CHAPTER 1 Introduction

1.1 What is a model?

The atmospheric science community includes a large and energetic group of researchers who devise and carry out measurements in the atmosphere. This work involves instrument development, algorithm development, data collection, data reduction, and data analysis. The data by themselves are just numbers. In order to make physical sense of the data, some sort of model is needed. This might be a qualitative conceptual model, or it might be an analytical theory, or it might take the form of a computer program.

Accordingly, a community of modelers is hard at work developing models, performing calculations, and analyzing the results by comparison with data. The models by themselves are just "stories" about the atmosphere. In making up these stories, however, modelers must strive to satisfy a very special and rather daunting requirement: The stories must be true, as far as we can tell; in other words, the models must be consistent with all of the relevant measurements.

A model essentially embodies a theory. A model (or a theory) provides a basis for making predictions about the outcomes of measurements. Atmospheric models can be conceptually grouped in various ways; one such classification follows:

- *Elementary models*. The disciplines of fluid dynamics, radiative transfer, atmospheric chemistry, and cloud microphysics all make use of models that are essentially direct applications of basic physical principles to phenomena that occur in the atmosphere. Many of these "elementary" models were developed under the banners of physics and chemistry, but some-- enough that we can be proud -- are products of the atmospheric science community. Elementary models tend to deal with microscale phenomena, (e.g. the evolution of individual cloud droplets suspended in or falling through the air, or the optical properties of ice crystals) so that their direct application to practical atmospheric problems is usually thwarted by the sheer size and complexity of the atmosphere. Because of their generality, elementary models often predict the existence of universal constants or functions.

- *Forecast models*. A model that predicts the deterministic evolution of the atmosphere or some macroscopic portion of it can be called a "forecast model." A forecast model could be, as the name suggests, a model that is used to conduct weather prediction, but there are other possibilities, e.g. it could be used to predict the deterministic evolution of an individual turbulent eddy. Forecast models can be tested against real data, documenting for example the observed development of a synoptic-scale system or the observed growth of an individual convective cloud, assuming of course that the requisite data can be collected.

We are often interested in computing the *statistics* of an atmospheric phenomenon, e.g. the statistics of the general circulation. It is now widely known that there are fundamental limits on the deterministic predictability of the atmosphere, due to sensitive dependence on initial conditions (e.g. Lorenz, 1969). For the global-scale circulation of the atmosphere, the limit of predictability is thought to be on the order of a few weeks, but for a cumulus-scale circulation it is on the order of a few minutes. For time scales longer than the deterministic limit of predictability for the system in question, only the statistics of the system can be predicted. These statistics can be generated by brute-force simulation, using a forecast model but pushing the forecast beyond the deterministic limit, and then computing statistics from the results. The obvious and most familiar example is simulation of the atmospheric general circulation (e.g. Smagorinski 1963). Additional examples are large eddy simulations of atmospheric turbulence (e.g. Moeng 1984), and simulations of the evolution of an ensemble of clouds using a space and time domains much larger than the space and time scales of individual clouds (e.g. Krueger 1988). Monte-Carlo simulations of radiative transfer (e.g. McKee and Cox, 1974) can be said to "forecast" the paths of individual photons, and statistics are computed from a large-number of such paths; we classify these Monte-Carlo radiative transfer models as "forecast models" for purposes of the present discussion.

The statistics simulated by these various models can be compared with statistics based on atmospheric measurements, most commonly with measurements collected in the case study mode. For example, statistics computed from the global meteorological observing network can be used to compute general circulation statistics, and these can then be compared with statistics computed from simulations of the general circulation.

As a second example, statistics computed from aircraft data can be compared with the results of large-eddy simulation models. These models are being used to predict universal functions that arise in connection with atmospheric turbulence (e.g. Moeng and Wyngaard, 1986, 1989). Through such applications, the large-eddy models are reaching or at least aiming for a stature comparable to that of "elementary models." Analogous applications of general circulation models can be imagined, but few such have been reported up to this time.

Forecast models are now also being used to make predictions of the time evolution of the *statistics* of the weather, far beyond the limit of deterministic predictability for individual weather systems. Examples are seasonal weather forecasts, which deal with the statistics of the weather rather than day-to-day variations of the weather and are now being produced by several operational centers; and climate change forecasts, which deal with the evolution of the climate over the coming decades and longer. In the case of seasonal forecasting, the predictability of the statistics of the atmospheric circulation beyond the two-week deterministic limit arises primarily from the predictability of the sea surface temperature, which has a much longer memory of its initial conditions than does the atmosphere. In the case of climate change predictions, the time evolution of the statistics of the climate system are predictable to the extent that they are driven by predictable changes in some external forcing. For example, projected increases in greenhouse gas concentrations represent a time-varying external forcing whose effects on the time evolution of the statistics of the climate system may be predictable. Over the next several decades measurements will make it very clear to what extent these predictions are right or wrong. A more mundane example is the seasonal cycle of the atmospheric circulation, which represents the response of the statistics of the atmospheric general circulation to the movement of the Earth in its orbit; because the seasonal forcing is predictable many years in advance[1], the seasonal cycle of the statistics of the atmospheric circulation is also highly predictable, far beyond the two-week limit of deterministic predictability for individual weather systems.

During the 1990s, an interesting development occurred: People began to compute statistics from the archived forecasts of numerical weather prediction models. This is now established as an important way in which the models can be used to learn about the atmosphere. Because the archived forecasts were initialized with real data and fall within the range of deterministic predictability, they are by no means pure simulations or “model products,” but at the same time they do contain errors that arise in part from weaknesses in the formulation of the model and/or the data- analysis scheme. Archived forecasts thus represent a middle ground between pure analyses of data and pure simulations of general circulation statistics. For example, general circulation statistics can be computed from an ensemble of *n*-day forecasts, and compared with observed (or “zero-day forecast”) general circulation statistics. Archived forecast datasets are being applied to studies of atmospheric predictability, and to investigate the systematic errors of forecast models (e.g. Lorenz, 1982; Heckley, 1985; Arpé and Klinker, 1986).

1. We can say without exaggeration that it is “known.”

- *Models that simulate statistics directly*. Most radiative transfer models describe the statistical behavior of extremely large numbers of photons. "Higher-order closure models" have been developed to simulate directly the statistics of small-scale atmospheric turbulence (e.g. Mellor and Yamada, 1974). Analogous models for direct simulation of the statistics of the large-scale circulation of the atmosphere may be possible (e.g. Green, 1970). These are examples of models that predict statistics directly; the dependent variables are the statistics themselves, and there is no need to average the model results to generate statistics after the fact. The predictions of such models can be compared with statistics computed from measurements made in case-study mode. Models that predict statistics directly can, in principle, predict the forms of universal functions.

  Conventional wisdom holds that the results of models that predict statistics directly are less reliable than statistics computed indirectly from forecast model results, so that, for example, large-eddy simulation results are generally considered more reliable than the results of higher-order closure models. The reason is that higher-order closure models generally contain more empirical parameters than large-eddy models. The role of such empirical parameters is discussed later.

- *Toy models*. We also build highly idealized models that are not intended to provide quantitatively accurate or physically complete descriptions of natural phenomena, but rather to encapsulate our physical understanding of a complex phenomenon in the simplest and most compact possible form, as a kind of modeler's haiku. For example, North (1975) discusses the application of this approach to climate modeling. Toy models are intended primarily as educational tools; the results that they produce can be compared with measurements only in qualitative or semi-quantitative ways.

A hypothesis is a prediction, based on a model or theory, of the outcome of a measurement. A hypothesis can be proven wrong, or "falsified." It can never be proven right, because there is always the possibility that some future measurement will be inconsistent with the hypothesis (Popper, 1959). Modelers need measurements first and foremost to test hypotheses. Of course, modelers also need measurements to suggest ideas about what is important and interesting, and what sorts of model output to look at.

Is a model a hypothesis? When a model is used to perform a calculation, it yields a prediction about the behavior of the atmosphere. To phrase this in terms of hypotheses, we can say that "we hypothesize that the prediction produced through calculations with the model is true." Atmospheric measurements can (or should) be able to falsify this hypothesis. If a prediction produced by a model is shown to be in conflict with measurements, then the model itself can be said to have been falsified.

1.2 Fundamental physics, mathematical methods, and physical parameterizations

Most models in atmospheric science are formulated by starting from basic physical principles, such as conservation of mass, conservation of momentum, conservation of thermodynamic energy, and the radiative transfer equation. In principle, these equations can describe the evolution of the atmosphere in extreme detail, down to spatial and temporal scales far below the range of meteorological interest.

Even if such detailed models were technologically feasible, we would still choose to average or aggregate the output produced by the models so as to depict the evolution of the scales of primary interest, e.g. thunderstorms, tropical cyclones, baroclinic waves, and the global circulation. In addition, we would want to *explain* why the solutions of the models turn out as they do. In practice, of course, we cannot use such high spatial and temporal resolution, and so we must represent some important processes parametrically. Such parametric representations, or "parameterizations", are a practical necessity in models of limited resolution, but even if we were using models with arbitrarily high resolution we would still need parameterizations to understand what the model results mean. Parameterizations are not dealt with in this course, but you can learn about them in courses on cloud physics, radiation, turbulence, and chemistry.

Obviously, mathematical methods are needed to solve the equations of a model, and in practice the methods are almost always approximate, which means that they entail errors. This course deals mainly with a survey of numerical methods that are particularly useful in atmospheric modeling, and an analysis of the errors involved and how they can be anticipated, analyzed, and minimized. This is a course about errors. All your life you have been making errors. Now, finally, you get to take a course on errors.

There is a tendency to think of numerical methods as one realm of research, and physical parameterization as a completely different realm. This is a mistake. The design of a numerical model should be guided, as far as possible, by our understanding of the essential physics of the processes represented by the model. This course will emphasize that very basic and inadequately recognized point.

As an example, to an excellent approximation, the mass of dry air does not change as the atmosphere goes about its business. This physical principle is embodied in the continuity equation, which can be written as

$$\frac{\partial\rho}{\partial t} = -\nabla\bullet(\rho\mathbf{V}) , \tag{1.1}$$

where ρ is the density of dry air, and $\mathbf{V}$ is the three-dimensional velocity vector. When (1.1) is integrated over the whole atmosphere, with appropriate boundary conditions, we find that

$$\int_{\text{whole atmosphere}} \nabla\bullet(\rho\mathbf{V})d^3\boldsymbol{x} = 0 , \tag{1.2}$$

and so we conclude that

$$\frac{d}{dt}\left\{\int_{\text{whole atmosphere}} \rho d^3\boldsymbol{x}\right\} = 0 . \tag{1.3}$$

Eq. (1.3) is a statement of global mass conservation; in order to obtain (1.3), we had to use (1.2), which is a property of the divergence operator with the appropriate boundary conditions.

In a numerical model, we replace (1.1) by an approximation; examples are given later. The approximate form of (1.1) entails an approximation to the divergence operator. These approximations inevitably involve errors, but because we are able to choose or design the approximations, we have some control over the nature of the errors. We cannot eliminate the errors, but we can refuse to accept certain kinds of errors. In particular, we refuse to accept any error in the global conservation of mass. This means that we can design our model so that an appropriate analog of (1.3) is satisfied *exactly*.

In order to derive an analog of (1.3), we have to enforce an analog of (1.2); this means that we have to choose an approximation to the divergence operator that "behaves like" the exact divergence operator in the sense that the global integral (or more precisely a global sum representing the global integral) is exactly zero. This can be done, quite easily. You would be surprised to learn how often it is *not* done.

There are many additional examples of important physical principles that can be enforced exactly by designing suitable approximations to differential and/or integral operators. These include conservation of energy and conservation of potential vorticity. More discussion is given later.

1.3 Numerical experimentation

A serious difficulty in the geophysical sciences such as atmospheric science is that it is usually impossible (perhaps fortunately) to perform controlled experiments using the Earth. Even where experiments are possible, as with some micrometeorological phenomena, it is usually not possible to draw definite conclusions, because of the difficulty of separating any one physical process from the others. For a long time, the development of atmospheric science had to rely entirely upon observations of the natural atmosphere, which is an uncontrolled synthesis of many mutually dependent physical processes. Such observations can hardly provide direct tests of theories, which are inevitably highly idealized.

Numerical modeling is a powerful tool for studying the atmosphere through an *experimental approach*. A numerical model simulates the physical processes that occur in the atmosphere. There are various types of numerical models, designed for various purposes. One class of models is designed for simulating the actual atmosphere as closely as possible. Examples are numerical weather prediction models and climate simulation models. These are intended to be substitutes for the actual atmosphere and, therefore, include representations of many physical processes. Direct comparisons with observations must be made for evaluation of the model results. Unfortunately (or perhaps fortunately), the design of such models can never be a purely mathematical problem. In practice, the models include many simplifications and parameterizations, but still they have to be realistic. To meet this requirement, we must rely on physical understanding of the relative importance of the various physical processes and the statistical interactions of subgrid-scale and grid-scale motions. Once we have gained sufficient confidence that a model is reasonably realistic, it can be used as a substitute for the real atmosphere. Numerical experiments with such models can lead to discoveries that would not have been possible with observations alone. A model can also be used as a purely experimental tool. Predictability experiments are examples.

Simpler numerical models are also very useful for studying individual phenomena, insofar as these phenomena can be isolated. Examples are models of tropical cyclones, baroclinic waves, and clouds. Simulations with these models can be compared with observations or with simpler models empirically derived from observations, or with simple theoretical models.

Numerical modeling has brought a maturity to atmospheric dynamics. Theories, numerical simulations and observational studies have been developed jointly in the last several decades, and this will continue indefinitely. Observational and theoretical studies guide the design of numerical models, and numerical simulations supply theoretical ideas and suggest efficient observational systems.

We do not attempt, in this course, to present general rigorous mathematical theories of numerical methods; such theories are a focus of the Mathematics Department. Instead, we concentrate on practical aspects of the numerical solution of the specific differential equations of relevance to atmospheric modeling.

We deal mainly with “prototype” equations that are simplified or idealized versions of equations that are actually encountered in atmospheric modeling. These include the “advection equation,” the “oscillation equation,” the “decay equation,” the “diffusion equation,” and others. We also use the shallow water equations to explore some topics including wave propagation. Emphasis is placed on time-dependent equations, but we also briefly discuss boundary-value problems. The various prototype equations are used in dynamics, but may of them are also used in other branches of atmospheric science, such as cloud physics or radiative transfer.