in large domains, violation of conservation results in the simulation of the dynamics of a distorted physical system(in comparison to the original system). The inheritance of the conservation properties of the continuous model system by the discrete model system can also be used as a requirement for evaluation for the numerical model. This study therefore considers numerical accuracy in a broader sense, by assessing the order of convergence, the conservation properties of the numerical methods used in the model system of interest, and the model's effective resolution as defined in the first paragraph of this chapter.

[¶]This is explained further and investigated in one of the next chapters

[‖]The term energy is used here to refer to the contribution of the harmonic components to the mean square value of the variable under considerations. This definition has been adapted from Mesinger and Arakawa (1976)

[**]The deviations from the solution of the continuous governing equations due to discretization of the equations is broadly referred to as discretization error, and if the exact solutions of both continuous and discrete set of equations exist, then their difference would be known as the solution error which in this case is equal to the discretization error.

1.1 Objectives

Considering the three fundamental properties *convergence*, *stability*, and *accuracy* of the numerical methods used for the discretization of the differential equations describing NWP and RCM models, credibility of the models' results demands fulfillment of all the three numerical properties to some degree below which the models can be rendered incapable of predicting weather and climate. Fulfilling these requirements is not only intuitive but has become a constraint in the design and development of dynamical cores of weather and climate models. Despite many years of development, state-of-the-art NWP models and RCMs for example WRF of NCAR/NOAA (see Wicker and Skamarock (2002)) and COSMO of DWD (see Baldauf (2008b)) still posses significant errors which can be improved by applying advanced numerical methods[††] for the solution of the models' system of equations. Most prominently the amplitude errors and the overall stability of the model systems can still be improved. Using a two-dimensional idealized mountain flow test case, Baldauf (2009) showed that the convergence rate of the spatial numerical methods used in the COSMO model is second order, even though the derivatives in the non-linear terms are discretized using second to sixth order accurate FD methods. Such results reduce credibility of the real case simulation results obtained by the model system, and the range of applicability. Investigating the linear stability analysis of the advection schemes in COSMO model, Baldauf (2008b) revealed that the inherently diffusive third order and fifth order upwind schemes used for discretization of the advection terms of the COSMO system of equations are more stable than the second, fourth, and sixth order centered finite difference schemes when used in combination with Runge-Kutta integration schemes. Another look into the overall stability of COSMO model reveals that, an artificial horizontal diffusion must be applied during time integration for model to remain stable as documented in Doms et al. (2011). The artificial diffusion term is meant to prevent non-linear instability in the model system. This procedure has an impact on the amplitudes of the variables for which small scale features are severely damped. In terms of the model's effective resolution, Skamarock (2004) has shown that the effective resolution of WRF model which uses similar numerical methods to discretize the model's system of equations as COSMO, is approximately six times the model's grid spacing($\approx 6\Delta x$) mainly affected by the artificial diffusion term. The consequence of such a low effective resolution is that a user have to set a relatively finer grid spacing to be able to simulate atmospheric features at cloud-resolving scale which could be quite costly in terms of computing resources and generally time consuming, otherwise, important small scale features cannot be resolved by the model.

The aim of this study is to investigate the potential for improvement of convergence, stability, and accuracy properties of discretization of the Euler equations of a state-of-the-art NWP and RCM model COSMO, by application of higher order schemes(traditional and quadratic conserving). The steps towards achieving the aim are:

1. A detailed theoretical analysis of quadratic conserving(symmetric) spatial schemes[‡‡] and traditional spatial schemes in terms of convergence, stability and accuracy. This is meant to justify advantages of the conservative schemes, which can be expected to be evident in real case applications.

[††]numerical methods and numerical schemes have been used interchangeably in this chapter for convenience to mean the same thing. However, after the current chapter, the finite difference methods will be commonly referred to as numerical schemes throughout

[‡‡]These schemes are known in the literature as *Quadratic conserving spatial schemes* for the reason of their property to conserve up to the second statistical moment of the prognostic model variable

2. Implement one of the higher order accurate quadratic conserving and traditional schemes in a dynamical core of a state-of-the-art operational mesoscale model.

3. Perform idealized numerical tests and analysis of the implemented numerical schemes, and carry out a real case study using real boundary conditions obtained from re-analyses data sets and evaluate the model results obtained using the new and the model's existing spatial schemes.

The new numerical schemes implemented in the COSMO model are the fourth order accurate Morinishi(symmetric) schemes (Morinishi et al. (1998) and Morinishi (2010)). The major advantages of these schemes are their quadratic conservation of an advected quantity property, and their higher order of convergence. Additionally, traditional fourth order scheme are obtained for the model system by combining fourth order interpolations with fourth order differencing for the existing COSMO schemes(Baldauf (2008b)). Schemes(of different orders of convergence) which are constructed in a similar way are generally referred to as higher order scheme(HOS) in this study. It can be expected that convergence, stability and accuracy properties of the model system can be improved by new[§§] numerical schemes. These methods will from here-on be referred to as Quadratic conserving higher order numerical schemes(QCHOS)[¶¶]. Up to the knowledge of the author, these spatial schemes are yet to be applied in a operational LAM like COSMO. It is the first time that such numerical methods are implemented and tested in a NWP and RCM model, and their properties for discretization of fully compressible system of equations of an atmospheric model, investigated and compared with numerical methods operationally used in NWP and RCM simulations. The author however, acknowledges that the 'new' numerical methods have been widely utilised in fluid mechanics for theoretical studies(e.g. Morinishi et al. (1998), Morinishi (2010), Kaltenbach et al. (2002)).

1.2 Outline

This study is arranged in three main parts (which are the first three parts presented) as a consequence of the objectives stated in the previous paragraph, and two additional parts for conclusions, outlook and appendices.

Part I: Fundamentals, Review and Theory

This is the first part, and it contains two chapters highlighted as follows: In *chapter two*, a review of different finite difference schemes in a staggered grid system with different orders of convergence applied in state-of-the-art NWP and RCMs is given. The HOS and QCHOS schemes are also described are their construction is explained. In *chapter three*, a comprehensive theoretical analysis of HOS and QCHOS from second to sixth order of convergence and the current operational schemes in COSMO and WRF models is done. For the analysis, accuracy of the methods in terms of; phase and phase speed errors, amplitude error, group velocity error, and aliasing error are investigated. The linear stability analysis of the HOS and QCHOS schemes in combination with the Runge-Kutta time integration

[§§] *'new'* is used here to refer to the status of the model's dynamical core in terms of the spatial schemes currently applied in the model for operational forecasting and climate simulations

[¶¶] These schemes are sometimes referred to as *symmetric schemes* due to the symmetric nature of their formulation schemes (Baldauf (2008b)) is also presented. The stability limits of the HOS and QCHOS schemes are then compared with the current operational schemes. In the same chapter, effective resolution of all spatial schemes investigated is analytically calculated based on the dispersion relation analysis Investigation of the the magnitude of alias error of the schemes which is considered an indication of the level of nonlinear instability is done as well. The comprehensive theoretical analysis in this chapter justifies the implementation of the HOS and QCHOS in the operational model system.

Part II: The Model System and Code Implementation

This part contains a single chapter which describes the operational non-hydrostatic model system under consideration (COSMO model) for this study, and also presents an in-depth documentation of the code development in the model's dynamical core in which the new schemes have been implemented. In *chapter four*, a full implementation documentation of fourth order accurate HOS and QCHOS horizontal schemes is given. For further elaborations, the fourth order scheme implemented are; first, is the traditional fourth discretization of the spatial derivatives in the model's Euler equations is extended by fourth order accurate interpolation of the advecting velocity in the non-linear term of the equations. This is considered an extension of the existing operational model's fourth order advection scheme (Baldauf (2008b)). The existing schemes are referred to as Quasi-higher order spatial schemes(QHOS) by the author. The second is a fourth order accurate QCHOS which is more promising due to its desirable conservative properties. In addition to nonlinear terms, the fourth order schemes are applied to all linear terms of the operational model's Euler equations, which makes the complete system fourth order accurate in horizontal space.

Part III: Code Verification and Real Case Study

This part consist of two chapters dedicated to; numerical experiments for verifying the new implementations in the computer code of the operational model system, and a chapter on the configuration, simulations, and results of a real case study. In *chapter five*, the numerical schemes implemented in the model system as documented in chapter four are tested using an idealized test case. In this chapter, the order of convergence of the schemes compared to the current operational schemes are calculated and compared. Stability of the model system using the new schemes is also numerically tested. In *chapter six*, the new schemes implemented are tested in climate mode using real boundary conditions. A series of 20-year long regional climate simulations over a European domain similar to that of EURO-CORDEX is carried out and analysed. Kinetic energy spectra are calculated from the simulated zonal wind velocities and compared with observed kinetic energy spectra. The climatologies of various model variables are also compared to the observations.

Part IV: Summary and Outlook

Summary and outlook of the study are presented in *chapter six*, conclusions based on the theoretical analyses and the numerical test results are given. Recommendations are then given for the application of QCHOS schemes in an operational NWP and RCM model.

Part V: Appendices and Bibliography

This is the final part which contains appendices and references used in the study. In the *appendices*, derivation of weighting factors for the finite difference schemes of arbitrary order of accuracy using Taylor series expansion technique is presented for further insights into the various FD schemes presented and discussed in the study. Numerical properties of QCHOS and upwind finite difference schemes as implemented in the model system are presented for better understanding of the properties of the QCHOS and upwind schemes.

Part I

Fundamentals, Review and Theory

CHAPTER 2

HORIZONTAL DISCRETIZATION METHODS ON A STAGGERED GRID

2.1 Introduction

A number of current atmospheric grid point models for weather forecasting and climate projections utilize staggered grid systems for the solution of their respective continuous governing systems of equations in discrete form. There are different types of grid staggering which have been used in atmospheric and oceanic prediction models (see: Arakawa and Lamb (1977)), and the most commonly used in the current operational models including COSMO and WRF is Arakawa C-grid. There is no fundamental difference between staggered and non-staggered grids, however, a number of analysis have shown that the propagation of waves and wave energy are better represented on a staggered grid than on unstaggered grid system(see, Duran (2010) and Thuburn (2011a)). All the discretizations of differential equations presented in the study are based on Arakawa C-grid as shown in figure 2.1. The aim of this chapter is to introduce, describe and discuss different centered finite difference schemes applied in current operational non-hydrostatic atmospheric grid-point models QHOS schemes, and the new HOS and QCHOS for compressible model equations.

Discussions on the required level of accuracy of finite difference(FD) schemes applied in atmospheric and oceanic fluid flow models have been presented in publications by a number of authors of which only some will be mentioned here. Kreiss and Oliger (1972) is an example of an early study and investigation on the need and benefits of using higher order spatial schemes(HOS)* on multi-dimensional large scale problems such as weather prediction. They used fourier analyses of finite difference methods for approximating hyperbolic PDEs to estimate the number of points per wavelength needed to achieve a particular accuracy for the systems. They found that, for problems where small errors or high accuracy is needed and for problems where long time integration is necessary, HOS is advantageous compared to second order accuarate methods. However, after the Kreiss and Oliger (1972)'s results were published, HOS remained sidelined in the weather and climate prediction models due to higher computational costs for a multi-dimensional simulations using HOS, and lack of improved predictability.

Advantages of using HOS for the descretisation of Partial Differential Equations(PDEs) as presented by Kreiss and Oliger (1972) have been recently reaffirmed by Gustafsson (2008). With results based on analysis of the numerical properties of a difference approximation applied to a single wave with a fixed wave number(von Neumann analysis), Gustafsson (2008) indicated that infact the gain of using HOS is more pronounced in multi-dimensional problems like weather and climate predictions. Gustafsson (2008) revealed that, if applying HOS in a single space dimension results to a reduction factor which is greater than one in

*As mentioned in chapter 1, traditional FD methods with orders of accuracy higher than second is referred to as HOS throughout this study