Chapter 15
A Perspective on the Role of the Dynamical Core in the Development of Weather and Climate Models

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Abstract This chapter aims to place the dynamical core of weather and climate models into the context of the model as a system of components. Building from basic definitions that describe models and their applications, the chapter details the component structure of a present-day atmospheric model. This facilitates the categorization of model components into types and the basic description of the dynamical core. An important point in this categorization is that the separation between 'dynamics' and 'physics' is not always clear; there is overlap. This overlap becomes more important as the spatial resolution of models increases, with resolved scales and parameterized processes becoming more conflated. From this categorization an oversimple, intuitive list of the parts of a dynamical core is made. Following this, the equations of motion are analyzed, and the design-based evolution of the dynamical core described in Lin (2004) is discussed. This leads to a more complete description of the dynamical core, which explicitly includes the specification of topography and grids on which the equations of motion are solved. Finally, a set of important problems for future consideration is provided. This set emphasizes the modeling system as a whole and the need to focus on physical consistency, on the scientific investigation of coupling, on the representation of physical and numerical dissipation (sub-scale mixing and filtering), and on the robust representation of divergent flows. This system-based approach of model building stands in contrast to a component-based approach and influences the details of component algorithms.

15.1 Introduction

This is a perspective on the design of physical models for use in the scientific investigation of weather and climate. This perspective follows from a career that involves both model development and the management of the development of institutional models. The point of view is anchored around the role of the dynamical core in

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atmospheric models. There are numerous books on atmospheric modeling, their history, their construction, and their applications (Trenberth 1992; Randall 2000; Mote and O'Neill 2000; Satoh 2004; Jacobson 2005; Washington and Parkinson 2005). The review paper by Rood (1987) contains many foundational references, and a basic introduction to the problem of numerical advection. The concepts associated with the works of Godunov (1959), Boris and Book (1973), and van Leer (1979) are particularly influential.

The perspective is outlined as follows:

- Definition and Description of the Model
- Construction of Weather and Climate Models
- Analysis of the Atmospheric Equations of Motion
- Numerical Expression of the Atmospheric Equations of Motion
- Synthesis and Future Directions
- Conclusions

15.2 Definition and Description of the Model

Dictionary definitions of model include:

- A work or construction used in testing or perfecting a final product.
- A schematic description of a system, theory, or phenomenon that accounts for its known or inferred properties and may be used for further studies of its characteristics.

In weather and climate modeling a scientist is generally faced with a set of observations of variables, for instance, velocity, temperature, water, ozone, etc., as well as either the knowledge or expectation of correlated behavior between the different variables. A number of types of models could be developed to describe the observations. These include:

- Conceptual or heuristic models which outline in the simplest terms the processes that describe the interrelation between different observed phenomena. These models are often intuitively or theoretically based. An example would be the tropical pipe model of Plumb and Ko (1992), which describes the transport of long-lived tracers in the stratosphere.
- Statistical models which describe the behavior of the observations based on the observations themselves. That is, the observations are described in terms of the mean, the variance, and the correlations of an existing set of observations. Johnson et al. (2000) discuss the use of statistical models in the prediction of tropical sea surface temperatures.
- Physical models which describe the behavior of the observations based on first principle tenets of physics (chemistry, biology, etc.). In general, these principles are expressed as mathematical equations, and these equations are solved using

discrete numerical methods. Detailed discussions of modeling include Trenberth (1992), Randall (2000), Mote and O'Neill (2000), Satoh (2004), Jacobson (2005), and Washington and Parkinson (2005).

In the study of geophysical phenomena there are numerous sub-types of models. These include comprehensive and mechanistic models. Comprehensive models attempt to model all of the relevant couplings or interactions in a system. Mechanistic models have prescribed variables, and the system evolves relative to the prescribed parameters. All of these models have their place in scientific investigation, and it is often the interplay between the different types and sub-types of models that leads to scientific advance.

Models are used in two major roles. The first role is diagnostic, in which the model is used to determine and to test the processes that are thought to describe the observations. In this case, it is determined whether or not the processes are well known and adequately described. In general, since models are an investigative tool, such studies are aimed at determining the nature of unknown or inadequately described processes. The second role is prognostic; that is, the model is used to make a prediction.

In all cases the model represents a management of complexity; that is, a scientist is faced with a complex set of observations and their interactions and is trying to manage those observations in order to develop a quantitative representation. In the case of physical models, which are the focus here, a comprehensive model would represent the cumulative knowledge of the physics (chemistry, biology, etc.) that describe the observations. It is tacit, that an accurate, validated, comprehensive physical model is the most robust way to forecast; that is, to predict the future.

The physical principles represented in an atmospheric model, for example, are a series of conservation laws which quantify the conservation of momentum, mass, and thermodynamic energy. The equation of state describes the relation between the thermodynamic variables. Because of the key roles that phase changes of water play in atmospheric energy exchanges, an equation for the conservation of water is required. Similarly, an equation for salinity is necessary to represent ocean dynamics. Models which include the transport and chemistry of atmosphere trace gases and aerosols require additional conservation equations for these constituents. The conservation equations for mass, trace gases, and aerosols are often called continuity equations.

In general, the conservation equation relates the time rate of change of a quantity to the sum of the quantity's production and loss. The production and loss for momentum follow from the forces described by Newton's Laws of Motion. Since the atmosphere is a fluid, either a Lagrangian or an Eulerian description of the flow can be used (Holton 2004). The Lagrangian description follows a notional fluid parcel, and the Eulerian description relies on spatial and temporal field descriptions of the flow at a particular point in the domain. In this chapter the Eulerian framework will be the primary focus. Holton (2004) provides a thorough introduction to the fundamental equations of motions and their scaling and application to atmospheric dynamics.

Table 15.1 Construction of an atmospheric model (see text for details)

Boundary/Initial conditions	Emissions, topography, sea surface temperature	ϵ
Representative equations	$DA/Dt = P - LA$	ϵ
Discrete/Parameterize	$\left(A_{t+\Delta t} - A_t\right)/\Delta t = \ldots$	ϵ_d,ϵ_p
Theory/Constraints	Geostrophy, Thermal wind	Scale analysis
Primary Products (i.e. A)	$T, u, v, H_2O, O_3, \ldots$	ϵ_b,ϵ_v
Derived Products	Potential Vorticity, Budgets	Consistent

ϵ_d = discretization error, ϵ_p = parameterization error, ϵ_v = variability error, ϵ_b = bias error

In order to provide an overarching background, it is useful to break down the process of the construction of an atmospheric model as shown in Table 15.1. The table lists six major elements (left column), a concrete example of the element (middle column), and a reminder that there are explicit errors, ϵ, at all stages of the construction (right column). The first element points to the boundary and initial conditions. For an atmospheric model, boundary conditions include topography, sea surface temperature, land type, vegetation, etc. Note that boundary conditions are generally prescribed from external sources of information.

The next three items in the table are intimately related. They are the representative equations, the discrete and parameterized equations, and constraints drawn from theory. The representative equations are the continuous forms of the conservation equations. The representative equations used in atmospheric modeling are approximations derived from scaling arguments (see Holton 2004); therefore, even the equations the modeler is trying to solve have *a priori* simplification which can be characterized as errors. Here a conservation equation for an arbitrary quantity, A, is written with an exemplary production, P, and loss, L. The continuous equations are a set of non-linear partial differential equations. The solutions to the representative equations are a balance amongst competing forces and tendencies.

The discrete and parameterized equations arise because it is not possible to solve the representative equations in analytical form. The strategy used by scientists is to develop a numerical representation of the equations. One approach is to define a grid of points which covers the spatial domain of the model. Then a discrete numerical representation of those variables and processes which can be resolved on the grid is written. Processes which take place on spatial scales smaller than the grid are parameterized. These approximate solutions are, at best, discrete estimates to solutions of the analytic equations. The discretization and parameterization of the representative equations introduce a large source of error. This introduces another level of balancing in the model; namely, these errors are generally managed through a subjective balancing process that keeps the numerical solution from producing obviously incorrect estimates.

While all of the terms in the analytic equation are potentially important, there are conditions or times when there is a dominant balance between, for instance, two terms. An example of this is the geostrophic balance and the related thermal wind balance in the middle latitudes of the atmosphere (Holton 2004). It is these balances, generally at the extremes of spatial and temporal scales, which provide the constraints drawn from theory. Such constraints are generally involved in the development of conceptual or heuristic models. If the modeler implements discrete methods which represent the relationship between the analytic equations and the constraints drawn from theory, then the modeler maintains a substantive scientific basis for the interpretation of model results.

The last two items in Table 15.1 represent the products that are drawn from the model. These are divided into two types: primary products and derived products. The primary products are variables such as temperature T, wind (u, v), water (H_2O), and ozone (O_3) – parameters that are, most often, transported by the fluid flow. The primary products might also be called the resolved or prognostic variables. The derived products are of two types. The first type describes those products which are diagnosed from the model's state variables, often in the parameterized physical processes. The second type follows from functional, $F(A)$, relationships between the primary products; for instance, potential vorticity (Holton 2004). A common derived product is the budget – the sum of the different terms of the discretized conservation equations. The budget is studied, explicitly, on how the balance is maintained and how this compares with budgets derived from observations or observations assimilated into predictive models.

In some cases the primary products can be directly evaluated with observations, and errors of bias and variability are estimated. The bias is, for example, the difference between time-averaged model predictions and observations. Variability errors follow from, for example, the representation of the distributions about the temporal mean. If attention has been paid in the discretization of the analytic equations to honor the theoretical constraints, then the derived products will behave consistently with the primary products and theory (see, Table 15.1). In this case consistency is used to state that budgets are balanced, and that the physically based, correlative relationship between variables is represented. In a consistent model, there will be errors of bias and variability, but when a budget is formed from the sum of the terms in the conservation equations, it will balance. That is, the discrete form of the conservation equation is solved.

15.3 Construction of Weather and Climate Models

Weather and climate models are an assembly of components that are composited together to construct integrated functionality. Composites are then composited together, yielding highly complex systems. For example, a physical climate model can be constructed from a sea ice model, a land surface model, an ice sheet model, an ocean model and an atmospheric model. Associated with these composited models are representations of chemical and biological processes important to the physical climate, for example, atmospheric ozone and plant respiration (i.e., carbon dioxide). These models communicate with each other through a coupler.

Big models are made from smaller models, and this concept cascades to increasing granularity. This method of model construction has been described as 'process splitting' or fractional steps and is described in, for instance, Yanenko (1971), Strang (1968), and McCrea et al. (1982). Historically, atmospheric models evolved from efforts focused on specific parts of the atmosphere: thermosphere models (e.g. Dickinson et al. 1981), middle atmosphere models (e.g. Schoeberl and Strobel 1980; Fomichev et al. 2002), and many models of the troposphere – often weather forecast models. The focus on specific parts of the atmosphere was driven by scientific interests, observational and theoretical foundations, and limited computational resources. A primary characteristic of, for example, a model focused on the middle atmosphere (i.e., the stratosphere and mesosphere) is special attention to the physical and chemical parameterizations that are important in the focus region. Connectivity, for example, the influence of the troposphere on the stratosphere is achieved in several ways. Mechoso et al. (1985) coupled the stratosphere to the troposphere with filtered observations at a lower boundary. A natural and comprehensive approach is to extend the domain of a tropospheric model upward or a middle atmosphere model downward with inclusion of appropriate physical algorithms. Only recently, whole atmosphere models have been routinely used for scientific research (e.g. Beres et al. 2005).

Using a specific model type to expose the component structure, a troposphere-stratosphere model might be constructed from a set of components that include, for example, algorithms that represent advection, mixing, the planetary boundary layer, gravity waves, radiation, cumulus convection and clouds. The component of the atmospheric model that represents clouds might then have sub-components that represent the different phases of water, sulfate aerosols (hence, sulfate chemistry), black carbon, etc. Components at all levels need to communicate with each other, and thus, in a generalized sense there is a requirement for coupling of components.

Figure 15.1 shows the Earth System Modeling Framework (ESMF, http://www.esmf.ucar.edu/about_us/) component architecture of the Goddard Earth Observing System, version 5 (GEOS-5) atmospheric model (Rienecker et al. 2008). From the top down, the structure shows the coupling of the atmospheric general circulation model ('agcm'), with the stored, digital 'history' files used in model initialization, diagnostics and application. Below 'agcm' there is a separation of the model components into 'dynamics' and 'physics,' and, again and throughout, the explicit need for coupling.

Those algorithms that are associated with advection and part of the sub-scale mixing (defined below) are often identified as 'the dynamics' and all of the other algorithms are identified as 'the physics'. The dynamical core is identified as 'fvcore' in Fig. 15.1. In this model the physical 'gravity_ wave_ drag' parameterization is counted as part of the dynamics. To be explicit, some algorithms identified with 'the physics' represent adiabatic dynamical processes such as 'turbulence' in the boundary layer. These mixing processes, gravity wave drag and turbulence, are at a resolution smaller than the grid can resolve, but associated with some physical cause not explicitly resolved by the dynamical core. This counting of dynamical processes in both 'dynamics' and 'physics' is a source of ambiguity in the definition of the dynamics of the model and the dynamical core – an ambiguity that becomes more important to address as resolution is increased.

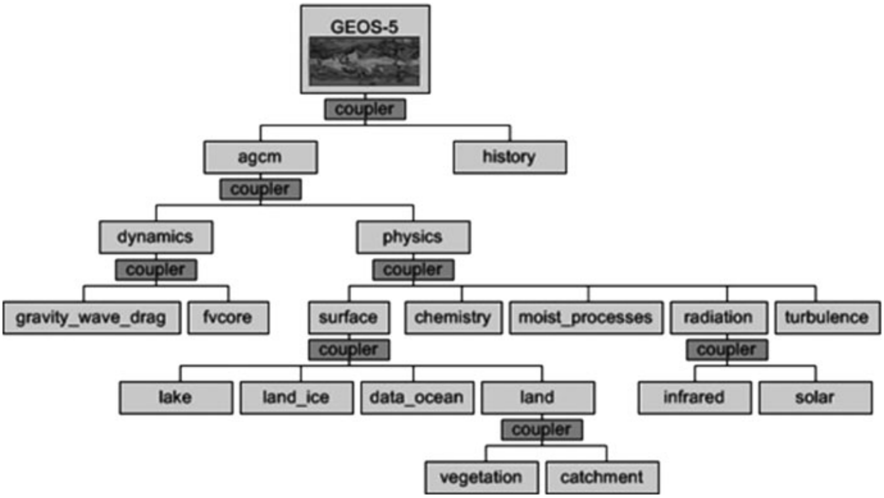

Fig. 15.1 Component architecture of the GEOS-5 atmospheric model

At the 'surface' the atmospheric model is coupled to needed information from other components of the Earth system – or the other components of a climate model. In this case the effects on the atmosphere of lakes ('lake') and ice and snow on the land ('land_ice') are explicitly specified. Data that represent the state of ocean are included in the standard configuration of the model ('data_ocean'). This is where an explicit, interactive ocean model could be coupled. Finally, the interaction of 'vegetation' on 'land' is included. Land-surface hydrology is represented on a spatial discretization based on water 'catchments', rather than the grid used for the atmospheric model.

There is no standard definition of the term 'dynamical core' (in short 'dycore'). Williamson (2007) defines the dynamical core 'to be the resolved fluid flow component of the model'. This definition is one that has been widely shared in model development centers, as is perhaps best represented by the model documentation (e.g. Collins et al. 2004). Within this chapter the following definition from Thuburn (2008b) is used: "The formulation of a numerical model of the atmosphere is usually considered to be made up of a dynamical core, and some parameterizations. Roughly speaking, the dynamical core solves the governing fluid and thermodynamic equations on resolved scales, while the parameterizations represent sub-grid scale processes and other processes not included in the dynamical core such as radiative transfer. Here, no attempt is made to give a precise definition of 'dynamical core' because, as discussed below, there are some open questions concerning exactly which terms and which processes should be included in a dynamical core".

In order to expose the building blocks of a dynamical core and to address the ambiguities and open questions suggested above, (15.1) is used to illustrate the 'dycore' part of the model more concretely. A representative conservation equation for a scalar quantity, A, can be written as

$$\frac{\partial A}{\partial t} = -\nabla \cdot \mathbf{u}A + M + P - LA \qquad (15.1)$$

P represents production and L represents a loss rate. $\mathbf{u}$ is the vector velocity and t is time. M represents dynamical mixing at spatial scales smaller than the grid size. A is, in this example, assumed to be a scalar parameter such as temperature or ozone. Formally in the dynamical core, A would include the velocity components, which yields a nonlinear equation and limits this illustration to only being demonstrative. In analogy with the atmospheric model described in Fig. 15.1, the P and LA terms are identified with 'the physics'. The flux divergence term is the resolved flow and is identified with the dynamical core. The flux term is where a specific advection algorithm (Rood 1987; Williamson 2007) is implemented. The dynamical mixing term, M, is also identified with the dynamical core; however, it may also be related to the mixing associated with the physics and is, hence, not cleanly separated. Part of the purpose of this chapter is to expose this ambiguity and refine the description of the dynamical core.

In their simplest expressions, dynamical cores are generally process split and include the following:

- The resolved advection in the horizontal plane.
- The resolved vertical advection.
- Unresolved sub-scale transport.
- A portfolio of filters and fixers that accommodate errors related to both the numerical technique and the characteristics of the underlying grid.

A more complete description of the dynamical core will be developed below, including discussion of how the dynamical core spans the equations of motion.

As revealed above, models are complex composites of sub-models. These sub-models are, most often, also complex, and they are approximations of varying accuracy that represent physical processes. At the finest levels these models are said to be parameterized, and the algorithms described as parameterizations. The function of the model as a whole is an amalgamation of all of the composites, and is therefore, a function of the errors associated with the components and how those errors are accumulated. For this reason, development of highly accurate sub-models and parameterizations often does not lead directly to an improved function of the model as a whole. The model needs to be rebalanced or tuned, a process that implicitly addresses the balance between both physical processes and error sources.

This description and the representation in Fig. 15.1 explicitly reveal the fact that there are many couplers in a model. Couplers are, *de facto*, yet more model components, and their construction influences the performance of the system as a whole. The robustness and the integrity of the model as a whole are often construed as being based on the construction and the quality of the component algorithms. Ultimately however, it is the function of the system as a whole that is of interest to the discipline scientist, e.g., the climate forecast user. Hence, the physics of the couplers also requires scientific scrutiny.

15.4 Analysis of the Atmospheric Equations of Motion

The equations of motion for the atmosphere in tangential spherical coordinates using the radial distance for the vertical coordinate (λ, ϕ, r) are given by (see also White et al. 2005)

$$\begin{aligned}
\frac{Du}{Dt} - \frac{uv\tan(\phi)}{r} + \frac{uw}{r} &= -\frac{1}{\rho r\cos(\phi)}\frac{\partial p}{\partial \lambda} + 2\Omega v\sin(\phi) - 2\Omega w\cos(\phi) + \nu\nabla^2 u \\
\frac{Dv}{Dt} + \frac{u^2\tan(\phi)}{r} + \frac{vw}{r} &= -\frac{1}{\rho r}\frac{\partial p}{\partial \phi} - 2\Omega u\sin(\phi) + \nu\nabla^2 v \\
\frac{Dw}{Dt} - \frac{u^2+v^2}{r} &= -\frac{1}{\rho}\frac{\partial p}{\partial r} - g + 2\Omega u\cos(\phi) + \nu\nabla^2 w \\
\frac{D\rho}{Dt} &= -\rho\nabla\cdot\mathbf{u} \\
c_v\frac{DT}{Dt} + p\frac{D\alpha}{Dt} &= J \\
p &= \rho R_d T \\
\alpha &= \frac{1}{\rho}
\end{aligned} \tag{15.2}$$

with

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla \tag{15.3}$$

t denotes the time, λ is longitude, ϕ is latitude, r is the radial distance to the center of the spherical Earth, Ω is the angular velocity of the Earth, g is gravity, ν is a coefficient of viscosity, c_v is specific heat at constant volume, R_d is the gas constant for dry air, ρ is density, T is temperature, p is pressure, $\mathbf{u}$ is the velocity vector $\mathbf{u} = (u, v, w)$, and J stands for the diabatic heating. The first three equations represent the conservation of momentum. The fourth equation is the mass continuity equation, and the fifth equation is the thermodynamic energy equation. The last equation in (15.2) is the equation of state for dry air.

In addition, equations are needed which describe the conservation of trace constituents. The generic form of these continuity equations are:

$$\frac{DQ_i}{Dt} + Q_i\nabla\cdot\mathbf{u} = P_{Q_i} - L_{Q_i} \tag{15.4}$$

Where Q_i is the density of a constituent identified by the subscript i. P_{Q_i} and L_{Q_i} represent the production and loss from phase changes and photochemistry. An equation for water in the atmosphere, $Q_i = Q_{H_2O}$, is required for a comprehensive atmospheric model. For water vapor, the production and loss terms are represented by evaporation and condensation. These are associated with significant consumption and release of heat, which must be accounted for in the heating J, the production and loss term of the thermodynamic energy equation. In the atmosphere below the stratopause, heating due to the chemical reactions of trace constituents are assumed not to impact the heat budget of the atmosphere. It is possible for the spatial distribution of trace constituents, for example ozone, to impact the absorption and emission of radiative energy; hence, there is feedback between the constituent distributions and diabatic processes in the atmosphere.

Dynamical cores are often developed, first, in the two-dimensional shallow-water model (for example Lin and Rood 1997). This brings focus to the momentum equation, with the presumption that if the numerical technique provides a good solution to the nonlinear momentum equations, then spanning the technique across the whole set of the equations of motion is relatively straightforward. The review of Williamson (2007) takes a focus on the 'horizontal aspects of the schemes' and describes the methods used to represent the advective terms in the equations of motion. The extension from two dimensions to three dimensions and consideration of real-world aspects of atmospheric modeling require addressing a set of fundamental issues. These issues lead to a more complete specification of the dynamical core, which will be exposed below.

There are a number of important points to be made directly from the atmospheric equations of motion. In general, the equations are scaled to expose the range of motions that are important to weather and climate models. Consideration of 'large-scale' dynamics, for example motions of spatial scales 1,000 km or greater, leads to a separation of the horizontal and vertical motions in the atmosphere. Similarly, it leads to the conclusion that the flow is dominated by rotational motion, as contrasted with divergent motion. Such scale analysis explicitly impacts the development of dynamical cores in numerical models; for example, the development of different algorithms to treat horizontal and vertical advection. In fact, the consideration of the large-scale characteristics of the atmospheric flow impacts the development of dynamical cores in ways that have such profound influence on the numerical performance that they require algorithmic archeology to expose their impact.

Returning to (15.2), consider the first two terms on the right hand side of the u and v equations. These are the horizontal pressure gradient terms and the Coriolis terms. They are often dominating terms and represent the geostrophic balance. From first principles, the pressure gradient initiates motion. As a large term important to the motion of the atmosphere, it is critical that the pressure gradient term be well represented. Alternatively, if the pressure gradient term is poorly represented, then there will be large negative consequences to the model performance.

Accuracy of the representation of the pressure gradient brings attention to the lower boundary condition and the specification of topography. A common practice in atmospheric modeling is to use a terrain following vertical coordinate (see Holton 2004; Satoh 2004). This eases the specification of the lower boundary. However, it introduces a major challenge in the representation of the horizontal pressure gradient in the presence of steep topography, hence, large pressure gradients, hence, large discretization errors. Though the pressure gradient and the Coriolis force are, abstractly, a momentum source term, these forces are a resolved part of the flow. Therefore, discretization of the pressure gradient term and specification of the Coriolis force are parts of the dynamical core.

There are in the continuous equations of motion, explicit dissipative terms. These include both the viscosity terms as well as the diabatic heating term (J), which includes damping of temperature perturbations. In the continuous equations the viscosity terms are usually very small. In the discrete equations viscosity takes on a far different character. In the estimation of numerical solutions, variability starts to form at the smallest spatial grid scale. This structure comes from a variety of sources ranging from physical advective cascade from large to small scales to numerical dispersion caused by different wavelengths propagating at different speeds. The grid-scale structure can come to dominate the estimated solution; hence, it requires dissipation both to account for a discrete representation of physical mixing and for remediation of unavoidable numerical errors. Therefore, real atmospheric dissipation becomes conflated with many forms of dissipation that are present in dynamical cores for both physical and numerical reasons. Further, this dissipation is not independent of that modeled in the planetary boundary layer parameterization and the gravity wave parameterization – both accounted for as part of the model 'physics'. There is no prescription from first principles on how to address the specification of dissipation, and the modeler is often left with the statement in Farge and Sadourny (1989) that the "validity (of the choice of dissipation) can only be judged on the grounds of numerical results". A thorough review of the dissipative processes in the dynamical cores of general circulation models is provided in Chap. 13.

Finally, consider the constituent continuity equations (15.4). As suggested above, the intuitive focus of the 'dynamical core' is on the algorithm used to solve the momentum equations, or alternatively, the vorticity and divergence equations. An atmospheric model, however, requires the solution of the thermodynamic equation and numerous constituent continuity equations. The mass conservation equation and the equation of state must be tied into the numerical solution. These equations all contain the advection of scalar quantities by the resolved flow, by definition, part of the dynamical core. The thermodynamic and constituent continuity equations can be addressed with different algorithms for the scalar advection than used in the momentum equation (see Rasch and Williamson 1991; Rasch et al. 2006). Without special attention, this explicitly introduces an inconsistency in the formulation of the model as a whole. This inconsistency can be interpreted as using a different vertical velocity for the advection of scalars than is estimated from the solution of the momentum equations (see Lin and Rood 1996; Jöckel et al. 2001; Machenhauer et al. 2008). This will be discussed more fully below.

Compared with the previous sections, the discussion and analysis presented in this section both refines and expands the components that make up the dynamical core. Namely, dynamical cores are generally process split and include algorithms that represent:

- The resolved advection of momentum in the horizontal plane.
- The resolved vertical advection of momentum.
- Unresolved sub-scale transport of momentum.
- A specification of the pressure gradient force.
- A specification of the Coriolis force.
- A specification of topography.

- The resolved advection of scalars in the horizontal plane.
- The resolved vertical advection of scalars.
- Unresolved sub-scale transport of scalars.
- A portfolio of filters and fixers that accommodate errors related to both the numerical technique and the characteristics of the underlying grid.

15.5 Numerical Expression of the Atmospheric Equations of Motion

There are many ways to approach the numerical estimation of solutions to the equations of motion for the atmosphere. A straightforward approach is to develop a discrete representation of variables and derivatives and to estimate, directly, the partial differential equations. It is reasonable to assume that accurate representation of the terms in the equation would lead to a credible numerical solution.

The equations of motions support many scales and types of motion. Some of these motions, such as sound waves, are not of direct relevance to weather and climate models. Unwanted scales are often eliminated either by recasting the continuous equations in such a way as to eliminate the unwanted scales or through numerical techniques such as filtering and scale-selective dissipation. When the discrete equations are formed new types of unwanted, computational motions might be created.

In addition, there are many important relationships that exist in the equations of motion. For example there are energy constraints, such as conservation of total energy for adiabatic, inviscid flows. Scaling arguments reveal strong relationships between, for example, the winds and the thermal structure and the vorticity and the pressure fields (see Holton 2004). Marching through the equation of motions making best estimates of the individual terms in the equations does not assure that these relationships are honored. Such inconsistencies in the discretization can lead to models composed of highly accurate elements that, collectively, do not provide credible simulations.

Therefore, experience suggests an alternative approach to the development of models. In this alternative approach design requirements are specified and numerical algorithms are developed to meet these requirements. Accuracy is sought in the context of integrated design.

This section will investigate the design-based approach of the Lin and Rood (1996) advection scheme and the full dynamical core which has been developed by Lin (2004). Model development by algorithm design is discussed thoroughly by Machenhauer et al. (2008).

The Lin and Rood (1996) advection scheme was motivated by attempts to model the high-quality aircraft observations collected to determine the chemical mechanisms responsible for the Antarctic ozone hole. Of special importance from these observations were the correlations between trace constituents (Fahey et al. 1990). These correlations are conserved in the absence of photochemical losses and sinks; that is, they are conserved in pure advection. Numerical simulations with conventional finite difference and spectral methods showed that correlations were not conserved, and that the lack of conservation was of sufficient magnitude to make comparisons with observations of little scientific value. The inability of these schemes to conserve tracer correlations was directly related to the filtering techniques used to counter the generation of negative tracer concentrations which arise from numerical errors. The strategy for addressing this problem was to adapt piecewise continuous schemes of the sort developed by Bram van Leer to atmospheric problems (see van Leer 1979; Allen et al. 1991). These are finite volume schemes which partition fluid volumes at each time step based on the velocity field. As posed in Lin and Rood (1996) the design criteria were:

- Conservation of mass without *a posteriori* restoration.
- Computation of mass fluxes based on the sub-grid distribution in the upwind direction.
- Generation of no new maxima or minima (ideally, maintain monotonicity).
- Preservation of tracer correlations.
- Computational efficiency in spherical coordinates.

These design criteria in combination with a mixture of higher and lower order numerical techniques led to credible results in a wide variety of chemistry-transport models (Douglass et al. 1997; Bey et al. 2001; Rotman et al. 2001). Implicit in the development was the reduction of numerical diffusion compared with the previously used methods (Allen et al. 1991). Also, implicit in this development is that the advection of well-resolved spatial scales, for example resolved by ten grid cells or more, is well represented. The number of grid cells required to resolve a feature accurately is not a strictly defined quantity. The choice of ten emphasizes that there is an order of magnitude between the number of grid cells and resolved scales; ten is drawn from the discussion of errors in Zalesak (1981). This criterion also directly states that there is a range of scales that are 'resolved,' but not accurately. The advection of accurately resolved waves in modern numerical advection schemes is expected, and therefore, does not serve as a good discriminator between algorithms.

The design features in the Lin and Rood advection scheme can be reframed to state that if a tracer distribution originally has no tracer gradients, then the tracer distribution will not change during the computation of advection. It was often true that chemistry-transport models did not have this feature, which is directly traceable to the underlying mass conservation equation (15.2) not being satisfied. This can be articulated as the vertical velocity that satisfies the momentum and mass conservation equations is not the same as the vertical velocity used in the calculation of the scalar advection. This design criterion is characterized as 'consistency,' where consistency represents the physical relationships that tie together the entire system of the equations of motion and the tracer continuity equations.

Known inadequacies of the Lin and Rood scheme at the time of development included splitting errors that generated negative concentrations in some instances and numerical diffusion related largely to the slope limiters. It was a design decision to take numerical errors in diffusion rather than in dispersion errors. Alternatively, diffusion is used to remedy, not cure, dispersion errors. In practice the scheme conserved constituent correlations in realistic test problems. However, the presence of splitting errors and the nonlinear application of the slope limiters means that there are potentially failures of both monotonicity and the conservation of correlations.

The Lin and Rood (1996) advection scheme was extended to the two-dimensional shallow water equations in Lin and Rood (1997) and to the three-dimensional primitive equations in Lin (2004). Both implementations utilized a regular, equal-angle, latitude-longitude grid. A major goal was to develop a numerical system that treated the momentum equations, the thermodynamic equation, and the tracer continuity equations ‘consistently,’ as defined above. Also in this development was the specification of quantities on the grid and use of averaging techniques to assure the correlative relationship between geopotential (i.e., a pressure-like variable in a coordinate system that uses pressure as a vertical coordinate) and vorticity. This design decision valued the accurate advection of vorticity. Therefore, the original development of the scheme was implicitly tuned towards the characteristics of large-scale dynamical features in a rotationally dominated flow.

Perhaps more important to model performance than the horizontal advection scheme was the development of methods to represent the horizontal pressure gradient and the treatment of vertical advection. Lin (1997) describes a piecewise continuous, finite volume method to represent the horizontal pressure gradient. This method, which integrates piecewise linear edges of the volume to calculate the balance of pressure forces on a volume, proved to be two orders of magnitude more accurate in the presence of steep topography than finite difference schemes used at the time.

The description of a Lagrangian formulation of the vertical velocity in Lin (2004) completes the development of the dynamical core. This calculation of vertical velocity originally relied on the hydrostatic approximation. It is analogous to the use of isopycnal coordinates in ocean modeling. This approach has a tremendous impact on the fidelity of the model, especially with regard to the representation of the mean meridional circulation important to the general circulation and tracer distributions (Schoeberl et al. 2003).

The design features discussed above suggest another attribute of the Lin (2004) dynamical core that was a desired feature. The net effect of the design is that the scheme is highly localized. The information that is used to calculate the atmospheric dynamics and tracer transport comes from nearby and primarily upstream grid points. This stands in contrast with spectral or pseudospectral methods, which use global basis functions and are formally more accurate (see Rood 1987). The local nature of the scheme has potential positive benefits for the representation of quantities that are derived from the model’s physical parameterizations. That is, the locality is relevant to the coupling between the dynamical core and the physics; the physics parameterizations are intrinsically local (see Bala et al. 2008).

The expression of the dynamical core described above in this section addresses the analysis of the equations of motion in the previous section. What has yet to be discussed is the portfolio of filters and fixers that are required for the scheme. The most obvious design feature of the model to address known errors is the slope limiter which is diffusion implemented locally when a new maximum or minimum will be created (see van Leer 1979). The use of slope limiting is a design decision. Slope limiting (van Leer 1979, and references therein) and flux limiters, pioneered by, e.g., Boris and Book (1973), were motivated by consideration of plasma shocks and the prevention of the generation of non-physical ripples at the shock front. This is an error that cannot be overlooked in reactive flow and combustion calculations. A physical analysis of the advective process reveals that advection cannot generate new maxima or minima in the scalar fields. That is, advection is monotonic, and if monotonicity is violated, then the scheme is 'non-physical'.

More generally, there are many errors in the calculation of advection that are non-physical. For example, without special consideration quadratic and higher moments of advected fields are not conserved in numerical algorithms. This is non-physical, and potentially important when considering conservation of energy, the propagation of variance and covariance in data assimilation, or modeling the distribution of droplets and aerosols. Prather (1986) developed a highly accurate advection scheme which conserves moments and vastly reduces numerical diffusion.

In Lin and Rood (1997) it was argued that the nature of the slope limiters, essentially a flow-dependent, nonlinear diffusion, was 'physical'. This argument is not formally true, but it is a statement that the mixing is localized and flow dependent, which is intuitively appealing. The diffusion associated with the limiter is large enough that it was not required to add an additional diffusion to the algorithm to eliminate grid-scale noise in scalar advection. The addition of diffusion is common in atmospheric models (for example Collins et al. 2004; Williamson 2007).

There are a variety of other filters and fixers in the scheme. There is a polar filter, which arises because of the decrease of the grid spacing on the equal-angle grid at high latitudes. More importantly, the scheme generates grid-scale noise, which manifests itself as localized divergent flows. This is countered by damping the divergent part of the flow. There is another digital filter which is used to manage grid-scale noise. All of these filters are ultimately diffusive, essential to the stability and performance of the dynamical core, and have a complex impact on the performance of the model. They are not an unusual portfolio of filters and are conflated with any representation of physical mixing, diffusion, and dissipation (see Chaps. 13 and 14).

15.6 Synthesis and Future Directions

The previous sections provide a high-level view of the structure and construction of weather and climate models. Atmospheric models are used to provide a concrete example. The point of view is from the role of the dynamical core in the model. Adcroft et al. (2004), Adcroft and Hallberg (2006), Adcroft et al. (2008) and White and Adcroft (2008) present a comprehensive representation of a modern oceanic dynamical core with many parallel attributes to what has been presented here for the atmosphere.

15.6.1 Model-Relevant Principles

1. Models are built from components, and the ultimate customers of models are interested in the results of the model as a whole. The application of the model strongly influences the priorities that are given weight in the building of a model. In the example provided in this chapter, correlated behavior of trace constituents and the conservation of advected variables have high priority. Given that model performance as a whole is ultimately required, balanced development of model components is necessary. The benefit of a highly precise algorithm, for say advection, is easily lost because other errors in the model or errors in the coupling of components are large.
2. The model as a whole is explicitly or implicitly optimized, i.e., tuned, towards applications at hand. This tuning includes the balancing of compensating errors. The introduction of a new, better founded algorithm is highly likely to degrade, initially, the performance of the model as a whole. This makes a barrier for the introduction of improved algorithms in models. New tuning is needed.
3. Formally, a validation plan that reflects the expected results of the model as a whole provides a framework for evaluating the impact of algorithms and their coupling. It is within the context of this validation plan that decisions on the potential benefits of improved algorithms should be made.

15.6.2 Lessons Learned about Dynamical Cores

15.6.2.1 Consistency

The enforcement of consistency in the development of dynamical cores has had significant payoff. In the field of tracer advection, the term consistency originally referred to what Machenhauer et al. (2008) call the mass-wind consistency; that is, the potential disconnection that can occur between mass conservation in the fluid and calculation of the transport of trace species (see also Jöckel et al., 2001). In this chapter, consistency is extended to include the theoretical constructs such as the thermal wind, the relation between vorticity and the pressure field obtained from scaling arguments, preservation of constituent correlations, specification of topography, etc. More generally, consistency refers to the correlative behavior that follows from theory, which is of tremendous value in the interpretation of observations and models. Correlative physics is crucial to studies of the attribution of climate change to human's activities (Santer et al. 2000). Attention to consistency improves the robustness of models. Development of consistent numerical schemes is a design decision based on developer's experience (and preference) defined by an application suite.

15.6.2.2 Locality

We have evolved to a state where we need to pay explicit attention to the interaction, that is, the coupling, between the dynamical core and 'the physics'. (see also Williamson 2007). This requires, minimally, presenting to the physics parameterizations physically realizable values of transported quantities with robust relationships to correlated parameters. Given that the physical parameterizations are local, it is intuitive that dynamical cores with localized grid stencils have potential advantage.

15.6.2.3 Horizontal Advection

The credible treatment of resolved horizontal advection is an essential performance criterion that is implicit in all modern dynamical cores. The metrics on which decisions are made are often experiential, and fall within an experiential range. Given that credible performance is realized by many schemes, horizontal advection of resolved scales has progressed to a standard and is not a discriminator of algorithms. All schemes have to balance intrinsic errors of dissipation and dispersion, and tolerance of such errors is a design and application-based decision. Conservation of advected variables without *a posteriori* restoration is, intuitively, a requirement for climate models; however, this, too, is a design decision. The importance of conservation of higher order moments, especially energy, will likely become more important in the future.

15.6.2.4 Vertical Velocity

The vertical velocity is central to the robust representation of weather and climate. Treatment of the vertical velocity is difficult because the vertical velocity is most often much smaller than the horizontal velocity. The vertical velocity is related to horizontal divergence, which is closely related to grid-scale noise and grid-scale forcing by the physical parameterizations. Therefore, the vertical velocity is strongly influenced by the sub-grid mixing, filters, and fixers. It is easy to corrupt the physical consistency of the vertical velocity. Treatment of the vertical velocity requires more attention in the development of dynamical cores.

15.6.2.5 Mixing, Filters and Fixers

The mixing algorithms, filters, and fixers have significant impact on model performance as e.g. discussed in Chaps. 13 and 14. The hydrostatic, geostrophic, and adiabatic balances in the atmosphere are powerful constraints on the flow and offer great theoretical insight. However, it is the difference from these balances that is often most important to weather and climate predictions. Fundamental theory, e.g. Andrews and Mcintyre (1978), shows that difference from balance is due to dissipation, nonlinearity and transience. Mixing algorithms, filters, and fixers are the locations where the artifacts of the discretization and numerical errors are addressed. The specifics of the mixing is important, especially with respect to the dissipation of waves. That mixing processes might be ‘small’ does not rationalize their being ignored. Far more attention is needed to the formulation and impact of mixing algorithms, filters, and fixers.

15.6.3 Future Directions

15.6.3.1 Divergence

The discussion in this paper reveals a number of facts about the treatment of divergence in atmospheric models. First, in the case of the Lin and Rood (1997) horizontal advection scheme, the development of the scheme is biased towards the advection of vorticity. This bias, implicitly, reflects large-scale, middle-latitude dynamics, and the importance of the conservation of vorticity. This is an acceptable situation for global climate models at resolutions of several hundred kilometers, where the flow is quasi-nondivergent. Second, in the Lin and Rood (1997) scheme, damping is added directly to the divergence in order to manage grid-scale noise and stability (see Collins et al. 2004).

Divergence damping is often used in atmospheric models and warrants more discussion. There are two primary paths of motivation. Bates et al. (1993) formally introduced two-dimensional divergence damping into the equations for the development of their semi-Lagrangian scheme. This damping was subsequently used in development and application (S. Moorthi, personal communication). Divergence damping is routinely used in the North American Model at the National Centers for Environmental Predictions to control noise in both the simulation and assimilation (S. Lord, personal communication). Farge and Sadourny (1989) discuss at length the use of dissipation on both the rotational and divergent parts of the flow to achieve adequate numerical performance. Their discussion is in the context of an investigation using a shallow water model with pseudospectral numerical schemes. They pursue a linear combination of a rotational and divergent form of dissipation (see also Vallis 1992; Gassmann and Herzog 2007).

The second motivational path for divergence damping follows from mesoscale modeling and the development of non-hydrostatic models. In this path the original line of reason was to incorporate three-dimensional divergence damping to remove meteorologically unimportant, computationally demanding acoustic modes (Skamarock and Klemp 1992; Dudhia 1993). Wicker and Skamarock (1998) note that not only are the acoustic modes eliminated, but that the stability of their numerical technique is improved. Therefore, in this path as well, the noise management and stability enhancements of divergence damping have emerged (see also Gassmann and Herzog 2007).

As global models and regional models resolve smaller and smaller scales, the divergent part of the flow becomes important. Furthermore there is forcing at the grid scale, which is formally not resolved, that is a source of physically based divergence. Therefore, these techniques to control noise impact important dynamical features and the interaction between large and small scales. Therefore, increased, direct attention to the physical role and representation of divergent flow is needed.

15.6.3.2 Mixing, Filters, and Fixers (Chap. 13)

The algorithms for mixing, filters, and fixers directly impact both the representation of divergence and the fundamentals of wave dissipation important for climate models. When the consequences of high resolution models are considered, the conflation of these algorithms with the model physics is realized to be even more complex. High resolution models will resolve more and more gravity waves, which are strongly divergent modes and are already ‘accounted for’ by the gravity wave parameterization. Therefore, the dynamical core and the physics parameterizations will not be as cleanly separated by scales. Similar realizations can be made for the relationship of the dynamical core with the planetary boundary layer parameterization and the convective parameterization. Far more attention is needed to the formulation and impact of mixing algorithms, filters, and fixers.

15.6.3.3 Non-Hydrostatic

As horizontal resolution is increased, the scales of the allowed motion are such that non-hydrostatic motion becomes important. Relaxing the hydrostatic assumption is realized in the vertical momentum equation. This provides a fundamental change in modeling. The strong relation of vertical velocity to small-scale divergence and the complex relationship between small- and large-scale programs again brings attention to the importance of the mixing algorithms, filters, and fixers.

15.6.3.4 Grids

Much attention is currently focused on types of grids (Randall 2000; Ringler et al. 2000; Putman and Lin 2009; Rančić et al. 2008; Walko and Avissar 2008; Thuburn 2008a). The excellent review of Williamson (2007) has a focus on how the development of dynamical cores is strongly influenced by the presence of the polar singularity on regular latitude-longitude grids. The Williamson (2007) review includes a large list of references to grids. Two grids that have received much attention are the cubic sphere (Sadourny 1972; Putman and Lin 2009) and the geodesic grid (Sadourny et al. 1968; Williamson 1968). There are both computational and physical advantages of these grids, and the grid and numerical methods used on the grids will reveal new consistency challenges. The grid has become another element of the dynamical core.

There is currently much discussion about grid artifacts; that is, the underlying grid can be 'seen' in the solutions. These comments also imply that present equal-angle, latitude-longitude grids are free of such artifacts. However, existing grids have a set of filters, especially polar filters, to remedy their artifacts. Indeed, as Williamson (2007) points out, the challenges of the equal-angle, latitude-longitude grid have been a great motivator to develop new techniques. Grid artifacts are currently a fact of modeling, and evaluation of their impact and development of remediation strategies are required; grid artifacts are not, *a priori*, an extraordinary flaw.

15.6.3.5 Coupling

Since climate models are composites of composites of components, there are couplings at many levels. It is easy to lose any advantage of a new numerical method to poor coupling. The coupling of the dynamical core to the physics is especially important because of the conflation of small and large scales at the grid scale and the conflation of numerical and physical mixing at the grid scale. Since model performance relies on the accumulation of the performance of interacting components, the physics of, the consistency of, and the performance of coupling need far more consideration (Staniforth et al. 2002; Williamson 2002, 2007).

15.7 Conclusions

The perspective provided here advocates looking at the function of the model as whole. The model as a whole is a system of interacting components. These components each have their error characteristics. Errors are balanced in the process of optimizing or tuning the model to address specific applications. Therefore, the development of specific components, without regard to the application and the interaction of one component with all components, is likely to have little obvious benefit. Model-building activities should include a formal step of system integration, which should be driven by an application-based validation plan.

With regard to dynamical cores – horizontal advection of resolved scales has evolved to a state of quality that is high compared with other sources of errors in the model. Therefore, in terms of performance it is essentially standardized. The choice of horizontal advection scheme does impact the requirements for filtering and fixers, which are of both theoretical and practical importance. The dynamical core needs to be considered as an integrated module, and the relation of the horizontal advection algorithm to algorithms for the vertical velocity and for mixing, filters, and fixers needs direct attention.

The discussion here brings attention to two items that might be considered values. These are consistency and locality. High value is given to these attributes because of experience in applications and, looking forward, focusing more attention on the coupling of the dynamical core with the physics. Specifically, there is the need to pass to the physics parameterizations physically realizable estimates of transported variables that represent the correlated behavior of the variables.

With these values the following is posed as the suite of elements in the dynamical core. It is implicit that these form an integrated, consistent module, informed by the interface with other components:

- A specification of the grid.
- A specification of topography.
- A specification of the pressure gradient force.
- A specification of the Coriolis force.
- The resolved advection of momentum in the horizontal plane.
- The resolved vertical advection of momentum.
- Unresolved sub-scale transport of momentum.
- The resolved advection of scalars in the horizontal plane.
- The resolved vertical advection of scalars.
- Unresolved sub-scale transport of scalars.
- A portfolio of filters and fixers that accommodate errors related to both the numerical technique and the characteristics of the underlying grid.

The representation of the divergent part of the flow and coupling of model components requires more attention. This demands attention to algorithms that represent mixing, filters, and fixers. High resolution simulations represent divergent circulations explicitly. Such models are poised to better represent the interaction of small and large scales, and ignoring the detritus of the dynamical core undermines efforts focused on the representation of processes from first principles.

The development of weather and climate models does not proceed through a well defined path from first principles. There is a mix of science, engineering, and intuition based upon experience and desired results. In the past decade both atmospheric and oceanic models, whose development has focused on design that gives priority to the underlying correlative physics, have had significant impact. Looking forward, the problems and applications being faced in climate modelers will bring attention to high resolution, the representation of small, divergent scales, and the interaction of small and large scales. This brings direct attention to the difficult and understudied problem of sub-scale mixing and the conflation of physical and numerical processes at the smallest scales. The interaction of the dynamical cores with the physics scheme, coupling in general, needs more rigorous attention and treatment; this is true for both parameterized and cloud-resolving models. Given the intrinsic nature of dissipation and dispersion errors in the numerical representation of advection, new strategies, such as more attention to the conservation of higher order moments, may be required to achieve fidelity between large and small scales.

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