LARGE-SCALE ATMOSPHERE–OCEAN DYNAMICS, I

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LARGE-SCALE ATMOSPHERE–OCEAN DYNAMICS

Volume I

Analytical Methods and Numerical Models

edited by

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University of Oxford

and

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 $Met \ Office$



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To the memory of Rupert Ford

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Preface

These two volumes provide an up-to-date account of the mathematics and numerical modelling that underpins weather forecasting, climate change simulations, dynamical meteorology and oceanography. The articles are a combination of teaching/review material and present results from contemporary research. The subject matter will be of interest to mathematicians and meteorologists, from graduate students to experts in the field. The articles have been written with the intention of providing accessible, interdisciplinary, accounts. The Introduction, which appears in both volumes, provides a guide to, and a perspective on, the subject matter and contents, and draws some tentative conclusions about the possible directions for future research.

The volumes are the result of the stimulus provided by the programme on *The Mathematics of Atmosphere and Ocean Dynamics* held at the Isaac Newton Institute for Mathematical Sciences in 1996, together with a follow-up meeting there in December 1997. The mathematical, scientific and computational challenge behind weather forecasting is why should we be able to forecast at all when the dynamical equations, the heat/moisture processes, and the billions of arithmetical calculations on 10–100 million unknowns involved in global forecasting each have associated instabilities and the potential for chaos? The overarching idea was to identify the stabilising principles and represent them effectively in mathematics that would lead to successful and efficient computation. Certain geometrical ideas are found to characterise the essential controlling physical principles, and the interplay of geometry and analysis makes for interesting new mathematics and helps to explain why computation of useful information becomes possible in the presence of chaos.

For obvious reasons, with over four years having elapsed since the conclusion of the original Programme, the subject matter has advanced as a result of work undertaken in the intervening period, both exploring ideas that were originally conceived in the Programme and developing new approaches. This has enabled new directions to be explored and this is reflected in the contributions. The Editors are indebted to all the contributors for both their perseverance and patience which has brought the project to fruition. While bringing the contributions together, we have received valuable help and encouragement from a number of people in addition to the support from the Met Office, Bracknell, and Lincoln College, Oxford. In particular, we would like to thank Terry Davies, Raymond Hide, Brian Hoskins and Emily Shuckburgh for reading various articles and providing useful comments. We would also like to thank Julian Hunt for his unstinting support for the programme from its inception, and John Toland for suggesting a programme on this subject matter in the first place! Much of the hard work in organizing the Programme was borne by the staff at the Newton Institute, and we would like to thank them,

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and the Director, Keith Moffatt, for valuable advice and assistance. Finally, David Tranah of the University Press showed us how to bring it all together.

Both the Programme and the volumes are forward looking, and history will decide on their success. However, it is with deep sadness that we record here the tragic passing of our much respected colleague Dr. Rupert Ford of Imperial College, who fell ill and died in March 2001 at the age of thirty-three. Although not making a written contribution to these volumes, Rupert was one of the most active and enthusiastic participants in the Programme itself, and a tremendous stimulus to us all. He stood astride the several disciplines that the organizers of the Programme sought to bring together. By the time of his death he had already published several outstanding contributions toward solving the problems with which the Programme was concerned. He will be sorely missed throughout a wide research community and we, the Editors and contributors, dedicate these volumes to his memory.

Ian Roulstone Met Office John Norbury University of Oxford

Introduction and Scientific Background

J.C.R. Hunt, J. Norbury and I. Roulstone

Because of the importance and excitement of recent developments in research on large scale atmosphere-ocean dynamics, in 1996 an intense programme was held at the Isaac Newton Institute in Cambridge bringing together about 300 scientists from a wide range of specialisms. The articles in these two volumes consist of reviews, up to date research findings, and challenging statements about problems for future research. These are based on presentations made during the programme and more recent developments in the research, resulting from the vigorous and continuing interactions between many of the participants.

Numerical weather prediction and ocean modelling are successful applications of mathematical physics and numerical analysis. Their scientific methodology is essentially reductionist, because it involves reducing the calculations of a complex environmental process into constituent parts, each of which can be understood scientifically and modelled (Hunt 1999). This involves combining quantitative representation at every point in space and time of physical processes, governing phase changes, radiation and molecular diffusion, with the mathematical modelling of fluid mechanics on a wide range of scales from thousands of kilometres to centimetres. In order that the predictions cover all the aspects of practical importance, as well as increasing their accuracy year on year, regular improvements are needed in the models of key processes and mechanisms; some are well understood such as phase changes and low amplitude waves, but others such as radiation and turbulence can only be approximately parameterised or modelled, using the latest research as it develops. Once these large systems of mathematical equations and boundary conditions have been fixed in any particular model, they are then further approximated by some form of discretisation, so as to be suitable for computation. Additional mathematical algorithms are introduced for the iterative recalculation of the equations for the 'assimilation' of the observational data as it continually arrives. Numerical analysis, mathematical and physical compromises are all necessary in these stages of the development of an accurate and practical operational system.

Typically 10¹⁰–10¹¹ equations have to be calculated in the operations of national and international meteorological organisations when they produce their regular forecasts for the global weather. They utilize both the largest computers in the world and 100 million observations per day which, according to the World Meteorological Organisation, now cost more than \$1 billion per year. The question of how to optimally incorporate satellite observations of particular atmospheric features, together with the more traditional ground

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and ship based observations, is one of growing importance both scientifically and economically. One could say that this effort has 'paid-off' because the errors, which increase with the number of days ahead for the forecasts, have been steadily decreasing, so that a 3-day forecast today is by many measures as accurate as a 1-day forecast 20 years ago. Forecasts for up to 7 days are now regularly issued and found to have useful accuracy on continental scales. However, to maintain this downward trend in errors, continuing research is essential.

In the 1980s prediction of global ocean currents began to be developed based on similar types of mathematical and computational methods, and fluid mechanics, but the models had to allow for the quite different thermodynamics and mixing processes of the watermass. Also the boundary conditions of the oceans at the surface, coasts and ocean floor are obviously different from those of the atmosphere. Although soundings from ships and buoys are now being supplemented by satellite borne measurements at the ocean surface, regular observations for initialising ocean models are only available over limited regions of the world. Nevertheless useful forecasts for global ocean temperatures and currents are produced every few days. Furthermore now that these models are working, it is possible to develop global climate models by coupling the atmospheric and ocean models together, and then to take up the challenge of predicting aspects of variability on seasonal timescales and climate change over the continents, oceans and icecaps for periods of the order of 100 years and beyond. As the models improve, their spatial discrimination is becoming finer.

On long climatic timescales processes have to be modelled that, on the shorter timescale of weather or ocean forecasts, either can be neglected, such as chemical reactions whose effects on weather are only significant over a period of months, or can be considered to be fixed boundary conditions, such as ice-sheets which change relatively slowly. On the climate timescale these otherwise neglected effects, such as the chemistry of the ozone hole, grow and decay significantly and affect the whole globe. As J.-L. Lions (1995) has pointed out, the mathematical properties of the governing equations may be transformed so substantially by the introduction of certain effects, such as modelling the dynamics of ice sheets, that it is no longer possible to prove an existence theorem! Despite such mathematical doubts, climate change computations converge to the same equilibrium state even over quite a wide range of initial conditions. The results for the key parameters, such as global temperature, now agree with measurements of the global climate taken over the past 150 years within the natural fluctuations of the system. Governments have accepted the reliability of these models as a basis for their policies to mitigate the effects of increases over the next century of global temperature and sea level because of their likely effects on human life and economic activities.

By the end of the nineteenth century, the equations of motion, of thermodynamics, and of transport of moisture, that are the essential components of

any model for forecasting the weather, had been worked out. However, it was also clear to those interested in such endeavours, for example Vilhelm Bjerknes (1914) and Lewis Fry Richardson (1922), that the problem of finding and computing solutions was extremely difficult. Although it was only 30-odd years between Richardson writing about a 'mere dream' of machines capable of performing such tasks and the advent of the first numerical forecasts (Charney, Fjørtoft and Von Neumann 1950), the intervening years witnessed the creation of ingenious methods for studying and analysing the atmospheric and oceanic flows that are still important in the context of weather and climate forecasting. Examples include fronts, ocean eddies and mid-latitude cyclones — such as the low pressure systems that cross the Atlantic and bring 'weather' to northern Europe.

The key idea behind these advances is to study the solutions of much simpler dynamical systems, whose solutions stay close for finite, but useful, time intervals, to those of the full fluid and thermodynamic equations. Indeed, much of modern dynamical meteorology is based on such studies, beginning with the pioneering work of Rossby (1936, 1940), Charney (1947, 1948) and Eady (1949). These approximate models usually correspond to some mathematical asymptotic state in which there is a dominant 'geostrophic' balance between the Coriolis, buoyancy and pressure-gradient forces on fluid particles so that the effects of acceleration of the particles (in the rotating frame of reference of the Earth) are relatively small. The asymptotic state arises from the rapid rotation and strong stratification of the Earth's atmosphere. Here, geostrophic balance (at its simplest) means horizontal flow around the pressure contours (Buys-Ballot's law), and this is coupled to the changes in the buoyancy force (hydrostatic balance between the vertical pressure gradient and gravity) in the vertical. Such approximations to Newton's second law are commonly referred to as *balanced models*. The Navier-Stokes equations for rotating, compressible, stratified fluid flow together with the equations of state and thermodynamics, commonly known in meteorology as the primitive equations, are the basis for numerical models used for atmospheric and oceanic predictions, and are therefore the starting point for the derivation of balanced models.

In the mid to late nineteenth century, classical hydrodynamics centred on the mathematical theorems of vortex motion, discovered by Helmholtz and Kelvin. The most notable of these governed the strength (or 'circulation'), the movement and the stability of vortices. Vortices persist even when their surroundings are quite disturbed or turbulent, as one observes by a simple experiment in one's bath. Vortices can move dangerously as tornadoes and swirling tropical storms, and last a long time over hundreds or thousands of rotation periods. Helmholtz' and Kelvin's theorem was formulated for a barotropic fluid in which the pressure is a function of the density alone, and therefore is too restrictive to represent air or sea water in motion because of the lack of thermodynamics.

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Vilhelm Bjerknes in 1897 (Friedman 1989) first made the link between theoretical fluid mechanics and meteorology, by generalising the circulation theorem to include the usual atmospheric and oceanic situations where vorticity is generated or destroyed by the variation of buoyancy forces involving temperature changes in the vertical. The application of these results to synoptic meteorology in the ensuing years is, perhaps, the most important advance in the subject (Petterssen 1956). However Bjerknes and his son Jakob are more famous for their observational description in the 1920s of how cyclonic disturbances develop, with converging air flow leading to the formation of fronts and the triggering of rain bands along the fronts. Through their advocacy and organisation of rapid international exchange of meteorological measurement, their ideas featured in public weather forecasts in the 1930s (Friedman 1989). Qualitative elements of frontal analysis and the further dynamical analysis of regions of convergence and divergence by Sutcliffe (1947) and his contemporaries provided the conceptual basis of practical forecasting until the 1990s. Rossby (1936, 1940) and Ertel (1942) provided the next important conceptual development in meteorology and oceanography with the unifying concept of 'potential vorticity' (PV). PV is proportional to the vertical component of the vorticity of a fluid parcel per unit mass, and is approximately conserved when the effects of friction and external heating are slow compared to the other changes that are occurring in an air mass as it moves horizontally and vertically, e.g. over another air mass or mountains. This dynamical insight about changing meteorological conditions constrained by the conservation of a scalar quantity was connected to the earlier ideas of geostrophic balance through the pioneering work of Charney (1947) on quasi-geostrophic theory and by Kleinschmidt (1950a,b; 1951) on the dynamics of cyclones. However, exploitation of this new variable (PV) had to wait until the introduction of super-computers and the greater availability of upper-air data in the 1980s. The concept of PV has become a useful tool in practical forecasting because this one scalar field determines (via so-called 'inversion') the wind, pressure, temperature and density fields. This is a conceptual simplification because the changing weather (or even errors in weather patterns) can be described very economically (and errors corrected) using this one variable at different levels (Hoskins, McIntyre and Robertson 1985). The mathematical significance of potential vorticity conservation is not only that it is a 'governing' variable, but also that its properties reflect the underlying symmetries of the fluiddynamical system which, in turn, determine conservation properties in both the infinite-dimensional, and numerical finite-dimensional, approximate 'models' of such systems.

In recent years a new appreciation has emerged of the central role, in controlling the behaviour of the equations and their solutions, of conservation laws of dynamical systems. This has been achieved by connecting them with the intrinsic geometric structure of the underlying equations of motion regarded as a hamiltonian dynamical system (i.e. one defined by its integral properties

such as mass, energy, potential vorticity). Recent research in mechanics and dynamical systems using this powerful concept is often not familiar to those working in theoretical fluid dynamics, meteorology and oceanography. Modern hamiltonian mechanics provides a natural framework for understanding phenomena such as nonlinear stability, integral invariants and constrained dynamical systems (such as balanced models), and also for developing improved numerical schemes that have reduced errors because the schemes reflect the intrinsic geometrical properties of the analytical equations (Budd and Iserles 1999). The interplay of geometry and analysis will have many applications in geophysical mechanics; forecasting and climate modelling being prime examples here. The Newton Institute programme was designed to help advance this understanding.

The lectures in these volumes explain why simplifications to Newton's second law applied to the complex motions in the atmosphere and oceans are needed to understand and solve the equations. Since the early work of Runge (1895), Kutta (1901) and Richardson (1911), mathematical analysis has enabled the accuracy of such approximations to be assessed systematically on what are now large scale computations. However, whereas meteorologists have sought patterns in the weather for over 300 years, mathematicians have only recently begun to use geometrical thinking to understand the structure behind the governing equations and their approximate forms. Here constrained hamiltonian mechanics, transformation groups, and convex analysis are used to control the potentially chaotic dynamics in the numerical simulations, and to suggest optimal ways to exploit observational data. Many of the chapters ¹ included in these volumes describe studies of the governing systems of equations, with all their complexities and approximations, although the main emphasis was on simpler systems whose integral properties and detailed solutions can be derived exactly. The approximations involved in deriving these idealised systems are controversial and have not always been mathematically consistent. Recent research, such as Cullen [I, 4], has centred on quantifying these approximations, by making full use of the latest results from the theory of stratified, rotating fluid dynamics. This book and its companion show how geometry and analysis quantify the concepts behind the fluid dynamics, and thus facilitate new solution strategies.

Any selection of contributions from an extensive subject such as weather and ocean forecasting necessarily reflects a particular viewpoint concerning both the historical significance of certain developments and their implications for future progress. The following brief commentary indicates the viewpoint taken and supplies a setting for the individual papers. However, the emphasis is always on large-scale atmosphere and ocean dynamical models that are useful in predicting changing weather patterns and climatic trends.

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¹They are designated hereafter by a number in square brackets [], with the volume number first, where needed. Other references are referred to by their date e.g. (1999).

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Introduction to Volume 1 — Analytical Methods and Numerical Models

The article A View of the Equations of Meteorological Dynamics and Various Approximations by White [1], is a pedagogical introduction to the mathematics of meteorological fluid dynamics, which includes the derivation of the governing equations from those for the conservation of mass, momentum, thermodynamics etc., making further suitable approximations consistent with the asymptotic regimes to be modelled. White reviews the problem of deriving simplified balance equations which, as he explains, requires certain assumptions. This article has been written for mathematicians and physicists who desire a compact introduction to the subject rather than the more extensive treatments to be found in good contemporary textbooks on meteorology. Attention is also paid to various recent developments which have received little exposure outside the research literature yet. The approximated models studied include the hydrostatic primitive equations, the shallow water equations, the barotropic vorticity equation, several approximately-geostrophic models and some acoustically-filtered models which permit buoyancy modes. Conservation properties and frame invariance are given special emphasis. A straightforward problem of small-amplitude wave motion in a rotating, stratified, compressible atmosphere is addressed in detail, with particular attention paid to the occurrence or non-occurrence of acoustic, buoyancy and planetary modes in these models. The concluding section contains a short discussion of basic issues in numerical model construction.

The motion of a rotating, stratified fluid governed by the hydrostatic primitive equations is studied by Allen *et al.* [2]. The hydrostatic approximation, as discussed by White, reflects the high degree of stratification in the atmosphere and oceans. Approximate models are derived from the hydrostatic primitive equations for application to mesoscale oceanographic problems. The approximations are made within the framework of Hamilton's principle using the Euler–Poincaré theorem for ideal continua (see Holm *et al.* [II, 7]). In this framework, the resulting eulerian approximate equations satisfy Kelvin's theorem, conserve potential vorticity of fluid particles and conserve a volumeintegrated energy. In addition, Allen *et al.* assess the accuracy of the model equations through numerical experiments involving a baroclinically unstable oceanic jet.

Roulstone and Norbury (1994) describe how one particular balanced model, the so-called semi-geostrophic (SG) equations, can be formulated in a manner similar to the Euler equations in two dimensions. Balanced evolution, which in this model entails the complete absence of fast inertia-gravity waves, is generated by a hamiltonian such that the solution is a sequence of minimum energy states, in a certain sense. Hoskins and Bretherton (1972) showed that the SG equations may be expressed in terms of lagrangian conservation laws. Thence a stable manifold within the dynamical system of the atmosphere is defined by

using a convexity principle to minimize the energy. An extra advantage of this principle is that it applies to variables which have discontinuities. Furthermore, Hoskins and Bretherton (1972) showed that there exists a transformation of coordinates under which the motion of the fluid parcels is exactly geostrophic. For this reason such coordinates are sometimes referred to as geostrophic coordinates. Singularities of this differentiable map can be interpreted as fronts.

For a solution to the semi-geostrophic equations on a plane rotating with constant angular velocity — a so-called f-plane — the Cullen–Norbury–Purser principle (Cullen et al. 1991) states that at each fixed time, the fluid particles arrange themselves to minimise energy. Rewriting the equations in terms of the so-called geostrophic coordinates (Sewell [II,5]), this principle yields a constrained variational problem (where the constraint evolves with time): at each fixed time t, minimize the energy over all possible fluid configurations, given that values of the geostrophic transformation are known on particles. The minimizer, if it exists and is unique, gives the actual state of the fluid (in terms of the geostrophic transformation) at time t. Assuming the geostrophic energy is finite, it has been proved (Douglas 1998) that there is a unique minimizer, equal to the gradient of a convex function. In this way, solutions can be viewed as a sequence of minimum energy states. The set of possible states is described by a set of rearrangements; the unique minimizer is the monotone rearrangement (see Brenier 1991).

Douglas [5] presents some mathematical ideas on rearrangements of fluid volumes that have found application in meteorology, and that promote the lagrangian viewpoint. An intuitive idea of when two functions are rearrangements is as follows. Let f be a function, defined on a bounded region, such as temperature or moisture content. Imagine that the bounded region is a continuum of infinitesimal particles, and suppose that we exchange the particle positions with each particle retaining its value of f, that is, we conserve the temperature or moisture on fluid particles. This yields a new function g, which describes the temperature or moisture at the new locations, which is a 'rearrangement' of f. The concept of rearranging a function can be applied to both scalar and vector valued functions, and Douglas [5] develops the theory for both cases. Examples are given to illustrate the key ideas. Essentially, rearrangements allow us to conserve quantities on fluid masses as the masses are transported through the atmosphere using a lagrangian rather than eulerian viewpoint.

We can rewrite the energy minimization problem as a 'Monge mass transfer problem', for which there already exists a significant mathematical theory and numerical solution procedure. We then find that the monotone rearrangement is the optimal mapping. Thus, the geostrophic energy-minimising arrangement of fluid masses can be related to local stability conditions that require convexity of certain pressure (or geopotential) surfaces in the atmosphere. Failure to satisfy these conditions is usually associated with a breakdown in balance and

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rapid change of atmospheric conditions, including storms. An introduction to the theory of rearrangements, together with a discussion of their application to the semi-geostrophic equations, is given by Douglas [5]. An alternative interpretation of this theory based on probability ensembles, considering in what sense maximum likelihood states are equivalent to the Cullen–Norbury–Purser principle in semi-geostrophic theory, is given in Baigent and Norbury [6].

Following the seminal work of Vilhelm Bjerknes, the method of numerical weather prediction (NWP) was first worked out by L.F. Richardson in 1922 (see, for example, Nebeker 1995). He anticipated that sufficient measurement of data would become available and that computations would become sufficiently fast and comprehensive that the accuracy of weather forecasts should eventually equal those for the stellar and planetary positions recorded annually in the Nautical Almanac. This presumption was essentially questioned by Lorenz (1963), who showed that even much simpler mathematical representations of fluid flow (3 coupled non-linear, first-order, differential equations) are intrinsically prone to errors, so that however small their initial value the magnitudes of errors generally grow. His broad conclusions have had a major influence on the interpretation of weather forecasts ever since, the first being that there is much more sensitivity to errors in some states of a system (e.g. near saddle points in the phase plane) than in others. The second is that errors can grow exponentially. The latter conclusion has been bowdlerised in much popular comment as implying that since errors grow rapidly the weather is so chaotic that it cannot be forecast at all! Reasons why this might not be true for large scale weather evolution were advanced during the Isaac Newton Institute programme and have been the basis of significant follow-up work. First it is necessary to think carefully about what is meant by forecast error. A new approach to the evaluation of weather forecast error is to decompose the error into a combination of displacement error and difference in qualitative features. Douglas [5], and Cullen [4], demonstrate this idea and give a precise formulation using rearrangements of functions.

Directly or indirectly, the papers in this volume show why useful predictions can be made in the presence of chaos. Cullen [4] explains how the errors for more complex systems than those considered by Lorenz often grow more slowly, one of the reasons being that typical atmosphere and ocean weather events have a localised or vortex nature rather than a wave-like form (Hunt 1999). Other papers (see Arnol'd 1998) show that whether the systems are simple or complex, whatever their growth rate over the first few days, the errors are limited because the range of possible solutions for small initial errors tend to be confined within certain 'basins of attraction' in the phase planes of the system. This geometrical interpretation reflects recent mathematical research in which the results of geometrical analysis of differential systems leads to a clearer definition of their 'global' (in the mathematical sense) properties. Babin, Mahalov and Nicolaenko [3] give a detailed derivation of the

errors involved in the balanced dynamics in the different asymptotic regimes of interest in atmospheric and oceanic dynamics. Babin *et al.* derive a new theorem for these error limits, and show how some of the standard approximations based on 'balance' and the neglect of the nonlinear time averaged effects of 'unbalanced' motion may be significant — reflecting perhaps the practical meteorologist's well known concern with waves on fronts, another example of further instability.

Weather forecasts are routinely computed for up to 10 days ahead, based on large quantities of wind, temperature and humidity data that are collected continuously, at random locations around the globe, and used to modify the computations. The data are of course insufficient to determine the exact state of the atmosphere. Since the data are very expensive to obtain there is a premium on their optimal exploitation. Therefore it is of the highest importance for numerical weather prediction to identify the dominant processes and flow features that determine how the large scale weather patterns develop. By ensuring that the continuous assimilation of data is consistent with these features the accuracy of the forecasts is greatly increased. Ocean modelling is beginning to develop similar data assimilation techniques. Cullen [4] explains how we can think of the atmosphere as evolving close to a dynamical system with high predictability which both explains the current success of operational predictions, and suggests that further useful progress can be made by exploiting this closeness more fully in the design of numerical prediction systems. Furthermore, using the notion of balance, and the associated transformation theory described by Sewell [II,5], Cullen suggests ways of using the incomplete observational data in more efficient ways, by exploiting the information implicit in the balance conditions to project the data onto the model grid in ways that respect the prevailing synoptic conditions. Babin *et al.* [3] provide a rigorous account of the asymptotic validity of these simpler systems. Cullen [4] argues that some recent results presented during the programme, from both atmosphere and ocean models, suggest that it is well worth making efforts to reduce the generation of spurious solutions arising from model and computational errors. Recent work supports the aim of building better numerical models that naturally support the desired simpler solutions.

Atmosphere and ocean models include approximate representations of sub grid scale processes and physical forcing; their best mathematical representation is not certain. Considerable progress is being made in showing how certain turbulence mixing processes that have been represented by diffusion-like terms can better be represented as effective advective transport terms. This could even affect conclusions about the large scale atmosphere and ocean circulation. Furthermore this change affects the form of the overall mathematical model, since these 'transports' have to be properly integrated with the rest of the dynamics. This issue too is discussed in the article by Cullen [4].

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Introduction to Volume 2 — Geometric Methods and Models

Salmon (1983, 1985, 1988) pioneered the systematic derivation of balanced models within the framework of Hamilton's principle. The rationale is to make approximations to the lagrangian without disturbing the symmetry properties of the functional, thereby ensuring that the resulting model retains approximations to the conservation laws of the primitive equations. The derivation and understanding of balanced models from the hamiltonian point of view was one of the key themes of the Newton Institute programme. The chapter *Balanced models in geophysical fluid dynamics: hamiltonian formulation, constraints and formal stability* by Bokhove [1], gives a step by step account of the basics of hamiltonian mechanics and proceeds to demonstrate how hamiltonian formulations of balanced models can be constructed such that fast inertio-gravity waves can be eliminated by imposing certain constraints.

Most fluid systems, such as the three-dimensional compressible Euler equations, are too complicated to yield general analytical solutions, and approximation methods are needed to make progress in understanding aspects of particular flows. Bokhove reviews derivations of approximate or reduced geophysical fluid equations which result from combining perturbation methods with preservation of the variational or hamiltonian structure. Preservation of this structure ensures that analogues of conservation laws in the original 'parent' equations of motion are preserved. Although formal accuracy in terms of a small parameter may be achieved with conservative asymptotic perturbation methods, asymptotic solutions are expected to diverge on longer time scales. Nevertheless, perturbation methods combined with preservation of the variational or hamiltonian structure are hypothesised to be useful in a climatological sense because conservation laws associated with this structure remain to constrain the reduced fluid dynamics. Variational and hamiltonian formulations, perturbative approaches based on 'slaving', and several constrained variational or hamiltonian approximation approaches are introduced, beginning with finite-dimensional systems because they facilitate a more succinct exposition of the essentials. (The more technical mathematical aspects of infinite-dimensional hamiltonian systems are not considered, see e.g. Marsden and Ratiu 1994.) The powerful energy-Casimir method which can be used to derive stability criteria for steady states of (canonical) hamiltonian systems is introduced and the hamiltonian approximation approaches to various fluid models starting from the compressible Euler equations and finishing with the barotropic quasi-geostrophic and higher-order geostrophically balanced equations is presented. The presentation of fluid examples runs in parallel with the general finite-dimensional treatment which facilitates a clear understanding of the methods involved.

An illustration of the concept of balance within the framework of a finitedimensional system is provided by Lynch [2]. The linear normal modes of the atmosphere fall into two categories, the low frequency Rossby waves and

the high frequency gravity waves. The elastic pendulum is a simple mechanical system having low frequency and high frequency oscillations. Its motion is governed by four coupled nonlinear ordinary differential equations. Lynch studies the dynamics of this system, drawing analogies between its behaviour and that of the atmosphere. The linear normal mode structure of the system is analysed, the procedure of initialization is described and the existence and character of the slow manifold is discussed. This allows non-specialists to see, in a very simple example, what is performed routinely with the enormous systems of equations in modern numerical weather prediction and why.

Balmforth and Morrison [4] develop a hamiltonian description of shear flow, including the dynamics of the continuous spectrum. Euler's equation linearized about a shear flow equilibrium is solved by means of a novel invertible integral transform that is a generalization of the Hilbert transform. The integral transform provides a means for describing the dynamics of the continuous spectrum that is well-known to occur in this system. The results are interpreted in the context of hamiltonian systems theory, where it is shown that the integral transform defines a canonical transformation to action-angle variables.

Many balanced models do not support gravity waves, indeed the elimination of these waves from the solutions is usually the aim in defining an appropriate balance. Caillol and Zeitlin [3] point out that although internal gravity waves are not normally associated with 'weather' (see also Cullen [I,4]), they play an important role in energy transport in atmosphere and ocean dynamics. In [3], Caillol and Zeitlin study statistically steady states of an ensemble of interacting internal gravity waves and the corresponding energy spectra. They derive a kinetic equation for a system of weakly nonlinear plane-parallel internal gravity waves in the Boussinesq approximation and solve them to find stationary energy spectra for wave packets propagating in the direction close to vertical. The result is a Rayleigh–Jeans energy equipartition solution and a Kolmogorov-type solution of the form $\epsilon_k \sim k_1^{-(3/2)} k_3^{-(3/2)}$ corresponding to a constant energy flux through the wave spectrum.

The canonical vortex structures, their interaction and slow evolution, may be described, in the semi-geostrophic model, by solutions to the non-standard (Monge mass transfer) optimization problem described by Cullen [I,4] and Douglas [I,5]. It has been shown, by Chynoweth and Sewell (1989) for example, that singularities arise from the convexifications of multivalued Legendre dual functions, such as the swallowtail, with a typical singular surface being identified with a weather front. Sewell [5] reviews many aspects of transformation theory including Legendre duality and other types, and of lift transformations and canonical transformations. Applications are mentioned in several branches of mechanics. A straightforward style is adopted, so that the paper is accessible to a wide readership. Developments in the semi-geostrophic theory of meteorology in the last fifteen years have prompted this review, but it draws upon earlier work in, for example, plasticity theory, gas dynamics,

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shallow water theory, catastrophe theory, hamiltonian mass-point mechanics, and the theory of maximum and minimum principles. Singularities need to be described in transformation theory, and the swallowtail catastrophe is one such example. The intimate relation between lift transformations and hamiltonian structures is described. New exact solutions in a semi-geostrophic central orbit theory are given and properties of constitutive surfaces in gas dynamics and shallow water theory are described.

Purser [6] demonstrates that, using transformation theory, one can construct different versions of the semi-geostrophic equations for the purposes of modelling non-axisymmetric vortices on an f-plane and hemispheric (variablef) dynamics. Both formulations retain a Legendre duality — a feature which is central to the construction of lagrangian finite-element methods. Note also that McIntyre and Roulstone [8] ask whether higher-order corrections to semigeostrophic theory may be constructed while retaining some of the mathematical features that facilitate the integration of the equations both analytically and numerically.

For semi-geostrophic theories derived from the hamiltonian principles suggested by Salmon it is known (e.g. Purser and Cullen 1987) that a duality exists between the physical coordinates and geopotential, on the one hand, and isentropic geostrophic momentum coordinates and geostrophic Bernoulli function, on the other hand. The duality is characterized geometrically by a *contact structure* as described by Sewell [5]. This enables the idealized balanced dynamics to be represented by horizontal geostrophic motion in the dual coordinates, while the mapping back to physical space is determined uniquely by requiring each instantaneous state to be the one of minimum energy with respect to volume-conserving rearrangements within the physical domain.

Purser [6] shows that the generic contact structure permits the emergence of topological anomalies during the evolution of discontinuous flows. For both theoretical and computational reasons it is desirable to seek special forms of semi-geostrophic dynamics in which the structure of the contact geometry prohibits such anomalies. Purser proves that this desideratum is equivalent to the existence of a mapping of geographical position to a euclidean domain, combined with some position-dependent additive modification of the geopotential, which results in the semi-geostrophic theory being manifestly Legendre-transformable from this alternative representation to its associated dual variables.

Legendre transformable representations for standard Boussinesq f-plane semi-geostrophic theory and for the axisymmetric gradient-balance version used to study the Eliassen vortex are already known and exploited in finite element algorithms. Here, Purser re-examines two other potentially useful classes of semi-geostrophic theory: (i) the *non*-axisymmetric f-plane vortex; (ii) hemispheric (variable-f) semi-geostrophic dynamics. We find that the imposition of the natural dynamical and geometrical symmetry requirements together

with the requirement of Legendre-transformability makes the choice of the f-plane vortex theory unique. Moreover, with modifications to accommodate sphericity, this special vortex theory supplies what appears to be the most symmetrical and consistent formulation of variable-f semi-geostrophic theory on the hemisphere. The Legendre-transformable representations of these theories appear superficially to violate the original symmetry of rotation about the vortex axis. But, remarkably, this symmetry is preserved provided the metric of the new representation is interpreted to be a pseudo-euclidean *Minkowski* metric. Rotation-invariance of the dynamical formulation in physical space is then perceived as a formal *Lorentz-invariance* in its Legendre-transformable representation.

Motivated by the remarkable mathematical structure of balanced models formulated in terms of a variational principle and their use in solving this class of problems, the last two articles consider more general and more accurate models of balanced atmospheric dynamics. The contributions by Holm, Marsden and Ratiu [7], and McIntyre and Roulstone [8], present recent developments in the theory of hamiltonian balanced models. Holm *et al.* [7] show how a number of models can be written in Euler–Poincaré form, and they propose a new modification of the Euler–Boussinesq equations which adaptively filters high wavenumbers and thereby enhances stability and regularity.

Recent theoretical work has developed the Hamilton's-principle analogue of Lie–Poisson hamiltonian systems defined on semidirect products. The main theoretical results presented in [7] are twofold: (i) Euler-Poincaré equations (the lagrangian analogue of Lie–Poisson hamiltonian equations) are derived for a parameter dependent lagrangian from a general variational principle of Lagrange-d'Alembert type in which variations are constrained; (ii) an abstract Kelvin-Noether theorem is derived for such systems. By imposing suitable constraints on the variations and by using invariance properties of the lagrangian, as one does for the Euler equations for the rigid body and ideal fluids, Holm et al. cast several standard eulerian models of geophysical fluid dynamics (GFD) at various levels of approximation into Euler–Poincaré form and discuss their corresponding Kelvin–Noether theorems and potential vorticity conservation laws. The various levels of GFD approximation are related by substituting a sequence of velocity decompositions and asymptotic expansions into Hamilton's principle for the Euler equations of a rotating stratified ideal incompressible fluid. They emphasize that the shared properties of this sequence of approximate ideal GFD models follow directly from their Euler-Poincaré formulations. New modifications of the Euler-Boussinesq equations and primitive equations are also proposed in which nonlinear dispersion adaptively filters high wavenumbers and thereby enhances stability and regularity without compromising either low wavenumber behaviour or geophysical balance.

The final article — epitomising the open-endedness of the Programme and the ongoing research it has stimulated — describes an unfinished journey, as

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well as presenting background tutorial material. Semigeostrophic theory and its contact structure and other formal properties are first of all reviewed in the simplest nontrivial context, f-plane shallow-water dynamics in $\mathbf{R}^2 = \{x, y\}$. A number of these properties are remarkably simple and elegant, and mathematically important. The authors ask which of those properties might generalize to more accurate hamiltonian models of balanced vortex motion. Many of the properties are intimately associated with the special canonical coordinates (X, Y) discovered by Hoskins (1975). The jacobian $\partial(X, Y)/\partial(x, y)$ of these coordinates with respect to the physical space coordinates (x, y) is equal to the absolute vorticity measured in units of the Coriolis parameter f; and Hoskins' transformation $(x, y) \mapsto (X, Y)$ is, in a natural sense, part of an explicitly invertible contact transformation (see also Sewell [5]). The invertibility is associated with a symmetric generating function. Unlike the flow in physical space $\{x, y\}$, the flow in the space $\{X, Y\}$ space is solenoidal, and its streamfunction $\Phi(X, Y, t)$ is obtainable by solving an elliptic Monge–Ampère equation expressing 'potential vorticity invertibility'. There are also certain Legendre duality and convexity properties, which make the model well-behaved, both mathematically and numerically, even when phenomena like frontal discontinuities occur (see also Cullen [I,4], Purser [6] and Sewell [5]).

No such canonical coordinates were known in simple analytical form for any other balanced model until the recent — and to fluid dynamicists very surprising — discovery by McIntyre and Roulstone (1996) of *complex-valued* canonical coordinates (X, Y) in a certain class of hamiltonian balanced models, some of which are more accurate than semigeostrophic theory. The general way in which these models and their canonical coordinates are systematically derived by constraining an unbalanced 'parent dynamics' (hence 'splitting' the parent velocity field into two or more different fields) is discussed, following the method of Salmon (1988). The coordinates (X, Y) are such that $\partial(X, Y)/\partial(x, y)$ is still real, and still equal to the absolute vorticity in units of f. The models include Salmon's L_1 dynamics and a new family of ' $\sqrt{3}$ models' that are formally the most accurate possible of this class. The authors pursue the question thus raised: do these new models, or any subset or superset of them, share significant properties with semigeostrophic theory beyond the underlying hamiltonian dynamical structure and the special canonical coordinates (X, Y) and their association with vorticity? The answer seems to be yes to the extent that the flow in (complex!) (X, Y) space is solenoidal — so that a complex streamfunction $\Phi(X, Y, t)$ must exist — and that elliptic Monge-Ampère equations expressing potential vorticity invertibility occur in all the new models, as well as in semigeostrophic theory. Otherwise, the answer is no. For instance the transformation $(x, y) \mapsto (X, Y)$ is no longer part of a contact transformation. However, the 'conjugate' transformation $(x, y) \mapsto (X, Y)$, where \overline{Y} is the complex conjugate of Y, is, by contrast, part of an explicitly invertible contact transformation with a symmetric generating function and a new transformed potential $\hat{\Phi}(X, \bar{Y}, t)$. This fact, discovered by Roubtsov

and Roulstone (2001), implies connections with hyper-Kähler geometry. The pair of transformations — taking (x, y) into (X, Y) and relating to vorticity, potential vorticity and elliptic Monge–Ampère equations, on the one hand, and taking (x, y) into (X, \overline{Y}) and relating to contact structure on the other — reveals that the structure underlying the whole picture is just that of a hyper-Kähler space or manifold, which in turn is part of a twistor space. The implications of this remain to be explored.

Conclusions

The Newton Institute programme successfully brought together ideas from geometry, analysis and dynamical systems theory, and showed their many benefits in numerical prediction used for weather forecasting, ocean and climate modelling. Various papers in these volumes advance the programme; and they suggest new problems and avenues for research in the theory of constrained dynamical systems, in particular for strongly stratified and rotating fluid flows where chaotic dynamics may be minimized.

From the material presented in these volumes we hope to gain new insights into the important issues surrounding various questions about the description of weather systems, on the large scale in both the atmosphere and the oceans, described by constrained variational principles. These issues include 'potential vorticity inversion' — the relationship between the potential vorticity and the balanced wind and temperature fields as described earlier in this Introduction — which usually involves solving a nonlinear elliptic problem (as in semi-geostrophic theory, for example). The convergence and practical stability of numerical schemes, and the relationship between stability of the flow and ellipticity of the operators, is far from being completely understood (for example, see comments in Ziemianski and Thorpe 2000 and also Knox 1997). For instance, Cullen [I,4] conjectures that 'elliptic PV inversion' constrains the enstrophy cascade, and hence controls the decay of fluid motions to turbulence. One direction in which work on these issues is proceeding is demanding more in terms of non-smooth analysis and ideas from rearrangement theory, as well as promoting a lagrangian view of fluid dynamics. Convex analysis plays a key role in many of the applications discussed here; in fact for the semi-geostrophic model, convexity, ellipticity and stability are directly related. From a purely mathematical perspective in terms of the lagrangian description of infinite-dimensional systems, and from a physical point-of-view relating to the stability of large-scale flows, convexity appears to limit chaotic dynamics.

There is increasing evidence to suggest that a major application of the hamiltonian dynamical aspects would be useful in numerical weather prediction. Numerical models based on Hamilton's equations pose a challenge to the numerical analyst working in partial differential equations and to the theorist who needs to find a hamiltonian formulation of the relevant constrained equa-

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tions of motion and their associated conservation properties. In particular, balance conditions are an important constraint for the new generation of data assimilation schemes which seek to minimise cost functions based on the fit of observations to four-dimensional integral curves of the equations of motion (Courtier and Talagrand 1990). The new techniques proposed here may therefore have a major impact on our ability to provide accurate and appropriately balanced initial conditions for numerical weather prediction. Such study of meteorological problems may also promote further insight into the theory of dynamical systems.

We draw three main conclusions for practical computation from the papers presented here. First, new approaches are now available for reducing errors in numerical schemes by considering local integral properties; secondly, the standard assumptions of geophysical fluid dynamics describing how flows are in approximate geostrophic balance can be used to reduce significant errors in certain forecasting situations, especially by making better use of assimilated data in each application; and thirdly, the growth rate and maximum level of errors caused by data uncertainty, when analysed using realistic local dynamics and global dynamics respectively, differ quantitatively and conceptually from those inferred from Lorenz's much simpler chaotic systems.

We conclude by noting that the past few years have witnessed a number of exciting parallel developments in both the mathematical aspects and the phenomenology of stratified, rotating fluid dynamics, with the promise of practically important spinoffs including improved analyses and prediction of weather systems. Recent mathematical advances have brought a new geometric viewpoint to these problems, in particular a new appreciation of the central role of potential vorticity and its connection with the symplectic geometric structure of the underlying equations of motion regarded as a hamiltonian dynamical system.

Weather forecasting and climate modelling are excellent examples of how these mathematical advances have practical applications in solving problems where there is a strong interplay of geometry and physics.

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