Dynamical Subgrid-scale Parameterizations for Quasigeostrophic Flows using Direct Numerical Simulations

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Declaration

This thesis is an account of research undertaken between March 2004 and December 2007 at CSIRO Marine and Atmospheric Research, Aspendale Laboratories, Victoria, Australia, and at The Department of Theoretical Physics, Research School of Physical Sciences and Engineering, The Australian National University, Canberra, Australia.

Except where acknowledged in the customary manner, the material presented in this thesis is, to the best of my knowledge, original and has not been submitted in whole or part for a degree at any other university.

Meelis Juma Zidikheri
December, 2007
I would like to thank my principal supervisor, Jørgen Frederiksen, for his continued support during my PhD candidature. Jørgen has been closely involved in all aspects of the research presented here, and he has invested a considerable amount of his time towards my training; I would like to express my gratitude to him for that. I would also like to thank the following people who have contributed in one way or another to the completion of my thesis: Rowena Ball and Bob Dewar, my supervisors at ANU, for their encouragement and making me feel welcome during my visits to Canberra; Terry O’Kane, formerly of CSIRO Marine and Atmospheric Research, for illuminating discussions and assistance with computational work, particularly during the early stages of my candidature; Steve Kepert, formerly of CSIRO Marine and Atmospheric Research, for assistance with computational work; Stacey Osbrough, of CSIRO Marine and Atmospheric Research, for assistance with some of the diagrams produced in this thesis; and staff at the CSIRO/Bureau of Meteorology High Performance Computing and Communications Centre (HPCCC), for assistance with computing issues, particularly Robert Bell and Aaron McDonough. I would also like to thank my family for their support: my mum, Reet; my sister, Asha; and my girlfriend, Kelly. Additionally, I would like to express my gratitude posthumously to my father, Ali Juma Zidikheri. As well as human resources, I have benefitted from material resources. I would like to thank the following organizations for their support: The Research School of Physical Sciences and Engineering of the Australian National University, for funding my PhD scholarship; CSIRO Complex Systems Science, for funding my supplementary scholarship; CSIRO Marine and Atmospheric Research, for providing me with a room and access to facilities; and the Australian Research Council, through the Discovery Projects funding scheme (Project No. DP0343765), for travel support to Canberra.
Preface

Chapter 1 is an introduction to the main ideas in this thesis. Chapters 2 and 3 (and Appendices C and D) contain descriptions of key concepts of geophysical fluid dynamics and turbulence that are used in this thesis. Many, but not all, of the concepts can be found in standards textbooks on these subjects; I have relied heavily on the textbooks by Salmon (1998) and Vallis (2006). The spectral form of the two-level QG equation in Section 2.7 and its related DIA closure expression in Section 3.3.3 originate from unpublished work by Jorgen Frederiksen. The aforementioned chapters and appendices are not meant to serve as a conventional literature review; rather, they are pedagogical in nature. Chapter 4 is a description of research on multiple equilibria and mode reduction in barotropic atmospheric flows that I have carried out under the supervision of Jorgen Frederiksen. A large portion of the material in Section 4.1 has been published, with me as the principal author (see Zidikheri et al., 2007). The numerical model that I use for the direct numerical simulation in Chapter 4 was developed at CSIRO Marine and Atmospheric Research by Jorgen Frederiksen, Anthony Davies, Robert Bell, and Terence O’Kane, with additional problem-specific code written by me. The FORTRAN code for implementing Brent’s Principal Axis algorithm has been written, and kindly been made available online, by John Burkardt. Chapter 5 is a literature review of the Subgrid-scale Parameterization problem. Chapters 6, 7, 8, and 9 are descriptions of research that I have carried out under the supervision of Jorgen Frederiksen on applying Frederiksen and Kepert’s (2006) subgrid-scale parameterization methodology to atmospheric and oceanic baroclinic flows. Appendices A and B are descriptions of material that can be found in research literature. Appendices E and F are descriptions of the numerical models used to generate the results of Chapters 6, 7, and 8. These models have been developed at CSIRO Marine and Atmospheric Research by Jorgen Frederiksen, Robert Bell, and Steve Kepert, with additional problem-specific code written by me. Appendix G contains a straightforward algebraic manipulation. Appendices H and I (and parts of Chapter 8) contain results that have been displayed using code written by Stacey Osbrough at CSIRO Marine and Atmospheric Research.
Abstract

In this thesis, parameterizations of non-linear interactions in quasigeostrophic (QG) flows for severely truncated models (STM) and Large Eddy Simulations (LES) are studied. Firstly, using Direct Numerical Simulations (DNS), atmospheric barotropic flows over topography are examined, and it is established that such flows exhibit multiple equilibrium states for a wide range of parameters. A STM is then constructed, consisting of the large scale zonal flow and a topographic mode. It is shown that, qualitatively, this system behaves similarly to the DNS as far as the interaction between the zonal flow and topography is concerned, and, in particular, exhibits multiple equilibrium states. By fitting the analytical form of the topographic stationary wave amplitude, obtained from the STM, to the results obtained from DNS, renormalized dissipation and rotation parameters are obtained. The usage of renormalized parameters in the STM results in better quantitative agreement with the DNS.

In the second type of problem, subgrid-scale parameterizations in LES are investigated with both atmospheric and oceanic parameters. This is in the context of two-level QG flows on the sphere, mostly, but not exclusively, employing a spherical harmonic triangular truncation at wavenumber 63 (T63) or higher. The methodology that is used is spectral, and is motivated by the stochastic representation of statistical closure theory, with the ‘damping’ and forcing covariance, representing backscatter, determined from the statistics of DNS. The damping and forcing covariance are formulated as $2 \times 2$ matrices for each wavenumber. As well as the transient subgrid tendency, the mean subgrid tendency is needed in the LES when the energy injection region is unresolved; this is also calculated from the statistics of the DNS. For comparison, a deterministic parameterization scheme consisting of $2 \times 2$ ‘damping’ parameters, which are calculated from the statistics of DNS, has been constructed. The main difference between atmospheric and oceanic flows, in this thesis, is that the atmospheric LES completely resolves the deformation scale, the energy and enstrophy injection region, and the truncation scale is spectrally distant from it, being well in the enstrophy cascade inertial range. In oceanic flows, however, the truncation scale is in the vicinity of the injection scale, at least for the parameters chosen, and is therefore not in an inertial range. A lower resolution oceanic LES at T15 is also examined, in which case the injection region is not resolved at all.

For atmospheric flows, it is found that, at T63, the matrix parameters are practically diagonal so that stratified atmospheric flows at these resolutions may be treated as uncoupled layers as far as subgrid-scale parameterizations are concerned. It is also found that the damping parameters are relatively independent of the (vertical) level, but the backscatter parameters are proportional to the subgrid flux in a given level. The stochastic and deterministic parameterization schemes give comparably good results relative to the DNS. For oceanic flows, it is found that the full matrix structure of the parameters must be used. Furthermore, it is found that there is a strong injection of barotropic energy from the subgrid scales, due to the unresolved, or partially resolved, baroclinic instability injection scales. It is found that the deterministic parameterization is too numerically unstable to be of use in the LES, and instead the stochastic parameterization must be used
to obtain good agreement with the DNS. The subgrid tendency of the ensemble mean flow is also needed in some problems, and is found to reduce the available potential energy of the flow.
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Chapter 1

Introduction

This thesis will be concerned mainly with mode reduction in large scale atmospheric and oceanic flows. The need for systematic mode reduction, also known as subgrid-scale parameterization, arises because such flows are turbulent, which implies that they involve coupled motions on very wide ranges of space and time scales. For example, in the atmosphere, the largest scales of motion are in the order of 10000 km while the smallest scales might be in the order of 1 cm (Holton, 1992). The range of time scales is similarly vast. The difficulty, of course, is that these motions are not independent; motions on very different space and times scale can and do interact. Given this, then any computation of motion at a particular scale, say the large scale, needs to involve some parameterization of the small scale motions, if as it often turns out be, it is impossible to compute the latter. One cannot simply study a particular scale of motion in isolation as can be done in many other problems in physics. To illustrate these ideas better we use a toy model of fluid motion as follows.

The acceleration of a particle with velocity $u(x,t)$ at position $x$ and time $t$ is just $a = \frac{\partial u(x,t)}{\partial t}$. However, if the particle is a parcel of fluid in motion, then if the position $x$ is measured relative to a frame moving with the fluid, we have

$$a = \frac{d}{dt}u(x(t),t) = \frac{\partial u}{\partial t} + \frac{\partial x}{\partial t} \frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x}, \quad (1.1)$$

which follows from the fact that the reference frame is moving so $x = x(t)$ and the chain rule for partial derivatives. It sufficient for our arguments to assume that the fluid is not accelerating, so

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \quad (1.2)$$

is a heuristic equation for fluid motion. Now assume that the motion consists of a time-independent part, $\bar{u}$, and a transient part, $u'$. Hence,

$$u(x,t) = \bar{u} + u'(x,t). \quad (1.3)$$

It is also convenient to assume that $\bar{u}$ is uniform in space as well. Then with this caveat, after substituting Eq. 1.3 in Eq. 1.2, we have the evolution equation for the transients (perturbations):

$$\frac{\partial u'}{\partial t} + \bar{u} \frac{\partial u'}{\partial x} + u' \frac{\partial u'}{\partial x} = 0. \quad (1.4)$$

In the absence of the $u' \frac{\partial u'}{\partial x}$ term, this equation is linear in $u'$. The trial solution $u'(x,t) = \exp[\i(kx + \omega t)]$ yields the frequency $\omega = -k\bar{u}$, which implies that $u'$ is always stable; that is, it does not grow exponentially with time. However, the model that
we are working with is very simplistic. In more realistic problems, flow instabilities, such as barotropic, baroclinic, and topographic instabilities for atmospheric and oceanic flows exist, so the frequency will in such problems have an imaginary component, making the solution unstable for some flow parameters. The instability will also typically have a peak at some wavenumber. In this toy model, the ‘missing’ instabilities can be represented by a transient forcing, \( f(t) \), in the equation of motion, Eq. 1.2. Hence,

\[
\frac{\partial u'}{\partial t} + \bar{u} \frac{\partial u'}{\partial x} + u' \frac{\partial u'}{\partial x} = f. \tag{1.5}
\]

It is illuminating to expand \( u' \) in terms of waves with wavenumbers \( k \), with corresponding length scales \( \lambda = \frac{1}{k} \). Hence,

\[
u'(x, t) = \sum_k u_k(t) \exp(ikx). \tag{1.6}
\]

Here, \( u_k \) is the amplitude of the wave with wavenumber \( k \). The flow, \( u' \), will be real if \( u_k^* = u_{-k} \). Similarly,

\[
f(x, t) = \sum_k f_k(t) \exp(ikx). \tag{1.7}
\]

Substituting Eqs. 1.6 and 1.7 in Eq. 1.5, we have

\[
\frac{\partial u_k}{\partial t} = \sum_p \sum_q A_{kpq}u_pu_q - ik\pi u_k + f_k. \tag{1.8}
\]

Here, \( A_{kpq} \) are interaction coefficients which depend on the wavenumbers \( k, p, \) and \( q \).

Now, imagine that the instability is initially confined to a single wavenumber \( k \). In the absence of the non-linear terms, the amplitude \( u_k \) would grow without bound. However consider a mode with wavenumber \( k' \), where \( k' \neq k \); the evolution equation for this mode is

\[
\frac{\partial u_{k'}}{\partial t} = \sum_p \sum_q A_{k'pq}u_pu_q - ik\pi u_{k'}. \tag{1.9}
\]

The amplitude \( u_{k'} \) will grow because when either \( p \) or \( q = k \), the non-linear term \( u_ku_q \) (or \( u_pu_k \)) will be large because the mode with wavenumber \( k \) grows exponentially due to an instability. Non-linear interactions, then, cause other modes, with wavenumbers \( k' \neq k \), to grow. In physical space, this corresponds to a motion of a particular scale, initially growing due to a (linear) instability of the flow, breaking up into motions of other scales. In three-dimensional fluids, these motions are generally of smaller scales, but in two-dimensional fluids, with atmospheric and oceanic fluids being examples thereof, it is possible for motions of larger scales to be generated as well. This phenomenon, whereby a fluid motion of a certain scale generates, via non-linear interactions, motions at numerous other scales, is understood to be turbulence, as far as this thesis is concerned. Clearly, an analytical solution is out of the question for such problems. However, numerical solutions are also problematic because one would have to resolve the smallest scales of motion, since all scales are coupled. This is out of reach of current computational technology for many problems of interest, including atmospheric and oceanic flows. In any case, even if such computational capabilities were to be available, they would be of no use for solving real-world problems in a deterministic sense, since it is not conceivably possible to measure the initial conditions of a physical system, such as the atmosphere or oceans, with such
precision. Instead, one can only hope to obtain flow statistics. The equations of motion of turbulent flows are thus inherently stochastic.

Flow statistics are impossible to compute directly from equations of type (1.8) since the tendency \( \frac{\partial \langle u_k \rangle}{\partial t} \) would involve a second-order moment \( \langle u_p u_q \rangle \), and the tendency for the second order moment would consequently involve the third order moments, and ad infinitum. This is called the closure problem of turbulence, and attempts to close the hierarchy of equations by additional assumptions regarding the flow statistics are called closure theories of turbulence. One can also use phenomenology to deduce some qualitative features of the flow statistics. So for example, in a two-dimensional fluid, the energy and enstrophy, which are flow statistics, are both conserved. This constrains the transfers of energy and enstrophy to be towards the large scales and small scales, respectively.

In many cases, one is interested in particular scales of motion, but has to carry around the computationally burdensome other scales. So, using our toy model as an example, we might be interested in looking at the interaction of a particular scale of motion with amplitude \( u_k \) with the background flow \( \bar{u} \):

\[
\frac{\partial u_k}{\partial t} = -i k \bar{\pi} u_k + f_k. \tag{1.10}
\]

This is a severely truncated, or reduced, model since we have ignored modes with wavenumbers other than \( k \). In some simple cases, one might be able to obtain an analytic solution to this problem. However, the neglected non-linear terms will have an effect on the flow, and these interactions have to be parameterized in some way. One way of doing this is to run a sufficiently high resolution simulation, with the non-linear terms included, and try to fit the analytic solution of the reduced-order model to the results of the higher resolution simulation by redefining some flow parameters. This is the first type of problem that we shall examine in this thesis (in Chapter 4) in relation to a barotropic (depth independent) atmospheric flow over topography.

The second type of problem involves choosing a cutoff wavenumber \( k_* \) in the flow, and, for wavenumbers \( k \leq k_* \), parameterizing the interactions with wavenumbers \( k > k_* \). This is called subgrid-scale parameterization, and is needed to run simulations truncated at wavenumber \( k_* \). Thus, we have

\[
\frac{\partial u_k}{\partial t} = \sum_{p \leq k_*} \sum_{q \leq k_*} A_{kpq} u_p u_q + g(u_k) - i k \bar{\pi} u_k + f_k. \tag{1.11}
\]

Here, \( g(u_k) \) is a function of the resolved scale amplitudes \( u_k \) which parameterizes non-linear interactions involving at least one wavenumber greater than \( k_* \). The simplest choice for this function is

\[
g(u_k) = a_k u_k + b_k. \tag{1.12}
\]

This form is justified by phenomenology and closure theories of turbulence. The parameters \( a_k \), if negative, are to be regarded as damping parameters, and \( b_k \) are random forcing functions. The parameters \( a_k \) and \( b_k \) are calculated from the statistics of a high resolution simulation, with wavenumbers \( k \leq k_* \) resolved. Generally, for reasons to be explained in latter parts of this thesis, it is sufficient to have the resolution of the high resolution simulation corresponding to a maximum wavenumber \( 2k_* \).

In large scale atmospheric problems, the main sources of instability are usually well resolved. This means that the most significant amplitudes of the forcing function, \( f_k \), in Eq. 1.8 are resolved. In oceanic problems, on the other hand, baroclinic instability
is responsible for the formation of mesoscale eddies of size in the order of 50 km, which are hard to resolve in complex models. Hence, the most significant amplitudes of the forcing, $f_k$, in Eq. 1.8 are not resolved in oceanic problems. If baroclinic instability is the only source of instability in the problem, and if $k_*$ is sufficiently small, then in fact the amplitudes $f_k$ that are resolved are relatively insignificant. Hence, in this respect, the oceanic problem is different to the atmospheric problem, and, for reasons to be discussed in the latter parts of thesis, is thus harder to parameterize. It should be noted that the toy model that we have presented here is just for illustrative purposes. In the rest of this thesis, we work with fairly realistic atmospheric and oceanic models, namely, the quasigeostrophic (QG) equations of motion. The outline for the rest of this thesis is as follows.

In Chapter 2, we introduce the QG equations of motion used in this study. We also show how the QG equations may be linearized to predict various atmospheric and oceanic motions such as Rossby waves, stationary topographic waves, and baroclinic instability. In Chapter 3, we look at turbulence, with a focus on QG turbulence. In the first part, we look at the phenomenology of QG turbulence, which leads to the prediction of various atmospheric and oceanic phenomena such as the inverse cascade, zonalization of flows, eddy-induced drag, and barotropization. In the second part, we examine closure theories of turbulence, with an emphasis on the Direct Interaction Approximation (DIA). This will help to justify the form of the subgrid-scale parameterizations used in this thesis.

In Chapter 4, we look at the tendency of barotropic flows over topography to generate multiple equilibrium states, which is thought to be related to the atmospheric phenomenon known as Blocking. A significant portion of this chapter is focussed on establishing the ubiquity of multiple equilibria in flows of various complexities; this includes severely truncated models (STM) and Direct Numerical Simulations (DNS) of the equations of motion. We also explore how to parameterize the non-linear interactions in a STM so that it is in better agreement with DNS.

In Chapter 5, we review the literature on subgrid-scale parameterizations, including advective-diffusive tensor subgrid-scale parameterizations and self-consistently calculated subgrid-scale parameterizations. By the latter we mean parameters calculated from the statistics of high resolution simulations, whether by closure methods or by DNS. We also introduce the methodology for subgrid-scale parameterizations used in this study, which is an extension of that outlined by Frederiksen and Kepert (2006). Finally, we attempt to relate Frederiksen and Kepert’s self-consistent DNS methodology to the advective-diffusive tensor methodology, and show that the latter is deficient in some respects.

In Chapters 6, 7, and 8, we examine subgrid-scale parameterizations for a variety of atmospheric and oceanic QG flows. In Chapter 6, we look at the equivalent layer problem. This is a highly symmetrical problem where the flow statistics in both layers are the same. It enables us to look at some aspects of the subgrid-scale parameterization problem without the complications induced by rotation and different forcing coefficients in the two layers. In Chapter 7, we introduce differential rotation and different forcing coefficients in the two layers. However, the forcing is of a very simple form, being confined to the largest scale only. The inclusion of rotation and different forcing coefficients in the vertical makes this problem closer to realistic atmospheric and oceanic flows.

In Chapter 8, we introduce zonal jets in the problem. This corresponds to mean forcing on a range of large scales, hence complicating the mean-transient interactions in the problem, but also raising the level of realism. The jets in the atmosphere correspond to mid-latitude jet streams, and in the ocean they are exemplified by the Atlantic Circumpolar-
lar Current, which flows around the globe in the vicinity of 60°S. In Chapter 9, we briefly summarize the main results of this thesis and discuss their implications.