Nonlinear Dynamics and Predictability in a Global Circulation Model of the Atmosphere

Dissertation

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I hereby declare, on oath, that I have written the present dissertation by my own and have not used other than the acknowledged resources and aids.

Hamburg, den
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This thesis is dedicated to my brother, my parents and my grandparents. Without their support all this would not have been possible.
Abstract

This study analyses the predictability of a global atmospheric circulation model in a dynamical systems framework. Error growth is evaluated by calculating global Lyapunov exponents for varying model setups in terms of resolution and driving temperature forcing. A clear relation between the forcing, the resolution and predictability is found. The global assessment is expanded toward a localised evaluation as finite time Lyapunov exponents are calculated. The fluctuations of these exponents are almost Gaussian distributed and there exists a non negligible probability to observe negative error growth. This is further assessed by linking error growth to the entropy production of dynamical systems. Negative entropy production is conceptually possible in the framework of the fluctuation theorem and the subsequent analysis shows that the fluctuations in error growth are compatible to the laws of the fluctuation theorem. Due to the approximated relation between error growth and entropy production a final proof remains open.

The spatial distribution of error growth and predictability is supported by traditional methods. Eady growth rate and potential vorticity deviations are compared to error growth patterns and similarities are found for potential vorticity, while the Eady growth rate analysis offers some different results. Different concepts of instability and predictability may be responsible for the observed results.

Blocking as an example for a possibly predictable atmospheric setup is analysed for correlation with error growth. Local Lyapunov exponents and blocking seem to be not correlated on a global level. Since a local assessment is not possible with the current framework, the connection between blocking and predictability in terms of error growth remains open.
Chapter 1

Introduction

1.1 Introduction

In this study an analysis of a global atmospheric circulation model as a dynamical system in terms of predictability is presented. While many models have previously been analysed this way, most famously the Lorenz-63 model (Lorenz, 1963), the analysis was never transferred to complex atmospheric circulation models. This study provides a new point of view on predictability by supplementing established methods to assess models by an analysis from the dynamical systems viewpoint.

Traditionally there are two ways of how models of the atmosphere are evaluated. The most common approach is to analyse specific phenomena like, for instance, blocking, cyclones or Rossby waves and either compare them with observations (Tibaldi and Molteni, 1990) or with an underlying theory of the phenomenon (Frederiksen, 1982). A model is often rated by its ability to reproduce the results demanded by theory or given by observations. These phenomena are related to predictability. Predictability can be defined in several ways, but here it is defined by the growth rate of an error. The higher the growth rate of the error, the lower the predictability.

Other studies have shown that although some of the aforementioned phenomena are very well represented, models can sometimes possess critical flaws. These flaws become apparent if a model is analysed as a physical system that has to obey the fundamental physical laws as a whole. Most models need sophisticated treatments to fulfil for example the energy conservation law (Boville and Bretherton, 2003). These methods advance the understanding of models in terms of physical systems.

Both these methods have helped to understand how models work, where they can represent the actual system that they are modelling and where the differences are. However in this study a third way is presented with the analysis of an atmospheric model as a dynamical system.
1.1.1 Dynamical systems point of view

In this study a global atmospheric circulation model is analysed from a dynamical systems perspective. Almost all physical systems can be seen or reduced to a dynamical system since the theory behind dynamical systems is based upon the dynamics of total differential equations of almost any kind. In this context, error growth and predictability can be seen as synonyms. High predictability denotes low error growth rates and vice versa. It is possible that a system is totally predictable, if errors do not grow or even shrink with time. One aspect of the dynamical systems analysis is that it analyses the model without any regard to the underlying processes that might be responsible for the observed behaviour of the system. Due to that they need to be analysed separately if connections are to be established.

The advantage of the dynamical systems analysis is that effectively one can describe the dynamics of the whole system including the evolution in time with a relatively low number of parameters. As such, comparison to other dynamical systems is very simple. Other dynamical systems could be different models or the same model, but run with a different set of parameters. Due to this, predictability can be assessed for a variety of systems easily.

Unstable processes are responsible for the unpredictable behaviour of the atmosphere. Barotropic and baroclinic instability are the possible unstable processes considered here as they are the only processes simulated by the model used in this study. Baroclinic instability is the focus of this investigation and several ways to describe this process are presented and compared to the dynamical systems analysis. This includes the calculation of potential vorticity deviations and the analysis of their spatial distribution and the evaluation of the results obtained by calculating the Eady growth rate.

1.1.2 Predictability and blocking

Blocking as an atmospheric phenomenon is often connected to predictability due to its uniquely stationary nature both in space and time opposite to baroclinic instability. Consequently, predicting blocking is very important. In this study a first simple approach is considered to investigate whether the dynamical systems analysis can help to detect phases of higher blocking activity without the need to analyse blocking directly. To test this hypothesis, blocking has to be automatically analysed and an efficient approach is presented.

1.2 Scope and contents of this thesis

This thesis aims at investigating predictability and non-linear dynamics in a global circulation model. The sensitivity of predictability on model parameters is investigated. The results are put into the context of various theories explaining the observed behaviour.
1.2 Scope and contents of this thesis

Chapter 2 provides the theoretical background of dynamical systems and describes the global atmospheric model.

Chapter 3 presents the experiment setups and results.

Chapter 4 offers a discussion about the results and puts them into further context.

Chapter 5 contains the summary and conclusions. The main findings of the thesis are highlighted. Additionally, future prospects on the basis of this study are discussed.
Chapter 2

Theory and models

This chapter describes the mathematical theory of dynamical systems and all related aspects like attractors or the Fluctuation Theorem. Furthermore the atmospheric circulation model is introduced and described. Finally, some meteorological indicators for predictability are presented.

2.1 Dynamical systems

This section provides a theoretical background on dynamical systems. It is explained how the atmosphere and an atmospheric model can be viewed as a dynamical system. Furthermore, different classes of dynamical systems are presented and evaluated in terms of applicability for the atmosphere or an atmospheric model. It is defined how to assess predictability in this context and how various system variables are defined.

2.1.1 Basics

A dynamical system is any system that can be written in a form such that

\[ \frac{d\vec{x}}{dt} = f(\vec{x}, K_1, \ldots, K_p, t) \] (2.1)

with \( K_1, \ldots, K_p \) being constant parameters of the system (Rothmann, 2010). The functional \( f \) describes how the state of the system \( \vec{x} \) changes with time. The state vector of the system lies in the phase space of the system, the space which represents all possible states of the system. For the atmosphere the state vector would practically have an infinite length as there are an infinite number of particles to consider and thus the system would have an infinite dimension. However, this is not the case for models of the atmosphere. Due to discretisation the state vector has a length of the number of grid points times the number of model variables. Depending on the resolution and complexity of the model this number can still be very large. For example an atmospheric model with 10 variables and a 2° horizontal resolution with 30 vertical layers would have a state vector with a length of 4.86 million. The phase space is not confined to grid point representations though and could contain
spherical harmonics instead of grid points or position and momentum of all particles in a multi-particle system.

Models in general are discrete in time. A time discrete dynamical system has the form

$$\vec{x}_{n+1} = f(\vec{x}_n, K_1, \ldots, K_p)$$  \hspace{1cm} (2.2)

with $\vec{x}_n$ the state vector at a discrete time $t_n$. If the initial condition ($\vec{x}_0$) is known the solution at any time can be calculated by

$$\vec{x}_n = f \circ f \circ \ldots f(\vec{x}_0, K_1, \ldots, K_p) \equiv f^n(\vec{x}_0, K_1, \ldots, K_p)$$  \hspace{1cm} (2.3)

where the successive functions ($\circ$) are used $n$ times. This is called the flow of the system. It is crucial to note that the equations for a large variety of models are partial differential equations rather than ordinary differential equations, which are necessary for it to be a dynamical system. This problem is resolved, however, if the model is used in discretised form which effectively removes the dependence on spatial coordinates.

A dynamical system is called dissipative if the divergence of the time tendencies ($f$) is negative or

$$\nabla \cdot f = \sum_{j=1}^{N} \frac{\partial f_j}{\partial x_j} < 0$$  \hspace{1cm} (2.4)

In such a case the phase space volume is shrinking. This is obvious if the Gaussian integral theorem is considered:

$$\frac{dV}{dt} = \oint \frac{d\vec{x}}{\partial V} \cdot \vec{n} da = \int_V \nabla \cdot \left( \frac{d\vec{x}}{dt} \right) dV = \int_V \nabla \cdot f dV < 0$$  \hspace{1cm} (2.5)

with $\vec{n}$ the unit vector perpendicular to the surface of the volume $V$.

If the dynamical system is not dissipative ($\nabla \cdot f = 0$), it is called conservative. Most systems and particularly atmospheric models are in the category of dissipative systems. This is because of irreversible processes such as friction which are dissipative and therefore volume shrinking.

2.1.2 Lyapunov exponents

When the phase space volume is reduced to zero in a dissipative dynamical system, the dynamics has reached the so called attractor. A system can have more than one attractor and even attractors of different kinds with their own basin of attraction are possible. The basin of attraction is defined as the region in phase space for which any initial condition ($\vec{x}_0$) collapses onto the attractor. The transition from the starting point onto the attractor is called transient.

The most basic attractor is the fixed point. The fixed point is a point in phase space and represents a stable equilibrium. If the system is in the state of the fixed point it will remain there indefinitely.
2.1 Dynamical systems

Other kinds of attractors include the limit cycle which is a closed trajectory in phase space (the solution of the dynamics is periodic, e.g. free harmonic oscillator) or the torus attractor which can be quasi-periodic.

In this study, however, it is concentrated on strange attractors instead. Strange attractors are defined by aperiodic system behaviour and sensitivity of initial conditions even when the initial point is already on the attractor. This behaviour is the result of the instability of the trajectory on the attractor which means that two adjacent (infinitesimal distance) trajectories diverge exponentially until the distance grows too large and non-linear effects become important. The most famous example of a strange attractor is the attractor of the Lorenz-63 model (Lorenz, 1963). A representation of this attractor is given in figure 2.1 which shows the typical ‘butterfly’ motive that has become widely known.

One method to characterise the stability of trajectories in phase space are the so called characteristic or Lyapunov exponents (Eckmann and Ruelle, 1985). A system is generally considered unstable or chaotic if nearby trajectories on the attractor diverge. The separation of two initially infinitesimally close trajectories \( \vec{x} \) and \( \vec{x}' \) after \( n \) time steps (or after time \( n \) for a continuous system) is

\[
\vec{x}_n - \vec{x}'_n = f^n(x_0) - f^n(x'_0)
\]  

and it has been shown (Eckmann and Ruelle, 1985) that this difference grows as

\[
\lambda = \lim_{n \to \infty} \log |D_{x_0}f^n \delta x(0)|
\]  

with \( \delta x(0) \) the initial distance or perturbation and \( D_x f = (\partial f_i / \partial x_j) \) evaluated
at $x = x_0$. For almost all choices of $\delta x(0)$ $\lambda = \lambda_1$ is the largest Lyapunov exponent. This exponent describes the mean growth rate of perturbations into the most unstable direction of phase space. If the initial perturbation has no component into the most unstable direction, the result will instead be a smaller exponent. Oseledecs theorem (Oseledec, 1968; Mané, 1983) states that there exist exponents $\lambda_1 > \lambda_2 > \ldots > \lambda_k$ and the corresponding Lyapunov subspaces $F_i$ with $F_k \subset F_{k-1} \subset \ldots \subset F_2 \subset F_1 = \mathbb{R}^k$ and $\mathbb{R}^k$ the space for which $\vec{x}$ is defined. If now (2.6) is used with an initial distance that lies only in a certain Lyapunov subspace $F_i$, the corresponding Lyapunov exponent $\lambda_i$ can be found.

For any Lyapunov subspace there exists an orthogonal basis of Lyapunov vectors such that $F_i = v_i \oplus v_{i-1} \oplus \ldots \oplus v_k$. It is evident that the vector $v_1$ points into the most unstable direction of phase space and corresponds to an optimal perturbation in the sense that it grows fastest. Furthermore the relation

$$\sum_{i=1}^{k} \lambda_i \leq 0 \quad (2.8)$$

must hold for all systems. For dissipative systems the sum has to be strictly smaller than zero.

There are several methods for the computation of these Lyapunov vectors and exponents. The standard method to compute the Lyapunov vectors and exponents involves an iterative process. At first an arbitrary orthonormal base of the system must be chosen. These vectors are then integrated along the model trajectory for some time interval $\tau$. Subsequently the resulting vectors are orthogonalized and normalized. The long time mean of the logarithm of the respective norms converges towards the Lyapunov exponent, while the vectors will evolve into the corresponding Lyapunov vectors.

A comparison of this technique with other methods has been given by Ramasubramanian and Sriram (2000). Furthermore, instead of these Lyapunov vectors covariant Lyapunov vectors have become increasingly popular to use (Ginelli et al., 2007) (Kuptsov and Parlitz, 2012). Covariant Lyapunov vectors are no longer orthogonal but are invariant under time reversal. In this study the Lyapunov spectrum is not computed directly due to the huge computational demand of the orthogonalisation. Instead another method is proposed that further classifies the attractor of the system and relates it to the Lyapunov exponents.

### 2.1.3 Attractor dimension

The focus of this study concentrates on the correlation dimension $D_2$ and the Lyapunov Dimension via the Kaplan-Yorke conjecture.

For the time discrete case the general attractor dimension or Renyi Dimension $D_q$ is defined as

$$D_q = \lim_{\epsilon \to 0} \frac{1}{1 - q} \log \frac{\{\sum_j [(\mu(C_j))]^q\}}{\ln (1/\epsilon)} \quad (2.9)$$
where $\mu(C_j)$ represents the number of phase space points within $\epsilon$-cubes (or spheres) which cover the whole attractor. While this general measure is not very informative in the scope of this study, it is noteworthy that for the case $q = 1$ this is called the information dimension and has the form

$$D_1 = \lim_{\epsilon \to 0} \frac{\sum_j \mu(C_j) \log \mu(C_j)}{\log(\epsilon)}$$

for the limit $q \to 1$ using L’Hôpital’s rule, while for $q=2$ it is called the correlation dimension. The information dimension is not calculated in this study directly, but it is the necessary link between the correlation dimension and the Lyapunov dimension due to the condition $D_1 \geq D_2$ (Grassberger, 1983). The correlation dimension ($q = 2$) can be calculated with a simple algorithm (Grassberger and Procaccia, 1983). First

$$S(\epsilon) = \sum_{i \neq j} u(\epsilon - |x_i - x_j|)$$

is defined. Here $u(y)$ is a step function such that $u = 1$ for $y \geq 0$ and $u = 0$ for $y < 0$. This means $S$ counts all trajectory points $x_j$ that are closer to $x_i$ than $\epsilon$ for all $x$ along the trajectory. Then $\log S(\epsilon)$ is plotted against $\log \epsilon$ and $D_2$ is estimated by the slope of a linear fit to the data. Therefore the correlation dimension can be seen as a geometric measure of the attractor. This is true for the information dimension albeit with a different metric. It has to be noted here that the points $x_i$ and $x_j$ must be independent from each other or the probability to observe $x_j$ in the $\epsilon$-sphere around $x_i$ must be equal for all $x, i, j$.

The Lyapunov dimension is defined as

$$D_L = k + \frac{\sum_{i=1}^{k} \lambda_i}{|\lambda_{k+1}|}$$

such that $k$ is the largest value where $\sum_{i=1}^{k} \lambda_i > 0$. The Lyapunov dimension is now linked to the information dimension through the Kaplan-Yorke conjecture that states

$$D_1 = D_L$$

for almost all systems (Kaplan and Yorke, 1979). This conjecture links the dynamical measure of the Lyapunov dimension to the geometric measure of the information dimension. This information dimension meanwhile is linked to the correlation dimension. Thus it is possible to get at least limited information about the dynamical aspect of the system by calculating the correlation dimension.

### 2.1.4 Error growth, entropy and the Fluctuation Theorem

Besides global dynamical measures such as Lyapunov exponents that do not depend on the current state of the system, it is possible to define local measures. These are called local Lyapunov exponents and are defined similarly to Lyapunov exponents,
but with two crucial differences. First, they are defined for a finite time interval, so instead of \( n \to \infty \) as in (2.7) \( n \) is a small number. Secondly, the initial perturbation has to point into the corresponding direction of phase space at the beginning already to ensure that the correct exponent is calculated. This is very difficult for the whole spectrum, but in the experiments here it is possible to get at least a very good representation of the most unstable direction along a trajectory. This is due to the experimental setup and is described in chapter 3.1.

The local measures are connected to ensemble forecasts produced by numerical weather forecast models. In most models the initial perturbations are pointing roughly into the most unstable direction (first Lyapunov vector) guaranteeing fast growth of errors. However, it has been shown by Keller et al. (2010) and others that perturbations pointing into other unstable directions are desirable for ensemble forecasts as well. Therefore, orthonormalisation methods are used to eliminate the most unstable direction(s) from the initial perturbations. Those are similar orthonormalisation methods that are used to calculate the Lyapunov spectrum as shown in section 2.1.2.

According to the arguments mentioned above it is impractical to calculate the whole spectrum of Lyapunov exponents locally because a high number of calculations has to be performed to cover most of the attractor. Instead the local largest Lyapunov exponent (\( \hat{\lambda} \)) is calculated.

\[
\hat{\lambda}(t, \tau) = \frac{1}{\tau} \log \frac{d(t, \tau)}{d_0} \tag{2.14}
\]

Here \( \tau \) is the time interval that has passed between the measurement of the initial perturbation \( d_0 = |x(t) - x'(t)| \) and the resulting perturbation \( d(t, \tau) = |x(t + \tau) - x'(t + \tau)| \). The dependence on the time \( t \) has to be noted. The local largest Lyapunov exponent can have different values depending on the current position on the attractor which is measured as the time elapsed since the experiment started. This is an arbitrary time measure and will not affect the results. The local largest Lyapunov exponent describes the instantaneous growth rate of the perturbation \( d_0 \).

If the perturbation points into the most unstable direction in phase space the time mean value of the local largest Lyapunov exponent is the largest Lyapunov exponent \( \lambda_1 \).

In addition to the Lyapunov exponents the entropy of a dynamical system can be defined as a measure to characterise the system. This entropy is called the Kolmogorv-Sinai entropy or metric entropy, and using Pesins formalism (Pesin, 1977) takes the form

\[
h_\mu = \int_M \Sigma(x) d\mu(x) \tag{2.15}
\]

where \( M \) is the whole phase space in the context of this study which can be replaced by a sum over the trajectory for \( t \to \infty \) due to ergodicity and \( \mu \) an invariant measure in \( M \). Furthermore, \( \Sigma(x) \) is the sum of all positive Lyapunov exponents. Benettin et al. (1976) have suggested an entropy-like quantity which is not the sum of all positive Lyapunov exponents but simply the largest Lyapunov exponent. Through
this one can deduce that the local largest Lyapunov exponent is a measure for the
growth (or increase) of the entropy-like quantity.

Entropy growth or entropy production is the main point of interest in the context
of the Fluctuation Theorem. However, there is not a single Fluctuation Theorem
that is applicable to all systems but rather a whole family of Fluctuation Theorems.
The first formulation of the Fluctuation Theorem was given by Evans and Searles
(1994) for thermodynamic systems in or near equilibrium. Gallavotti and Cohen
(1995) introduced a formulation of the Fluctuation Theorem for dynamical systems,
and subsequently many formulations (Evans and Searles, 2002) for various systems
and dynamics haven been proposed. Furthermore, there are two distinct classes of
Fluctuation Theorems, one being steady state fluctuation theorems which are only
valid in the limit for $t \to \infty$, and transient Fluctuation Theorems which are valid
for all times $t$. In this study it is investigated if the observed behaviour of the local
largest Lyapunov exponent can be explained by a steady state Fluctuation Theorem.

The fluctuation theorems generally state that for a finite time $\tau$ and for a low
number of degrees of freedom the quotient of the probability to observe an entropy
production $\Sigma = +a$ and the probability to observe the negative entropy production
$\Sigma = -a$ grows exponentially with the length of the observation interval $\tau$. They
have the general form

$$\frac{P(\Sigma = +a)}{P(\Sigma = -a)} = \exp(a\tau \bar{\Sigma})$$

with $\bar{\Sigma}$ the mean entropy production rate.

These fluctuations have been observed for several systems, for example thermo-
dynamic (Bustamante et al., 2005) and dynamical (Maes and Netocny, 2008). This
study suggests that fluctuations in accordance with the Fluctuation Theorem can
be observed in an atmospheric circulation model. No rigorous proof of this is pre-
sented as the entropy production $\Sigma$ is not computed directly but approximated by
the entropy-like quantity. The increase of this quantity is identified as the largest
local Lyapunov exponent which is accessible for long time series.

2.2 The Portable University Model of the Atmosphere

The dynamical system investigated in this study is a global atmospheric circulation
model. In this section this model which represents a dynamical core model is in-
troduced. The dynamics of the model are explained as well as its relation to more
complex climate or weather forecast models. Furthermore, the versions used are
presented and the differences are highlighted. This section is mainly based on the
PUMA Users Guide (Fraedrich et al., 2011) and references therein.

2.2.1 Model description

The global atmospheric circulation model used in this study is the Portable Univer-
sity Model of the Atmosphere or PUMA for short. PUMA is a global circulation
model which solves the primitive equations on a rotating sphere. The primitive equations are an approximated form of the Navier-Stokes equations for the atmosphere. It is assumed that the atmosphere is hydrostatic

$$\frac{\partial p}{\partial z} = -\rho g$$

(2.17)

Here $p$ is the atmospheric pressure, $z$ is the vertical coordinate, $\rho$ is the density of the air and $g$ is the acceleration due to gravity which in PUMA is fixed to $9.81 \text{m/s}^2$. Currently models solving the primitive equations are still widely used in climate sciences (e.g. ECHAM6 (Stevens et al., 2013)) while currently used weather forecast models employ the non-hydrostatic equations. The main reason to use PUMA is because it is a dynamical core of more complex models. This means that the fundamental dynamical equations are the same in all weather and climate models as long as they are hydrostatic. They may be implemented differently on the numerical level, however. Furthermore, PUMA is able to simulate all dynamical processes (or adiabatic processes) in the atmosphere, but needs a fraction of the computing power compared to more complex models. A comparative graph between PUMA and the more complex ECHAM model is given in figure 2.2. Another advantage is that dynamical core models in general are easier to validate which has been done in the 2012 Dynamical Core Intercomparison Project\(^1\). Another advantage that is crucial for this study is the high degree of flexibility. Almost all parameters of the model (like for instance friction) can be changed through a namelist file, so it is very simple to perform sensitivity experiments. Horizontal and vertical resolution can be changed as well as the time step. All these features combined make it an excellent tool to study an atmospheric circulation model from a dynamical systems perspective. While non-hydrostatic models are better suited for weather prediction due to their higher accuracy in forecasts, they tend to be too computationally expensive to be used as modules for climate models. In comparison to the atmospheric component of climate models like for instance ECHAM the PUMA model could be called simple. There is no water vapour present and consequently no clouds, no rain and no evaporation or latent heat flux. Other processes like radiative transport are crudely parametrised. However, in the context of this study this is not even a disadvantage since discontinuous processes like precipitation cannot be assessed as a dynamical system. The PUMA model does not need to be limited in its dynamics due to the dynamical systems analysis.

2.2.2 Model equations

As stated in the previous section, PUMA is based on the primitive equations. These equations are based on the fundamental physical principles of conservation of momentum, energy and mass. PUMA uses spherical coordinates and the sigma system in the vertical direction. The sigma coordinate is a pressure coordinate defined as $\sigma = p/p_s$ with the surface pressure $p_s$. All variables are dimensionless through

\(^1\)http://earthsystemcog.org/projects/dcmip-2012/
appropriate scaling. Divergence and Vorticity are scaled by the Earth rotation $\Omega$, pressure is scaled by the mean sea level pressure which is prescribed as 101 100 Pa, temperature is scaled by $(a^2\Omega^2)/R$ with $a$ the planet radius and $R$ the gas constant.

If orography is used it is scaled by $(a^2\Omega^2)/g$.

Conservation of momentum is expressed by the vorticity equation

$$\frac{\partial (\zeta + f)}{\partial t} = \frac{1}{(1 - \mu^2)} \frac{\partial F_v}{\partial \lambda} - \frac{\partial F_u}{\partial \mu} + P \zeta$$

(2.18)

and the divergence equation

$$\frac{\partial D}{\partial t} = \frac{1}{(1 - \mu^2)} \frac{\partial F_v}{\partial \lambda} + \frac{\partial F_u}{\partial \mu} - \nabla^2 \left( \frac{U^2 + V^2}{2(1 - \mu^2)} + \Phi + T_0 \ln p_s \right) + P_D$$

(2.19)
coupled with the hydrostatic approximation

\[ \frac{\partial \Phi}{\partial \ln \sigma} = -T \]  

(2.20)

Here \( U = u \cos \phi \), \( V = v \sin \phi \) and \( \mu = \sin \phi \) with \( u \) the zonal wind velocity, \( v \) the meridional wind velocity and \( \phi \) the latitude is used. Furthermore, the abbreviations

\[ F_u = V (\zeta + f) - \sigma \frac{\partial U}{\partial \sigma} - T' \frac{\partial \ln p_s}{\partial \lambda} \]

and

\[ F_v = -U (\zeta + f) - \sigma \frac{\partial V}{\partial \sigma} - T' (1 - \mu^2) \frac{\partial \ln p_s}{\partial \mu} \]

are used. The relative vorticity is denoted by \( \zeta \), the divergence by \( D \), \( T \) is the temperature, \( T_0 \) is the reference temperature, \( T' \) is \( T - T_0 \), \( \lambda \) is the latitude, \( \Phi \) is the geopotential and \( \dot{\sigma} \) is the vertical velocity in the sigma system. \( P_\zeta \) and \( P_D \) are parametrisations for friction and hyperdiffusion.

Conservation of mass is expressed by the continuity equation

\[ \frac{\partial \ln p_s}{\partial t} = - \int_0^1 A d\sigma \]  

(2.21)

with \( A = D + \vec{V} \cdot \nabla \ln p_s \) and \( \vec{V} \) the horizontal velocity with components \( U \) and \( V \).

Conservation of energy is given by the first law of thermodynamics in the temperature equation

\[ \frac{\partial T'}{\partial t} = - \frac{1}{(1 - \mu^2)} \frac{\partial (UT')}{\partial \lambda} - \frac{\partial (VT')}{\partial \mu} + DT' - \dot{\sigma} \frac{\partial T}{\partial \sigma} + \kappa \frac{T}{p} \omega + \frac{J}{c_p} + P_T \]  

(2.22)

Here \( \kappa \) is the adiabatic coefficient \( R/c_p \) and \( c_p \) the heat capacity of dry air at constant pressure respectively, \( \omega \) is the vertical velocity in the \( p \)-system and \( J \) is the diabatic heating rate.

The model is driven by the diabatic heating term which together with the parametrisation term is defined as

\[ \frac{J}{c_p} + P_T = \frac{T_R - T}{\tau_R} + H_T \]  

(2.23)

\( H_T \) is the hyperdiffusion of temperature and \( T_R \) is the restoration temperature field, not to be confused with \( T_0 \) which is a global constant.

The restoration temperature \( T_R \) is used in this study with two different setups. It is used as the driver of the model and describes the temperature profile of the atmosphere in radiative equilibrium. The usual setup of PUMA uses the following restoration temperature

\[ T_R(\phi, \sigma) = T_R(\sigma) + f(\sigma) T_R(\phi) \]  

(2.24)
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\[ T_R(\sigma) = (T_R)_{tp} + \sqrt{\left[ \frac{L}{2} (z_{tp} - z(\sigma)) \right]^2 + S^2 + \frac{L}{2} (z_{tp} - z(\sigma))} \] (2.25)

the vertical part and

\[ T_R(\phi) = (\Delta T_R)_{NS} \frac{\sin \phi}{2} - (\Delta T_R)_{EP} \left( \sin^2 \phi - \frac{1}{3} \right) \] (2.26)

the horizontal part. Here \( z \) is the geometric height, \( z_{tp} \) the height of the tropopause, \( L \) is the vertical restoration temperature gradient and \( (T_R)_{tp} \) is the temperature at the tropopause which is calculated by the parameter \( (T_R)_{grd} \) and the vertical gradient \( L \) as well as the chosen tropopause height by \( (T_R)_{tp} = (T_R)_{grd} - L z_{tp} \). The parameter \( S \) provides a smoothing of the vertical profile at the tropopause. The horizontal part of the restoration temperature is further smoothed by \( f(\sigma) \) which is 0 for \( \sigma < \sigma_{tp} \). For \( \sigma \geq \sigma_{tp} \) \( f(\sigma) \) is defined by

\[ f(\sigma) = \sin \left( \frac{\pi}{2} \left( \frac{\sigma - \sigma_{tp}}{1 - \sigma_{tp}} \right) \right) \] (2.27)

The tropopause height in sigma coordinates is calculated by

\[ \sigma_{tp} = \left( \frac{(T_R)_{tp}}{(T_R)_{grd}} \right)^{g/LR} \] (2.28)

In the horizontal part of the restoration temperature, \( (\Delta T_R)_{EP} \) is the temperature gradient between the poles and the equator which is a constant for any given experiment. The expression \( (\Delta T_R)_{NS} \) describes a temperature asymmetry between the hemispheres which is used for an annual cycle. This is not further explained here since an annual cycle is not used in this study. Consequently \( (\Delta T_R)_{NS} \) is always zero.

In (2.23) \( \tau_R \) is the time scale which determines how fast the model temperature is forced towards the restoration temperature profile. This parameter is usually dependant on height but in almost all experiments here this is constant throughout the whole atmosphere.

In addition to this standard profile of the relaxation temperature, the Held-Suarez (Held and Suarez, 1994) setup is used. This setup has the form

\[ T_R = \max \left\{ 200 K, \left[ 315 K - (\Delta T)_y \sin^2 \phi - (\Delta \theta)_z \log \left( \frac{P}{P_0} \right) \cos^2 \phi \right] \left( \frac{P}{P_0} \right)^{\kappa} \right\} \] (2.29)

The Held-Suarez setup features larger temperature gradients especially in the mid-troposphere. Values near the surface are almost identical. This setup is used for a special case where the standard setup failed to deliver meaningful results with respect to blocking activity. The details are described in the results section.
2.2.3 Numerics

In PUMA the prognostic variables \((\zeta, D, T, p_s)\) and some supporting fields like for instance orography are transformed into the spectral domain. In the spectral domain all linear computations are executed, while the non-linear parts of the model are computed in the grid point domain. This means that the model variables are defined by a series of spherical harmonics. The spectral representation of any model variable \(B\) is given by

\[
B(\lambda, \mu, t) = \sum_\gamma B_\gamma(t) Y_\gamma(\lambda, \mu)
\]

(2.30)

where \(Y_\gamma\) are the spherical harmonics and \(B_\gamma\) the corresponding complex amplitudes with \(\gamma = (n, m)\) the spectral modes with \(n\) the total wavenumber and \(m\) the zonal wavenumber. Due to the triangular truncation the relation \(|m| \leq n\) has to be satisfied. The grid is an alternating Gaussian grid. At any given time step the model variables have to be transformed from the grid point domain into the spectral domain to perform the linear computations. This is done by a series of Legendre and Fourier transformations optimised for fastest computation. The model is integrated using a leap-frog time step. The two time levels are linked by a Robert-Asselin time filter to prevent decoupling of the time levels.

The vertical coordinate is discretised by equidistant \(\sigma\)-levels as described in section 2.2.1. The model variables are calculated at the full levels with the boundary conditions that the vertical velocity \(\dot{\sigma}\) vanishes at the lower \((\sigma = 1)\) and the upper \((\sigma = 0)\) boundaries. An example for the vertical discretisation with 5 levels is given in figure 2.3. Vertical advection is implemented as

\[
(\overline{\dot{\sigma} \delta_{\sigma} B_\sigma})_k = \frac{1}{2} \left( \dot{\sigma}_{k+\frac{1}{2}} \frac{B_{k+1} - B_k}{\Delta \sigma} + \dot{\sigma}_{k-\frac{1}{2}} \frac{B_k - B_{k-1}}{\Delta \sigma} \right)
\]

(2.31)

for any model level \(k\).

Due to the spectral representation the model resolution is given in spectral modes rather than grid points. A resolution T21 for example has a maximal total wavenumber of 21. The T stands for the type of truncation and in this case means the triangular truncation. Table 3.2 is a reference which shows how the grid point resolution is related to the spectral resolution.

2.2.4 Parametrisations

The parametrisation for the diabatic heating is given in section 2.2.2 and is the driver of the model. It replaces radiation and functions as the driver of the model. Without this process the circulation would slowly come to a halt due to dissipation by friction.

The friction parametrisation emulates dissipative processes like surface drag and momentum transport through turbulence in the boundary layer. The approach used in PUMA is a linear Rayleigh friction. The relative vorticity \(\zeta\) and the divergence
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<table>
<thead>
<tr>
<th>Level</th>
<th>$\sigma$</th>
<th>Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.0</td>
<td>$p = 0$, $\dot{\sigma} = 0$</td>
</tr>
<tr>
<td>1.0</td>
<td>0.1</td>
<td>$\zeta$, $D$, $T'$</td>
</tr>
<tr>
<td>1.5</td>
<td>0.2</td>
<td>$\dot{\sigma}$</td>
</tr>
<tr>
<td>2.0</td>
<td>0.3</td>
<td>$\zeta$, $D$, $T'$</td>
</tr>
<tr>
<td>2.5</td>
<td>0.4</td>
<td>$\dot{\sigma}$</td>
</tr>
<tr>
<td>3.0</td>
<td>0.5</td>
<td>$\zeta$, $D$, $T'$</td>
</tr>
<tr>
<td>3.5</td>
<td>0.6</td>
<td>$\dot{\sigma}$</td>
</tr>
<tr>
<td>4.0</td>
<td>0.7</td>
<td>$\zeta$, $D$, $T'$</td>
</tr>
<tr>
<td>4.5</td>
<td>0.8</td>
<td>$\dot{\sigma}$</td>
</tr>
<tr>
<td>5.0</td>
<td>0.9</td>
<td>$\zeta$, $D$, $T'$</td>
</tr>
<tr>
<td>5.5</td>
<td>1.0</td>
<td>$p = p_s$, $\dot{\sigma} = 0$</td>
</tr>
</tbody>
</table>

$D$ are damped towards the state of rest ($\zeta, D = 0$) with a prescribed time scale $\tau_F$. This parametrisation is used in (2.18) and (2.19) as

$$P_\zeta = \frac{\zeta}{\tau_F} + H_\zeta$$

(2.32)

$$P_D = \frac{D}{\tau_F} + H_D$$

(2.33)

The time scale $\tau_F$ is usually set to $\infty$ for the free atmosphere which indicates no friction. In the lower atmosphere the time scale for $\tau_F$ is usually in the order of one day. The exact setup depends on the experiment.

The terms $H_\zeta$, $H_D$ and $H_T$ in (2.32), (2.33) and (2.23) describe the hyperdiffusion in the model. The hyperdiffusion parametrisation is necessary to incorporate effects of horizontal mixing and the energy cascade towards small scales and its dissipation at the Kolmogorov scale. Hyperdiffusion is implemented in the form

$$H_\gamma = -\frac{1}{\tau_H} \left( \frac{n(n+1)}{n_T(n_T+1)} \right)^h B_\gamma(t) Y_\gamma(\lambda, \mu)$$

(2.34)

with $B$ being any model variable and $n_T$ the resolution-dependant highest total wavenumber. This implementation intensely damps the shortest waves ($n = n_T$), while the global means ($n=0$) are not dampened. The exponent $h$ which is set to the default value of 4 for all experiments here further restricts the dampening to larger wavenumbers. The hyperdiffusion time scale is set to its standard value of $\tau_H = 1/4d$ for all experiments.
2.2.5 Model versions

PUMA is part of a model suite that includes the Shallow Ocean Model (SOM), the Shallow Atmosphere Model (SAM) and the Planet Simulator. The version of the model suite used for this study is version 16. However, certain experiments were done with slightly more advanced versions (16.19 for example). These versions did not change the code in PUMA in critical places but mostly in the Planet Simulator model and the overarching model starter program. The most notable change for PUMA compared to previous versions is the possibility to run two instances of the model parallel with the option to exchange information between the instances. The most obvious application for this mode of operation are synchronisation experiments where the two models are coupled to one another by varying degrees to find out how strong the coupling has to be before full synchronisation is achieved. This mode of operation is used for the calculation of Lyapunov exponents.

2.3 Dynamical systems analysis of PUMA

This section describes the major subroutines that are added to the PUMA model in order to perform the dynamical systems analysis. The change of the output is a practical decision. The Lyapunov subroutine, however, is the major subroutine where error growth and the Lyapunov exponent are calculated.

2.3.1 The Lyapunov Exponents

The general setup involves two instances of the PUMA model that are executed in a parallel fashion. But rather than using several CPU cores to speed up the computation, each of the two models is run on one core and communicates with the other model instance through the message passing interface (MPI). At any time step after the computations in the spectral domain are complete, the Lyapunov subroutine is called. But only every half-day or day (depending on the experiment) the subroutine is executed further. This subroutine is executed for one of the model instances, the other model is unaffected. A description of all important steps of the subroutine follows.

1. The difference fields between the two model instances is calculated directly with the built-in functions of the message passing interface. They are transformed from spectral to the grid point domain for computation.

2. The euclidean distance of all variables at all grid points between the two model instances is calculated. This distance is weighted with the Gaussian weights to consider the larger distance between grid points near the equator compared to the polar regions. The sum of these weighted distances is the total distance $d$ between the two model instances. This is done at the start of an experiment (time step zero) to calculate the initial distance $d_0$ that is then used for the rest of the model run.

3. The quotient $d/d_0$ is calculated and from this the local largest Lyapunov exponent as described in (2.7). These values are stored in a separate output file.
4. The distance $d$ is rescaled to the distance $d_0$. This is done by adding the scaled distance which is calculated by multiplying all difference fields with $d_0/d$. This scaled difference is added to the fields of the unaffected model instance to generate the new perturbed model run. It has to be stressed here that this method merely changes the amplitudes of the difference but not its pattern. From the dynamical systems standpoint only the length of the difference vector is affected, not its direction in phase space.

5. Eady growth rate and potential vorticity are calculated. The rescaling has no effect on these computations since the changes to the overall model variables are negligible due to the smallness of the distance $d$.

6. All model variables are transformed back to the spectral domain and the normal PUMA time step routine continues.

Steps three through six are not executed for the first time step where the initial separation of the trajectories is calculated. The source code of this subroutine is available in the second part of the appendix.

2.3.2 Direct output

All new variables and fields that are added through the Lyapunov subroutine are stored in text format (ASCII). The advantage is that the values can be checked immediately even during the model run and it is very easy to read these files into further post-processing programs such as MATLAB. The disadvantage is that since these files are not compressed they take up to 8 times more storage space compared to the same output in the standard PUMA format. Overall the text format turned out to be more practical.

All other output is generated through the PUMA post-processor with its built-in interpolation methods to generate derived fields such as geopotential height not only on model levels but on pressure levels as well.

2.4 Blocking, Eady growth rate and potential vorticity

PUMA is used as a tool to investigate meteorological phenomenons and concepts which are related to predictability. The results are subsequently compared to find similarities and differences. Blocking is one of the few synoptic-scale weather patterns that is long lasting and nearly stationary. It is thus possible that blocking and less chaotic regimes of the global circulation coincide.

The Eady growth rate is often used to identify regions with strong potential for cyclogenesis and potential vorticity is another indicator for the same process. In the scope of this study it is discussed which of these indicators is similar to the error growth pattern obtained through the dynamical systems analysis.

While the Eady growth rate and potential vorticity are calculated within separate subroutines of the model, blocking is analysed through the standard output of the
Model using the post-processor, a program which calculates derived fields such as the geopotential height from the existing model data.

2.4.1 Blocking

Blocking anticyclones are among the most impactful weather patterns in the mid-latitudes. Through their spatial stationarity and longevity they can influence the atmospheric conditions in the affected regions for whole seasons. Extreme events are often linked to blocking with the Russian heat wave of 2010 being a very prominent example (Matsueda, 2011).

Despite the importance of blocking, predicting the onset and decay is still a major challenge for weather forecast models (Watson and Colucci, 2002). There are several different ways to automatically detect blocking. The traditional method is presented here as it is used as a basis or reference in most related studies (Barriopedro et al., 2006).

2.4.2 Blocking detection

Automated blocking detection is a necessary tool to analyse long time series for blocking. There are, however, different methods to detect blocking. Most of them are based on the phenomenological description of blocking given by Rex (1950). According to Rex there are five criteria the atmospheric flow has to fulfil in order to be blocked:

1. The westerly jet has to be split up into two parts.
2. Both parts of the jet have to transport meaningful amounts of mass.
3. The zonal extent must be larger than $45^\circ$.
4. At the point of the jet split the flow has to change from zonal to meridional.
5. The configuration has to remain stable for 10 days.

Current detection algorithms are often less strict especially concerning points three and five, due to the different methods for the detection.

The Tibaldi-Molteni method

One particular method that is often used (Kreienkamp et al., 2010) is the Tibaldi-Molteni method (Tibaldi and Molteni, 1990). Even though this method is as well based on the description by Rex (1950) it is less strict. The method is based on analysing the geopotential height field at the 500 hPa level in the northern Hemisphere but it can be used on the southern hemisphere as well with the respective values for the calculation of the gradients. There are two geopotential height gradients defined, a northern one

$$GHGN = \frac{Z(\phi_N) - Z(\phi_0)}{\phi_n - \phi_0}$$

(2.35)
and a southern gradient

\[ GHGS = \frac{Z(\phi_0) - Z(\phi_S)}{\phi_0 - \phi_S} \] (2.36)

with

\[
\begin{align*}
\phi_N &= 78.75^\circ + \Delta \\
\phi_0 &= 60^\circ + \Delta \\
\phi_S &= 41.25^\circ + \Delta
\end{align*}
\]

and

\[ \Delta = -3.75^\circ, 0, 3.75^\circ. \]

Here \( Z \) denotes the geopotential height at the respective latitudes \( \phi \). For every longitude these gradients are calculated and blocking is registered if the following conditions are true:

\[
\begin{align*}
GHGS &= 0 \\
GHGN &= -10 \frac{m}{\text{lat}}
\end{align*}
\] (2.37)

This means that the geopotential height profile along a longitude must have a local maximum near the \( \phi_0 \) region.

**The modified Tibaldi-Molteni method**

While the Tibaldi-Molteni method is able to detect blocking cases it has the disadvantage of falsely detecting similar atmospheric setups that are not blocking. Most prominent are cut-off low pressure systems. These systems produce the same geopotential height profile as blocking. Furthermore, the Tibaldi-Molteni method does not check if the detected blocking regions are large enough, since the longitudes are considered separately. Finally is is not checked whether the blocked regions are persistent as demanded by Rex’s criteria.

To overcome these problems a modified blocking index has been proposed (Schalge et al., 2011). It uses the same calculations for the geopotential height gradients, but with a small difference concerning the latitudes. Instead of the original latitudes it uses

\[
\begin{align*}
\phi_N &= 78.75^\circ + \Delta' \\
\phi_0 &= 60^\circ + \Delta \\
\phi_S &= 41.25^\circ + \Delta''
\end{align*}
\]

\[ \Delta, \Delta', \Delta'' = [-3.75^\circ, \ldots, 3.75^\circ] \]

with the difference that instead of constant \( \Delta \)-value for all three latitudes, different values are possible. Furthermore the three fixed latitudes are replaced by a band of latitudes with the actual number of latitudes being dependant on the resolution
of the data. This change is introduced to account for high-resolution data. The initial detection yields slightly more blocking with this setup due to additional combinations of possible latitudes. After this step of the detection, blocked regions that are less than 10° separated are merged. This is done due to failure of this detection method near the centre of blocked regions when the first of the conditions \((GHGS > 0)\) is not fulfilled. The disadvantages of the Tibaldi-Molteni method, the false detection of cut-off low pressure systems and the missing checks for spatial and temporal extent are not solved by this change and therefore three filters are introduced.

The quantile filter is designed to eliminate the false detection of cut-off lows. It is a simple additional condition that is added to the conditions of (2.37) and demands that the geopotential height in the centre region must be higher than a specified quantile \(Q\) for the respective latitude and time step.

\[
Z(\lambda, \phi_0) - Z_Q(\lambda, \phi_0) > 0 \quad (2.38)
\]

All blocked regions that are detected by the conditions above but do not meet this requirement are no longer considered.

The extent filter introduces spatial dependence. As proposed by Rex a blocking high has to have a certain longitudinal extent. The extent filter checks if blocked longitudes are connected to other blocked longitudes and subsequently disregards all regions without a specified minimum width.

The persistence filter deals with the problem that blocking is a long-lived phenomenon. At every time step the blocked regions are tracked in the sense that it is investigated whether this blocked region has existed before. The total time of occurrence for every blocking event is calculated and all events that do not meet the minimum required lifetime are eliminated. A blocked region at a specific time step is considered to be part of a blocking episode if at least one longitude that is blocked is blocked as well at a previous or a following time step.

If all filters are combined the resulting detections correspond to synoptic scale blocking events with much higher probability. It has been shown (Schalge et al., 2011) that although the overall blocking frequency is considerably reduced, the actual distribution of blocking is not affected severely.

### 2.4.3 Eady growth rate

Most of the variability and therefore most of the error growth in the mid latitudes is thought to be caused by baroclinic instability. Baroclinic instability is one of the major features of the atmospheric dynamics that is fully resolved in PUMA. It therefore stands to reason that regions with high values of error growth and regions of high baroclinicity coincide.

A commonly used measure for baroclinicity is the maximum Eady growth rate. It is defined as (Vallis, 2006)

\[
E = 0.31 \frac{f}{N} \frac{\partial |\vec{\nu}|}{\partial z} \quad (2.39)
\]
2.4 Blocking, Eady growth rate and potential vorticity

with the Brundt-Vaissala frequency

\[ N^2 = \frac{g}{\Theta} \frac{\partial \Theta}{\partial z} \quad (2.40) \]

determining the stability of the air column. These two parts of the Eady growth rate combine local (in-)stability (Brundt-Vaissala Frequency) and large scale atmospheric conditions. The large scale conditions are represented by \( \partial |\vec{v}|/\partial z \) which outside of the frictional boundary layer is the thermal wind. As such the Eady growth rate is zero for barotropic setups and indicates regions with high baroclinicity. However, the local part can become important as these large scale baroclinic setups are dampened by stable stratification. The general factor 0.31 is a theoretical value of the maximum growth rate of the most unstable setup (Eady, 1949). This Eady growth rate has since been used to analyse baroclinic instability in observations (Simmonds and Lim, 2009) as well as model results (Yin, 2005).

The Eady Growth Rate is calculated on the third model level (which can vary in height due to vertical resolution, but it is always in the frictionless area). The vertical gradients of wind \( \vec{v} \) and potential temperature \( \Theta \) are approximated by choosing height values \( z \) of the model levels for the mean state rather than calculate the heights of the model levels at every time step. The error introduced due to this is not larger than the typical ratio of surface pressure variance versus mean surface pressure values apart from regions with significant orography, in cases where orography is used. The Eady growth rate is calculated within the Lyapunov subroutine so it is calculated in one of the model instances and at certain time steps, not continuously for every time step. However, the Eady growth rate is not calculated from the mean fields but rather the instantaneous fields as suggested by Simmonds and Lim (2009).

2.4.4 Potential vorticity

Potential vorticity is important in dynamical meteorology as it remains constant for an air parcel along a trajectory (Hoskins et al., 1985). Variations of potential vorticity are therefore indicators for baroclinic instabilities since they are regions with fast changing values of vorticity. In contrast to the Eady growth rate potential vorticity is important for barotropic instability as well. The necessary condition for barotropic instability to occur is a change in the sign of the horizontal potential vorticity gradient (Vallis, 2006). However, within the framework of this study, setups that support barotropic instability are rare, but they cannot be excluded.

Potential vorticity is usually calculated on isentropic levels and has the form (Hoskins et al., 1985)

\[ PV = -g(f + \zeta \Theta)/\frac{\partial p}{\partial \Theta} \quad (2.41) \]

where the \( \Theta \) subscripts indicate that they are calculated on isentropic levels.

In this study the potential Vorticity is not computed on isentropic levels but on model levels instead. This is done to achieve the highest possible comparability.
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between the different methods that assess predictability. The potential vorticity (PV) on sigma levels is defined as

\[
PV = -\frac{g}{p_s} \left( (f + \zeta) \frac{\partial \Theta}{\partial \sigma} + \frac{1}{a \cos \phi} \left( \frac{\partial (u \cos \phi)}{\partial \sigma} \frac{\partial \Theta}{\partial \phi} - \frac{\partial v}{\partial \sigma} \frac{\partial \Theta}{\partial \lambda} \right) \right)
\]  

(2.42)

with \(p_s\) the surface pressure, \(\Theta\) the potential temperature, \(a\) the planetary radius and all other variables as for (2.18). It is calculated in the model similarly to the Eady growth rate within the Lyapunov subroutine. The subroutine for the calculation of the potential vorticity has mainly been programmed by Hartmut Borth.

2.5 Statistics

The investigation of all kinds of measurements requires statistical tools to distil the important information out of large sets of observations or in this case model output. The used methods are described here.

The k-th moment of a random variable is defined as

\[
m_k = \int_a^b x^k f(x) dx.
\]  

(2.43)

The first moment is known as the expected value \(\mu\) while the second moment is the variance \(\sigma^2\) describing the fluctuations around the expected values. The third moment is called skewness \(S\) which is used to analyse how symmetrical or asymmetrical the distribution is and the fourth moment is called the kurtosis \(K\) which is a measure to identify distributions with so called fat tails. In fat tail distributions the probability to observe a realisation far from the expected value is larger than expected by the value of the variance.

In addition to moments, the quantiles of distributions are used in this study. The \(p\)-quantile is defined as

\[
P(X \in (-\infty, x_p)) = p
\]

\[
P(X \in [x_p, \infty)) = 1 - p,
\]

meaning that the probability to observe values larger than \(x_p\) is \(p\). If \(p = 0.5\) this is called the median and it defines the middle of the distribution in the sense that there is equal probability to observe larger or smaller values.

In this study, the well known Gaussian distribution is used. It is defined as

\[
f(x) = \frac{1}{\sqrt{2\pi}\sigma_D} e^{\exp \left( -\frac{1}{2} \left( \frac{x - \mu}{\sigma_D} \right)^2 \right)}.
\]  

(2.44)

The Gaussian distribution is defined by the first two moments. All other moments are are zero with the exception of the Skewness which is three. If one wants to find deviations from Gaussianity, investigating the higher moments is advisable. Cristelli
et al. (2012) found a relationship between skewness and kurtosis for several systems with very different but complex dynamics. Alberghi et al. (2002) meanwhile have found a similar relationship for the dynamics of the sea breeze. In this study the error between the two models is investigated for a similar relationship. To this end the total time series of the investigated parameter is cut into slices, each consisting of 100 subsequent time steps. This has been done for the local largest Lyapunov exponent on a global scale as well as on a more localised scale where the local largest Lyapunov exponent calculation is restricted to the tropics or mid-latitudes.

2.6 Conclusion

In this chapter the theory of dynamical systems relevant for the present study is briefly summarised. The importance of Lyapunov exponents for characterising the stability of a dynamical system is discussed. More advanced methods to classify a dynamical system are given such as the attractor dimension. The Fluctuation Theorem is introduced as a concept that might be applicable to low-resolution atmospheric models.

The PUMA Model is introduced, the model equations presented and the spectral computation highlighted. Its advantages as a tool to be analysed in a dynamical systems perspective are shown.

Three additional meteorological concepts that are supposed to be linked to predictability and error growth are introduced. They will serve as comparison and validation of the results from the dynamical systems analysis.
Chapter 3

Experimental setup and results

In this section the results of the dynamical systems analysis are presented. At first the experiment and model setup is shown and the choice of parameters explained. Then the result of the Lyapunov analysis is given and related to the Fluctuation Theorem. Finally the dynamical systems results are compared to results from traditional meteorological methods to assess stability and predictability.

3.1 Model setup

In this section the experimental setup is described. If a specific parameter or constant is not mentioned here it always has the standard value that the PUMA model uses as defined in the user’s guide (Fraedrich et al., 2011).

The general setup used here is an experiment where two instances of the model are run simultaneously, a so called identical twin experiment. One of these runs serves as the reference run. It is not influenced in any way and is integrated normally while the main run is weakly influenced by the Lyapunov subroutine as described in section 2.3.1. Both runs use the same set of parameters and are identical with the exception of the actual values of the model variables. Since the models are identical they have the same attractor and, therefore, this setup is used to perform the dynamical systems analysis.

The run is initialised with a restart. This means that rather than starting from a state of rest as usual, an existing run is continued from a previous saved state. This saved state is already integrated so far, that all the initial spin-up time of the model has passed. During this spin-up phase all additional subroutines such as the Lyapunov subroutine are skipped. These runs are created using the same parameters as the actual run but after a certain time it is stopped and saved. However, the saved state is changed slightly. For both runs the time step has been reset to zero. In addition to that the main run features a perturbation that is prescribed on the surface pressure field in grid point representation. The time step is set to zero to always have the same starting time step for the different experiments, where the length of a time step can vary depending on the resolution. The perturbation is
random and always less than 0.01% of the actual value at the respective grid point. This ensures that the initial distance $d_0$ is indeed small enough so that non-linear effects can be disregarded. Furthermore after the perturbations are applied and the surface pressure field transformed back into spectral form, the global mean is set again to a previously saved value to ensure that the total mass in both runs is equal. Since the perturbations are random to begin with the expected value of the difference in the global mean is zero, but for every application it is of course slightly non-zero. The final surface pressure field is then saved to the restart file.

When the model is subsequently started it is clear that due to the arbitrary initial perturbation the difference between the models will not grow with the value of the largest Lyapunov exponent. It can instead be assumed that the initial perturbation will align itself into the most unstable direction over some time. For this reason, the first 4800 time steps of the experiment are not used for the calculation of local Lyapunov exponents. That means that their respective time series are always 4800 time steps (100 or 50 days depending on resolution) shorter. The global Lyapunov exponent is not affected, since it is a mean over a very long time series and the initial values do not change the result since it is defined as a limit for $t \to \infty$.

Depending on the experiments some of the parameters are varied. Table 3.1 shows the range of values and their impact on the model. It has to be noted that the most significant change in the choice of parameters compared to the standard setup are the friction and relaxation temperature time scales. These have been chosen to be identical to synchronisation experiments of Lunkeit (2001) since synchronisation experiments provide another possibility to estimate the largest Lyapunov exponent. This will be highlighted in the following section 3.2 where the results are compared.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Name</th>
<th>Range of values</th>
<th>Impacts</th>
<th>PUMA standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>DTNS</td>
<td>North-South temperature gradient</td>
<td>0</td>
<td>No annual cycle, hemispherically symmetric</td>
<td>0 or -70</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>conditions</td>
<td></td>
</tr>
<tr>
<td>DTEP</td>
<td>Equator-Pole temperature gradient</td>
<td>20-100, usually 70</td>
<td>Strength of mean temperature gradient or jet</td>
<td>60 or 70</td>
</tr>
<tr>
<td>MPSTEP</td>
<td>Minutes per time step</td>
<td>30, 15 for T42</td>
<td>Shorter time steps stabilize numerically, longer computation</td>
<td>60 for T21, 45 for T31, 30 for T42</td>
</tr>
<tr>
<td>TFRC</td>
<td>Reciprocal friction time scale</td>
<td>0 if $\sigma &lt; 0.8$, 1 if $\sigma \geq 0.8$</td>
<td>Strength of friction and dissipation of kinetic energy</td>
<td>$\exp(10(1 - \sigma))$ for $\sigma \geq 0.8$, 0 otherwise</td>
</tr>
<tr>
<td>RESTIM</td>
<td>Restoration temperature relaxation time scale</td>
<td>30</td>
<td>Strength of the diabatic heating forcing</td>
<td>$\min(30, 158/(\pi \arctan(1 - \sigma)))$</td>
</tr>
<tr>
<td>NYEARS</td>
<td>Length of the simulation in 360-day years</td>
<td>usually 200 also 100, 2000, 3000, 8000</td>
<td>No restart file</td>
<td>1, with restarts</td>
</tr>
<tr>
<td>NSYNC</td>
<td>Switch to define if model instances can communicate</td>
<td>1</td>
<td>They do communicate</td>
<td>0</td>
</tr>
<tr>
<td>SYNCSTR</td>
<td>Synchronisation strength between instances</td>
<td>0, handled via rescaling</td>
<td>Deactivated for this study</td>
<td>0, since NSYNC = 0</td>
</tr>
<tr>
<td>REVEPS</td>
<td>Defines the model instance for Lyapunov subroutine</td>
<td>0 for reference run, 1 for main run</td>
<td>Can disable Lyapunov subroutine if 0</td>
<td>Not available</td>
</tr>
</tbody>
</table>

Table 3.1—A description of all parameters, their numeric range as well as their impact on the model. All values with a ‘usually’ tag comprise the standard setup used in this study, while the standard setup of the PUMA model is given in a separate column.
3.2 Lyapunov exponents

The dynamical systems analysis here concentrates on the assessment of Lyapunov exponents. Lyapunov exponents describe how fast nearby trajectories on the attractor diverge and thereby how predictable a system is. Any system with a largest Lyapunov exponent larger than zero is considered to be chaotic while systems with a vanishing largest Lyapunov exponent have attractors like fixed points or limit cycles and are considered non-chaotic. The largest global Lyapunov exponent can not become negative, however, local or finite time growth rates can be negative even for otherwise very chaotic systems which will be discussed in an forthcoming section.

3.2.1 The largest Lyapunov exponent

The largest Lyapunov exponent is a general measure for the predictability of a system. Due to the observed chaotic behaviour it must be assumed that the largest Lyapunov exponent is positive for an atmospheric circulation model (Eckmann and Ruelle, 1985). The actual value can give an estimate of the predictability limit. Since model results are investigated and not, like in weather forecast validation, the relation to the actual atmospheric development, a sensitivity study of the largest Lyapunov exponent suggests itself. The main focus lies on the question how the model resolution and the prescribed temperature gradient of the relaxation temperature affects the result. A larger temperature gradient of the relaxation temperature will result in a larger mean temperature gradient in the model. The larger gradient results in a larger vertical wind gradient and therefore stronger jets. As described in section 2.4.3 a stronger vertical wind gradient indicates higher baroclinicity and since it is assumed that for our model baroclinic instability is the primary contributor to the chaotic behaviour it can be expected that the largest Lyapunov exponent increases with the temperature gradient. It has to be noted that a similar experiment was performed by Guerrieri (2009) where such a relation was found. In this section this study is repeated with a newer version of the model and (possibly) with a different set of parameters chosen as not all of their choices were specified.

For these experiments the models have been run for 36000 days or 100 years according to the PUMA 360 day calendar to ensure a robust result. It turns out that the largest Lyapunov exponent deviates less than 5% of its final value (after 200 years) after about 20 years.

Figure 3.1 shows the relation between the largest Lyapunov exponent and the horizontal gradient of the relaxation temperature. The x-axis shows the values for the parameter \((\Delta T_R)_{EP}\) as used in equations (2.25) and (2.26). The setup for this experiment is a horizontal resolution of T21, five vertical levels and the standard parameters from table 3.1 with the exception of the relaxation temperature gradient \((\Delta T_R)_{EP}\) which is varied between 20 and 100. The values obtained by Guerrieri (2009) are analysed from their figures and are accurate to about 5%. The figure shows that the largest Lyapunov exponents for \((\Delta T_R)_{EP}\) values below 40 is indeed zero or even slightly negative. Since it is not allowed for the largest Lyapunov
3.2 Lyapunov exponents

The largest Lyapunov exponent versus the pole-equator temperature forcing $(\Delta T_R)_{EP}$ for the resolutions T21. The red values are obtained by Guerrieri (2009).

exponent to become negative it can be assumed that this effect is due to initial values that are slightly negative and the finite time of integration. For $t \to \infty$ the values should become zero. This result indicates that the temperature gradient is too weak for baroclinic instabilities to form and the flow is perfectly zonal and laminar. For larger values the Lyapunov exponent increases sharply and finally begins to saturate although it is still growing for the largest values chosen here. Larger values could not be investigated since the model becomes numerically unstable if the wind speeds induced by the high gradient become too large. When compared with the results by Guerrieri (2009) it can be seen that their results are consistently higher than the new results, but the slope is very similar. Furthermore, their cut-off point for a vanishing Lyapunov exponent is slightly lower between $30 - 40$ K rather than $40 - 50$ K.

In figure 3.2 a similar experiment is conducted but for a horizontal resolution of T42. Again the red markers indicate the previous results from Guerrieri (2009). The most striking difference compared to the results of the T21 experiment is that vanishing Lyapunov exponents are found for $(\Delta T_R)_{EP}$ gradients below 20 K which is a substantial reduction compared to the T21 case. It stands to reason that the smaller scale structures introduced through the higher resolution are helpful in the development of baroclinic instabilities. In addition to this change the largest Lyapunov exponent is nearly twice as large as in the low resolution experiment for $(\Delta T_R)_{EP}$ in the range between 50 K and 80 K. It has to be reasoned here as well that the smaller scales are important for the development of instabilities. The comparison

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure3.1.png}
\caption{The largest Lyapunov Exponent versus the pole-equator temperature forcing $(\Delta T_R)_{EP}$ for the resolutions T21. The red values are obtained by Guerrieri (2009).}
\end{figure}
with the Guerrieri (2009) results shows that the difference between the experiments has become larger with the higher resolution. However, the slope remains similar for the experiments.

It has to be noted that the mean state of the atmospheric circulation is almost identical in both resolutions and that the changes in the dynamics as detected by the Lyapunov exponent can only be explained by a change in the transient behaviour. This will be investigated further in the context of the Fluctuation Theorem in section 3.2.3. In addition to the Lyapunov exponent there are further methods to quantify the dynamical properties of the model.

The attractor dimension can give additional hints with respect to the dynamics of the system as mentioned in chapter 2.1.3. To this end the correlation dimension $D_2$ for the PUMA attractor has been calculated as described. The experimental setup for this calculation is slightly different from the setups of the sensitivity experiments. Only the reference run is used and the integration time is 2000 years for T21, 8000 years for T31 and 3000 years for T42. The experiment in T42 should have been even longer than the T31 experiment, but due to computational constraints in the evaluation program a longer time series could not be calculated. The short time series for the T21 case is due to some data corruption but should not have any influence on the result as it is the lowest resolution here and therefore needs the shortest trajectory for robust results. In order to ensure independence of the system states, a state is measured every 40 days. This value is chosen since it is about four times larger than the typical (actually the high end) synoptic time scale of 10 days for large systems. However, due to the low resolution individual systems tend to

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**Figure 3.2**— As figure 3.1 but for T42 resolution.
exist longer than in higher resolution experiments (see appendix for the video and figures 4.2 and A.2). To make sure to still have independent states, a secure time frame of 40 days is chosen. Since integrations over such a long time period take a long time even with the PUMA model, only one experiment is performed for each resolution with a $(\Delta T_R)_{EP}$ value of 70. The resolutions considered are T21, T31 and T42. While it would certainly be interesting to investigate higher resolutions like T63 or T85 the time to create such a long time series is too immense for the scope of this study. Furthermore the memory requirements of the subsequent calculation of the individual distances would have been too large as well.

The slope of $\log S(\epsilon)$ is plotted against $\log \epsilon$ to calculate $D_2$ and the result for the linear regime is shown in figure 3.3. The whole figure including the non-linear parts is available in the appendix as figure A.1. $S(\epsilon)$ is the number of unique pairs of states with a distance less than $\epsilon$. The slope is calculated in the linear regime (small $S(\epsilon)$) with a least square fit. For T21 $D_2 = 13.1$, for T31 $D_2 = 48.4$ and for T42 $D_2 = 77.7$. According to the rough estimate of the number of positive Lyapunov exponents given in section 2.1.3 the first guess number (1/3 of $D_2$) of positive Lyapunov exponents in PUMA is 5 for T21, 15 for T31 and 26 for T42.

### 3.2.2 The local largest Lyapunov exponent

While the largest Lyapunov exponent and the attractor analysis can be used to assess the global dynamical properties of a system, a local view is preferred. This study concentrates on temporal localisation by looking at finite and short time intervals.
Table 3.2— All investigated horizontal and vertical resolution combinations and their degrees of freedom.

<table>
<thead>
<tr>
<th>Name</th>
<th>Levels</th>
<th>max. wave number</th>
<th>grid points</th>
<th>Degrees of freedom</th>
</tr>
</thead>
<tbody>
<tr>
<td>T15L3</td>
<td>3</td>
<td>15</td>
<td>24x48</td>
<td>2240</td>
</tr>
<tr>
<td>T15L5</td>
<td>5</td>
<td>15</td>
<td>24x48</td>
<td>3584</td>
</tr>
<tr>
<td>T21L3</td>
<td>3</td>
<td>21</td>
<td>32x64</td>
<td>4400</td>
</tr>
<tr>
<td>T21L5</td>
<td>5</td>
<td>21</td>
<td>32x64</td>
<td>7040</td>
</tr>
<tr>
<td>T21L10</td>
<td>10</td>
<td>21</td>
<td>32x64</td>
<td>13640</td>
</tr>
<tr>
<td>T21L20</td>
<td>20</td>
<td>21</td>
<td>32x64</td>
<td>26840</td>
</tr>
<tr>
<td>T31L5</td>
<td>5</td>
<td>31</td>
<td>48x96</td>
<td>15360</td>
</tr>
<tr>
<td>T42L5</td>
<td>5</td>
<td>42</td>
<td>64x128</td>
<td>26880</td>
</tr>
<tr>
<td>T42L10</td>
<td>10</td>
<td>42</td>
<td>64x128</td>
<td>52080</td>
</tr>
<tr>
<td>T42L20</td>
<td>20</td>
<td>42</td>
<td>64x128</td>
<td>102480</td>
</tr>
</tbody>
</table>

(Schalge et al., 2013). Other forms of localisation are the restriction of the analysis to certain regions or individual grid points. Some insight into the spatial aspect is gained due to the Lyapunov vector. As defined in section 2.1.2 the Lyapunov vector is the vector that points into the most unstable direction of phase space. By the design of the experiment, the perturbation between the two model instances grows freely and will therefore unavoidably align towards the most unstable direction. It can therefore be assumed that the difference between the instances is the Lyapunov vector of the largest Lyapunov exponent. However, the largest Lyapunov exponent is a global measure while the Lyapunov vector is dependant on the current state of the system at any time due to the rescaling. In this case the Lyapunov vector can not be defined without the state of the system. The growth rate of the Lyapunov vector is not equal to the global Lyapunov exponent but rather a finite time or local Lyapunov exponent. The time average of the growth has to be equal to the global Lyapunov exponent. In order to analyse the model the local largest Lyapunov Exponent ($\hat{\lambda}$, (2.14)) is calculated. In addition, the results from the global Lyapunov calculation are used as a reference.

The experimental setup is identical to the setup for the global Lyapunov exponents with the change that the total length of the time series is 200 years and the $(\Delta T_R)_{EP}$ values are fixed to 70 K. The longer time series provides reduced uncertainties while the restriction to one relaxation temperature keeps the computational effort manageable to compute a larger range of combinations of horizontal and vertical resolutions. Table 3.2 shows the list of all used resolutions and their respective degrees of freedom. The degrees of freedom are calculated from the spectral perspective with the restrictions that all imaginary parts of zonally symmetric spherical harmonics are always zero and therefore disregarded.

Figure 3.4 shows an arbitrary time slice of the time series of the local Lyapunov exponent for the T42 case with 5 vertical layers for different values of $(\Delta T_R)_{EP}$. This is a supplement to the global analysis to show how the Lyapunov exponents behave locally. It is evident that the fluctuations of the local largest Lyapunov exponent...
increase with the relaxation temperature gradient and that too low values cause the system to become non chaotic and the local largest Lyapunov exponent zero. Even more remarkable is that the local largest Lyapunov exponent becomes negative for certain time periods for all gradients that are large enough to show generally chaotic behaviour. This means that close trajectories converge rather than diverge during these periods. Consequently the system is not sensitive to initial conditions, at least within a certain range for the perturbations. These time series are further analysed for different resolutions since they change the degrees of freedom of the system.

3.2.3 Towards the Fluctuation Theorem

Occurrence of negative local largest Lyapunov exponent can be attributed to a behaviour similar to the one predicted by the Fluctuation Theorems. Here a simplified and non-rigorous version of the theorem is used. The Fluctuation Theorem states

$$\frac{P(\Sigma = +a)}{P(\Sigma = -a)} = \exp(a \tau \Sigma)$$

(3.1)

with $\Sigma$ the entropy production identified by the local largest Lyapunov exponent.

In figure 3.5 the probability distribution for the local largest Lyapunov exponent is assessed for the T21L5 case. The distribution is nearly Gaussian as indicated by the fit, however, especially in the tails a different distribution cannot be ruled out. The Gaussianity of the distribution is no trivial result as there is no clear reason why the local largest Lyapunov exponent should be Gaussian. However, the fact
that it is nearly Gaussian is a good hint towards the validity of equation (3.1) since this relation follows trivially if $\Sigma$ is Gaussian. Apart from the Gaussianity the next striking observation is the large portion of values less than zero. About 17% of all values are negative so there is a significant occurrence of these events.

The sensitivity of this phenomenon has been investigated and the results are shown in figure 3.6 and 3.7 respectively for a fixed error growth time of $\tau = 100$ hours.

Figure 3.6 shows the dependence on vertical resolution. In this case the horizontal resolution is kept constant at T21, but the vertical resolution is changed with values of 3, 5, 10 and 20 levels. For clarity the Gaussian fits are shown in this figure and it can be seen that larger vertical resolutions mostly increase the fluctuation effect. The distribution is broader, but the mean shifts very little to more positive values. Furthermore it seems that vertical resolutions larger than 10 levels add nothing further to the dynamics as a saturation effect becomes visible for this low horizontal resolution.

The dependence on the horizontal resolution is shown in figure 3.7 where the vertical resolution has been kept constant at five levels, but the horizontal resolution is changed. T15, T21, T31 and T42 are used and as before only the Gaussian fits are shown. Between T21, T31 and T42 the major difference is a shift of the distribution to the positive side of the graph. The distributions become marginally broader, but this is a minor effect compared to the shift of the mean to much larger values for higher horizontal resolutions. The resolution T is a special case. Its mean is as assumed lower than the means of the other resolutions, but the distribution is much
sharper than expected by the results from the other resolutions.

Figure 3.6 — The relative frequency of the Gaussian fit of the local largest Lyapunov Exponent ($\hat{\lambda}$) for the T21 resolution with different numbers of vertical levels.

Figure 3.7 — The relative frequency of the Gaussian fit of the local largest Lyapunov Exponent ($\hat{\lambda}$) for 5 vertical levels and different horizontal resolutions.
Equation (3.1) does not solely depend on $\Sigma$ but on the growth times $\tau$ as well. To get the respective behaviour for different error growth times $\tau$ the local largest Lyapunov exponent is calculated every 6 hours over the course of 10 days or 240 hours. 240 hours are equivalent to 480 time steps in T21 and T31 and 960 time steps in T42. The result is presented in figure 3.8 where for the T21 case with 5 levels the median of the distribution as well as the .9 and .99 quantiles are shown. The median does not change, however, the distribution slowly sharpens with $\tau$ as the quantiles move closer to the median. In the limit $\tau \to \infty$ the distribution should collapse to the single value of the median which is the global Lyapunov exponent. With increasing $\tau$ the probability to observe negative values does decline due to the sharpening of the distribution.

All the previous observations indicate that the Fluctuation Theorem is applicable here. For this reason the validity of equation (3.1) has been tested for the T21 case with 5 levels. Figure 3.9 shows the results for fixed values of the growth time $\tau$. For all cases a robust linear relationship between the logarithm of the left hand side of equation (2.16) and the approximated entropy production $\Sigma$ is evident. It has to be noted that for larger values of $\Sigma$ this relation becomes increasingly more uncertain due to the data scarcity in this regime. Larger growth times run into this problem earlier since their distribution is already sharper in accordance with the results from figure 3.8. It remains reasonable that the local largest Lyapunov exponent fulfils the Fluctuation Theorem with respect to the entropy production rate $\Sigma$. 

Figure 3.8 — Quantiles of the local largest Lyapunov Exponent ($\hat{\lambda}$) versus the growth time $\tau$ for the T21 resolution with 5 vertical levels.
Figure 3.9— The right hand side of (2.16) against the values of $\Sigma$ for different growth times $\tau$.

Figure 3.10— The logarithmic slope from figure 3.9 against the growth time $\tau$. For all $\tau > 160$ h a least square fit that passes through the origin is calculated.
The relation with the growth time is assessed in figure 3.10. It should be log-linear with $\tau$, however, this relation does not hold for very small $\tau$. The results indicate that such a relationship can be found for values of $\tau$ larger than 160 hours. For this regime a least square fit that is forced to go through the origin is computed as shown in the figure. Since the data is scattered around this line for the mentioned regime it can furthermore be assumed that equation (2.16) also holds with respect to $\tau$ for $\tau > 160$ h.

### 3.3 Nonlinear error growth

An important question with regard to weather forecasts is how large the initial error can grow before non-linear interactions change the error growth characteristics of the system. To this end an experiment with the standard setup (T21, 5 levels) has been conducted where the initial error has been increased. Additionally all variables are perturbed and not only the surface pressure to increase the total error and for it to be independent of the number of vertical levels. If the surface pressure is perturbed, the total error will be larger in an experiment with few vertical levels. The total error is around 1% of the total values which translates to temperature differences of $3K$ for example.

It turns out that at least for PUMA and for this resolution and setup there is no difference in the error growth statistics. Over large time periods the Lyapunov exponent (or equivalent measure for non infinitesimal distances) is identical.

### 3.4 Error growth and Eady growth rate

In the analysis above, globally integrated values like the local largest Lyapunov exponent were considered. For the dynamics, the distribution of regions with high fluctuations are interesting as well as they indicate regions of baroclinic instability.

The error growth is investigated through the local largest Lyapunov exponent and the difference vector between the two model instances. This vector describes the fastest growing direction and the Lyapunov exponent the growth rate. Consequently the regions with the largest average growth rates are the regions with the largest average values of the Lyapunov vector. Since the model setup is zonally symmetric the long time averages are zonally symmetric as well and zonal averages are almost identical to the individual values at a longitude. Level dependant variables (Vorticity, Divergence and Temperature) are evaluated for level three (around 500 or 300 hPa depending on resolution) to be conform with the Eady growth rate as described in section 2.4.3. Since the variables have very different magnitudes of values, they are scaled to fit into one diagram in figure 3.11 together with the Eady growth rate. The scale for error growth is arbitrary as only the distribution but not the overall magnitude is important. The setup for this experiment is the standard setup (Table 3.1) with a horizontal resolution of T21 and five vertical levels.
3.4 Error growth and Eady growth rate

Figure 3.11— Zonal mean distribution of the Eady growth rate (black), the temperature difference (red) and the surface pressure difference (blue). To accommodate all distributions in one plot they are scaled as described.

Figure 3.12— Distribution of the Eady growth rate for the T42 case with 10 vertical levels and orography.
It can be seen that the maximum of variability of all model variables is approximately at the same latitude, while the maximum of the Eady growth rate is further towards the equator in accordance with the position of the jets. It stands to reason that in PUMA the vertical wind gradient is the dominant factor for the Eady growth rate compared to the stability of the atmosphere.

The Eady growth rate and error growth has furthermore been calculated for a case with topography in T42 horizontal resolution as shown in figure 3.12. Here a zonal average representation is not possible especially for the northern hemisphere. The southern hemisphere shows very similar results compared to the previous setup, but on the northern hemisphere the mean circulation is more influenced by topography and therefore the growth values as well. It has to be noted that the Eady growth rate in mountainous regions is calculated poorly due to the simplified computation method. The final result for the northern hemisphere is similar to the standard setup as it shows that the highest values of Eady growth rate are further to the equator near the jet maximum. However, there are distinct differences. The region downstream of the Himalaya mountains shows a double-jet structure that is unique to this region. The jet is furthermore slightly shifted to the north.

In addition to the time mean growth rate a smaller time frame is selected as a sample to investigate the Lyapunov vector during some time. A small video was produced, where it can be seen that the Lyapunov vector changes slowly and that the largest values are found near baroclinic eddies which for this coarse resolution are low pressure systems. This video is available in the appendix and a panel with some frames from the video is given in figure 4.2. These frames illustrate the general life-cycle of instabilities in the model. For this special case the Lyapunov vector is recorded at every time step for the considered time period, but rescaling is done every day, which can be partly seen in the video, while the panel shows frames that are one day apart, so no rescaling is visible. It can therefore be assumed that either the Lyapunov Vector changes slowly with respect to the simulation time scales or that the Lyapunov vector slowly aligns towards the most unstable direction. The latter option seems unlikely since the instabilities move consistently with the mean flow.

In addition to the spatial distribution of error growth rate and Eady growth rate the distribution of all values is compiled in figures 3.13 and 3.14. The figures show the relative probability to observe a certain value of error growth or Eady growth rate at any grid point. All grid points are used for this analysis, however, error growth is represented by the surface pressure difference only. As such the scale of the difference values is arbitrary, but the slope or form of the distribution represents the total error growth. The major difference between the distributions is that the relative frequency of the surface pressure difference is monotonically deceasing while the Eady growth rate features a local minimum near 0.15 and a local maximum around 0.3 while the relative frequency decreases sharply for values larger than 0.5. Between 0.1 and 0.5 the relative frequency to observe any value of Eady growth rate is very similar and the distribution is almost flat. The error growth, however, shows an almost exponential decay in relative frequency with the value of the error.
### 3.4 Error growth and Eady growth rate

![Graph](image.png)

**Figure 3.13** — Relative frequency of Eady growth rates.

![Graph](image.png)

**Figure 3.14** — As figure 3.13 but for error growth represented by the surface pressure error.
3.5 Potential vorticity and error growth

Potential vorticity and error growth have been analysed in the same manner as Eady growth rate and error growth. The distributions of the error growth (scaled) and potential vorticity for the standard case are shown in figure 3.15. In contrast to the results with the Eady growth rate the variability of potential vorticity and error growth are extremely similar. The shape of the distribution is almost identical and the maximum values are also found at the same latitude.

As before for error growth and Eady growth rate, the distribution of the potential vorticity deviations is analysed. Figure 3.16 shows the relative frequency similar to figures 3.13 and 3.14. The distribution of the potential vorticity deviations shows three regimes where it is nearly log-linear with different slopes. The difference in the slope between the last two regimes between 0.05 and 0.3 as well as 0.4 and 0.6 is small, while an initial decay is strongest. This initial strong decrease is also featured by the other two distributions.

3.6 Skewness and kurtosis

The time series of the local largest Lyapunov exponent has been analysed for deviations from Gaussianity. Alberghi et al. (2002) and Cristelli et al. (2012) among others have found that there are distinct relationships between skewness and kurtosis.
3.6 Skewness and kurtosis

for a wide variety of complex dynamical systems. The skewness-kurtosis relationship found by Cristelli et al. (2012) demands $K = N^{1/3}S^{4/3}$ while Alberghi et al. (2002) used the statistical limit of $K \geq S^2 + 1$ as an additional reference. The time series of the local largest Lyapunov exponent is split into segments of $N = 100$ values each and the distribution over this limited time frame is subsequently analysed. Skewness and kurtosis are calculated for the individual distributions as well as for the full time series. For this experiment, the resolution is T21L5 with all other parameters as before for the Eady experiments. Different regions are defined, the tropic region between $-30^\circ$ and $30^\circ$, the mid-latitudes from $45^\circ$ to $60^\circ$ and $-45^\circ$ to $-60^\circ$ respectively and the global analysis. The results are shown in figure 3.17. Most of the distributions are in a cloud around the values for the Gaussian distribution (3 for kurtosis and 0 for skewness) with some shift towards lower kurtosis values. For the mid-latitudes, however, the distributions shows a shift to larger kurtosis and skewness values indicating fat-tail distributions for some of the time slices. The values for the full time series are indicated with plus symbols and generally show kurtosis values larger than three and marginally positive skewness values. The global distribution is closest to Gaussianity. The skewness-kurtosis relationship from Cristelli et al. (2012) that demands $K = N^{1/3}S^{4/3}$ is indicated in all of the figures. It is evident that neither of the results seems to follow the skewness kurtosis relationship. Most of the values are too close to the Gaussian values and the more extreme cases are not distributed according to the relation but rather between the proposed relation and the statistical limit.

![Figure 3.16](image_url) — As figure 3.13 but for potential vorticity deviations.
Figure 3.17— Skewness and Kurtosis of the local largest Lyapunov exponent for time slices limited to 100 values for the global analysis (top), for the mid-latitudes only (middle) and for the tropics (bottom).
3.7 Blocking and stability

Blocking can be interpreted as a transient stable phase of the atmosphere due to its persistent nature. Models often have shown difficulties in the prediction of onset and end of blocking periods (Watson and Colucci, 2002). The aim of this part of the study is to investigate if the stability analysis with local largest Lyapunov exponents can be used to detect blocking periods or find some predictive skill.

The most challenging task, however, is to first get a model setup that produces enough blocking, but at the same time does not take too long to compute. A study (Schalge, 2010) about blocking in PUMA has shown that resolutions below T42 do not produce blocking. Furthermore topography is essential if one wants to get blocking. With these points considered an experiment is conducted in T42 with topography and all other settings set to standard values, identical to the experiment in section 3.1 and for the Eady growth rate. It turns out, however, that this setup does not produce enough blocking for a meaningful analysis.

On the basis of the aforementioned study, the setup is changed and the standard relaxation temperature is switched to a Held-Suarez setup as defined in section 2.2.2. Furthermore the relaxation time scale is set to PUMA default values resulting in much stronger relaxation near the surface. Lastly the friction values are set to PUMA standard values and not the otherwise used 0, 1 case (compare table 3.1).

With this setup blocking is found roughly similar to the results in the mentioned study, with peak values of about 5% if the original Tibaldi-Molteni method is used as specified in section 2.4.2. The distribution of the blocking frequency according to the original Tibaldi-Molteni method is shown in figure 3.18 and the only difference to the previous study is the sharp peak around 150° longitude. This feature is reduced in prominence if the modified method is used instead. This method reduces the overall blocking frequency so that the largest values barely reach 2%. On average the distributions are still similar. Simultaneously to the blocking frequency, the error growth and local largest Lyapunov exponent are computed. However, negative values of error growth are already very rare in the T42 case. Despite this, correlation between negative growth rates and blocking periods is investigated.

It turns out that there is no correlation (0.06) between a time series of total blocking (the sum of all blocked longitudes at every time step) and the negative episodes of the local largest Lyapunov exponent. In summary, the experiments conducted here are not conclusive whether the dynamical systems analysis is a helpful tool to analyse blocking.

3.8 Conclusions

In this section all results are presented. The discussion of the results will follow in the next chapter. It is shown how unstable or unpredictable the PUMA model is globally but on a temporal local scale in the form of the local largest Lyapunov exponent. The local largest Lyapunov exponent is furthermore used to investigate
the spatial distribution of the error growth and by that the spatial distribution of the predictability. Furthermore, a probability distribution is calculated for the local largest Lyapunov exponent and a nearly Gaussian distribution is found. Consequently, the local largest Lyapunov exponent as a representation of an entropy-like quantity fulfilled the Fluctuation Theorem at least within the more certain range of values.

The growth rate and local largest Lyapunov exponent are compared to other often used tools to study atmospheric instabilities, namely the Eady growth rate and the potential vorticity. It is found that potential vorticity and error growth are very similar in its distribution, while the Eady growth rate differed in terms of the location of the maximum values.

Finally, it is attempted to connect the atmospheric phenomenon of blocking with the error growth rate and dynamical analysis in general. It proved to be difficult to get enough blocking in PUMA and a special setup is necessary. Despite this there is no correlation or other connection between blocking and the dynamical parameter investigated before.

Figure 3.18— Distribution of the blocking frequency in PUMA.
Chapter 4

Discussion

In this chapter the results from the previous chapter are evaluated. They are compared to existing studies of similar systems as well as analysed from a theoretical point of view.

4.1 Lyapunov analysis

The first part of the analysis is a sensitivity study of the largest Lyapunov exponent with respect to horizontal resolution and relaxation temperature gradient. Such a study was performed before with an older version of the same model (Guerrieri, 2009). Most of the time the results are similar. Both investigations show that below certain values of relaxation temperature gradient the Lyapunov exponent becomes zero. For both studies this happened at approximately at the same values, with smaller thresholds for the Guerrieri (2009) results. Furthermore, both studies have found a sharp increase in the Lyapunov exponent for slightly higher gradient values and a slower increase with even higher gradient values. The exact numerical values, however, in this section are different. The older study shows higher values in general than the results outlined here. The main reason why this could happen is the choice of parameters to run the model with. The authors of the original study have used the same values for friction, but the other parameter values were not specified. It is possible that a slight difference in the choice of parameters could have a large impact on the dynamics of the model. It is therefore crucial to make sure the parameters are correct and the same for a true comparison. In this case it is therefore unknown if the results are compatible. They show qualitatively the same behaviour, but quantitatively they are different. Another reason why this could be the case are changes in the numerics of the model. The exact version of the model in the original study is unknown too, but it can be assumed that since this study is from 2009 the model might have changed significantly in the mean-time. Ideally a change in numerics should have no impact on the dynamics. However, the Dynamical Core Model Intercomparison Project from 2012 where PUMA took part has shown that the different dynamical cores indeed produce different results.
Neither result is outside the realm of possibility or plausibility and reflects how much influence different numerical schemes can have.

One question that remains is why the parameters for the PUMA model were chosen the way they are. The main reason is to have the same parameter as a synchronisation study by Lunkeit (2001). This study investigated how strong two models have to be coupled until they synchronize. This method can also be used to calculate the largest Lyapunov exponent. Since the exponent is the mean rate of divergence of the two model instances, the synchronisation parameter must be approximately as strong. It can be seen, however, that locally the rate of divergence behaves very different. It can therefore be assumed that slightly lower coupling strength is sufficient to reach synchronisation if the time is still finite. Of course the definition of the Lyapunov exponent is for \( t \to \infty \) so a coupling strength has to be found where total synchronisation occurs after infinitely long time. Such an experiment was conducted in the mentioned study and the values obtained for the largest Lyapunov exponent are practically identical to the results found here. The values obtained in the study have to be doubled since the synchronisation term acts on both models at the same time and not on one of them as in the experiments in this study. The PUMA parameters were therefore chosen to have another method to compare the results to. As mentioned the results depend heavily on the choice of parameters. So choosing the same parameters should, even if changes in the numerics of the model have some minor effects, deliver comparable results.

The analysis of the local values of the largest Lyapunov exponent is to the knowledge of the author new for atmospheric circulation models governing the primitive equations. Most studies (Kazantsev, 1999; Snyder and Hamill, 2003; Vannitsem and Nicolis, 1997) have investigated the local Lyapunov exponents or Lyapunov exponents in general for simpler systems (quasi-geostrophic) with fewer degrees of freedom. While it has to be expected that the local largest Lyapunov exponent (\( \hat{\lambda} \)) is not constant in time the result that it can become negative is surprising. Results with quasi-geostrophic atmospheric models did not show a similar behaviour as shown in the above-mentioned studies. Negative values of the local largest Lyapunov exponent mean that locally nearby trajectories converge rather than diverge. However, theory states that on a strange attractor nearby trajectories always diverge unless they are already too far apart so that non-linear effects become important. In this study it is taken care of this fact by choosing the separation of the two trajectories to be very small. To this end the model is even run in double precision mode to ensure no numeric effects to become visible. In some other studies (Dellago and Hoover, 2000) (Eckhardt and Yao, 1993) of local Lyapunov exponents it is sometimes shown that negative values are possible or even common for very short time frames, however they are found for simple systems compared to PUMA.

There remains a discrepancy between the quasi-geostrophic results and the results for PUMA. It can be assumed that the additional dynamics introduced by the primitive equations are responsible for this negative error growth.

If one were able to properly visualize the PUMA attractor, one would find re-
regions where trajectories converge over short distances. The short distances can be assumed due to the typical length of such a negative episode which is usually less than a day as shown in figure 3.4. Longer periods, however, are possible as figure 3.8 suggests where after ten days the probability to observe negative local largest Lyapunov exponents is not negligible. After ten days the two states of the system will still have a high correlation. This then means that they cannot have a very huge distance between them in a phase space diagram and that means that the regions of convergence are rather small compared to the total size of the attractor. These regions can actually be observed for simpler systems. A study by Sprott (1993) showed many representations of strange attractors where at some points the trajectories seem to be channelled together. The same would be visible for the PUMA attractor. However, since the PUMA attractor has at least 2240 dimensions (table 3.2) a reduction to two or three dimensions for a visualisation will loose too much information.

The main reason why the negative episodes are so interesting is because during these short time periods the system is not sensitive to the initial conditions if they are not too far from each other. And this is observed here for a global circulation model. This means that for these time periods the system is predictable. Initial errors would not lead to a rapid deterioration of the forecast skill over the respective time interval. Moreover, if a forecast is done and the local largest Lyapunov exponent is negative during the forecast period, the prediction would even become better from that point onwards. This is referred to in weather forecasts as return of skill (Anderson and Van Den Dool, 1994). Most of these cases are local features and said regions have been identified as regions with low effective dimensionality in models (Patil et al., 2001). It seems therefore, that a low number of effective dimensions and return of skill are connected. It is therefore logical that for higher resolved experiments very few periods of negative local largest Lyapunov exponents on the global scale remain. In PUMA it is unlikely to find similar localised effects as in the aforementioned study since there are no physical processes present on these scales that could induce them. Instead, it is likely that local time series of local largest Lyapunov exponents will look similar to global time series but with broader distributions. Indeed an experiment where the analysis is restricted to certain regions is conducted and the result is shown in figure 4.1. This figure shows the distributions of different regions, with the regions the same as in figure 3.17. The distributions are very similar, they have practically the same mean or median values, but the variance of the distributions is different. The variance is much larger in the mid-latitudes, while in the tropics the variance is close to the global variance.

The differences in the distributions of the local largest Lyapunov exponent might depend on the effective degrees of freedom of the system. The effective number of degrees of freedom can be assessed by the fractal dimension of the attractor. As seen in figure 3.3 the fractal dimension of the attractor increases with resolution. This is a good estimate to see how much information or detail of the system is lost purely by the coarser representation. The effect is very large. The number of effective degrees of freedom increases sharply between T21 and T31 from 13.1 to
48.4, so it has a 3.7 times larger effective dimension. The increase from T31 to T42 is only from 48.4 to 77.7 or a 1.6 times increase in effective dimension. These results suggest that the small scales introduced especially between T21 and T31 have a major impact on the general dynamics of the system, while even smaller scales that are introduced when the resolution is increased to T42 have less impact. The small scales seem to add the part which makes the model chaotic or fractal enough to nearly disregard periods of negative local largest Lyapunov exponents as they are very rare in resolutions beyond T21. Due to the reasons given before, this should still be valid for a regionally constrained analysis.

The attractor analysis provides another interesting result. As visible in figure 3.3, the slope of the T42 experiment is greater than the T31 or T21 experiments. Additionally the distances between the phase space points is larger than before, since the curve is below the other ones. This means that the extent of the attractor is much larger in the T42 case than the other cases. This is mainly due to the additional possible directions. The Euclidean distance that is used to measure the distance between the phase space point could be potentially misleading. That is due to the constraint of the imaginary parts of the spherical harmonics. They are cyclic with respect to the interval \([0, 2\pi]\) meaning a value of 0 or a value of \(2\pi\) produces the same pattern. However, this is not accounted for with the Euclidean metric so the imaginary parts could possibly experience jumps in distance between two states, even if they are correlated. The fact that the states are supposed to be uncorrelated should alleviate the mentioned problem with the metric, but not eliminate it.

Figure 4.1 — Distribution of the local largest Lyapunov Exponent evaluated for specific regions. The means are almost identical, the variances differ greatly.
4.1 Lyapunov analysis

One of the reasons why the attractor analysis is done is to find a connection to the Lyapunov spectrum. The spectrum, as mentioned in chapter 2.1.2, together with the Lyapunov vectors define all the dynamics of the system. However, computing the spectrum, especially the global spectrum where long time series are necessary, is extremely time intensive and costly in terms of computer resources. Furthermore, conducted tests have shown that the commonly used method to compute the spectrum (Ramasubramanian and Sriram, 2000) which is based on an orthonormalisation routine is numerically unstable for more than approximately 3000 vectors. The orthonormalisation fails for the last vectors after some time, even in double precision mode. The more vectors are used, the faster the method fails and there were no meaningful results attainable. For that reason it is desirable to at least get an estimate of how the Lyapunov spectrum might look like. For the global spectrum this can be done through the attractor dimension. As mentioned in chapter 2.1.3 the correlation dimension \( D_2 \) is connected to the Lyapunov dimension \( D_L \) via the information dimension \( D_1 \) through the relation \( D_L = D_1 \geq D_2 \). Often the difference between \( D_1 \) and \( D_2 \) is small (Grassberger and Procaccia, 1983) so the same is assumed for this case and that the Lyapunov dimension and the correlation dimension are equal. The Lyapunov dimension furthermore is slightly larger than \( k \) with \( k \) the largest integer such that \( \sum_{i=1}^{k} \lambda_i > 0 \) is fulfilled. This is the relation to the Lyapunov spectrum or at least a small part of the spectrum. The spectrum has as many exponents and vectors as there are dimensions in phase space, but the attractor dimension is much lower than that. The ballpark assumption for the number of positive Lyapunov exponents is now that it is one third the value of \( k \). This is of course a very uncertain assumption. The guess of one third is inspired by results of quasi-geostrophic experiments where the Lyapunov-Exponent distribution was convex for the largest ones (Vannitsem and Nicolis, 1997; Snyder and Hamill, 2003). The relation that must always be true is that the sum of the negative exponents is larger than the sum of the positive exponents (dissipative system). But the negative exponents that just balance the positive ones like here could be very different. In theory it would even be possible that there is only one positive exponent and then several negative exponents that balance this single positive one. However, for a complex model such as PUMA it is unlikely that there is only one positive exponent. This is another reason why the assumption of one third of the value of \( k \) is chosen.

Under the previous assumption the dimension of the attractor is directly related to the number of positive Lyapunov exponents or the number of expanding directions in phase space. This can be an important property to know, for example for ensemble predictions in weather forecasts. There is no sense in choosing an initial condition whose perturbation is pointing in a direction with a negative Lyapunov exponent. This run will not grow apart from the control run. However, all runs initialized into an unstable directions will. And since they are orthogonal they all will produce different results and will not all align into the most unstable direction as random perturbations would. Calculating some orthogonal vectors however still is a problem with traditional methods as mentioned before. Still this method has been proposed
to be used for ensemble weather predictions (Keller et al., 2010).

Figure 4.2—Panel of the surface pressure difference between the model instances. Time elapsed between the plots is one day or 48 time steps.
4.2 Fluctuation Theorem

The Fluctuation Theorem has got a lot of attention over the last years as many cases of applicability in physics (Ciliberto et al., 2004) or micro-biology (Collin et al., 2005) were discovered. Here the Fluctuation Theorem is adopted from a dynamical systems perspective. Instead of using a version with thermodynamic entropy (Bustamante et al., 2005), the entropy of a dynamical system (Young, 2003) is used instead. As mentioned in section 2.1.2 the Lyapunov spectrum is required to calculate the entropy of a dynamical system. The previous chapter showed that the Lyapunov spectrum cannot be attained easily for a system with comparatively large number of degrees of freedom. To this end an approximated version of the entropy is used as defined by Benettin et al. (1976). In their study they showed that this entropy-like quantity has some similarities to the entropy, however, some relations that are proven for the entropy are not true for this property. This property remains a way to approximate the concept of the fluctuation theorem. Since not the entropy itself but its production is needed for the Fluctuation Theorem the entropy production must be known. The entropy production (Young, 2003) is defined as less or equal the sum of all positive Lyapunov exponents for dissipative dynamical systems. This means if the largest local Lyapunov exponent is negative, the entropy production is negative as well. Therefore the local largest Lyapunov exponent is in this context in close relation to the actual entropy production. Since there is to the knowledge of the author no other simple way to approximate the entropy production, this method is used.

The results are split so that they could be assessed for individual growth times $\tau$. When the results are compared to results of turbulent flows using the full entropy (Gilbert, 2004) some similarities can be found. The probability distribution (Figure 1 in their study) for the measured values is similar to the results obtained here, even though the actual values are much smaller. The distribution is almost Gaussian with the possible exception of the tails which are represented much further than here due to more available data. This is the reason why they were able to get a much more reliable linear relationship for the left hand side of equation (2.16). Another study by Ciliberto et al. (2004) has very similar results for experimental data rather than simulations.

The results in this study regarding the validity of the Fluctuation Theorem in the context of atmospheric circulation models is shown in figure 3.9 and 3.10. The former figure establishes the necessary relationship between the left hand side of equation (2.16) and the entropy production $\Sigma$, while the latter figure confirms the relationship with respect to the growth time $\tau$. With respect to the entropy production the uncertainty of the data points becomes increasingly larger with the value $a$ of the entropy production. This is because of the data available from the histogram on which this analysis is based. If the number of observations in the bin for the value $-a$ is very small, it becomes very sensitive. If for example the value for $+a$ was 500 and the value for $-a$ was 3, the logarithm of the left hand side would be 5.12. However, if the value for $-a$ was 2 instead, the result would be 5.52. So a small
change in the value for $-a$ has a large influence if it is very small. In this case this is the reason why the data points become more uncertain. In addition to that the number of data points plotted is restricted up to the point where the first empty bin in the histogram is encountered. A much longer time series can resolve this issue and it would be possible to establish the relation for larger values of the entropy production as well. Furthermore, the larger the resolution, the lower the probability to observe negative values of entropy production at all. Consequently, to show the same relation for higher resolutions even longer time series would be necessary.

With respect to the relation with $\tau$ figure 3.10 shows that the relation is found for values of $\tau$ larger than 160 h. This is not an issue though since the relation is valid for large $\tau$ (Evans and Searles, 1994). The solid line in this figure is created by a least-square fit to all data points with $\tau \geq 160$ h with the additional requirement to go through the origin. Since there is no drift of the data points to one or another direction visible it can be assumed that the relation with respect to $\tau$ holds.

While the above results strongly suggest that the Fluctuation Theorem is valid for PUMA in a low resolution environment, future studies that consider the whole spectrum of Lyapunov exponents are needed to validate this result.

An important question with regard to the more complex general circulation models is if any of the results found here are important for these models as well. There is some evidence that the effect described by the Fluctuation Theorem can be important in these models even in high resolutions. However, this effect will probably be very localised both in time and space. If the degrees of freedom within the considered local framework are in the same order of magnitude than for the PUMA model, the effects described by the Fluctuation Theorem could occur. A counter argument would be that on these then much smaller spatial scales the dynamics are no longer restricted to the few processes that are available in PUMA. This could change the dynamical behaviour fundamentally such that the Fluctuation Theorem is no longer applicable. On the other hand there are some smaller scale phenomenons like for instance fronts that could be similar to the PUMA model as the underlying dynamics are similar albeit on different spatial scales. In the end it is not clear if the effects found here can be transferred to more complex models.

4.3 Skewness and kurtosis

Deviations from Gaussianity are assessed by calculating the higher moments of the observed distributions of the error growth in PUMA for the global analysis as well as for spatially confined regions. The results in section 3.6 show no clear skewness-kurtosis relationship as the results from Alberghi et al. (2002) and Cristelli et al. (2012). The size of the sub-samples is chosen to be 100 and there might be some problems connected to this choice. For once the individual samples need to be independent. In this case the 100 samples are directly 100 subsequent results for one day error growth. Two nearby values are therefore not independent. The length of 100 should be long enough such that there are sufficient independent samples,
4.4 Nonlinear error growth

however, this can not always guaranteed. Extending the individual sample size to 1000 did not change the result. Figure 4.3 shows the result for the global case for $N = 1000$. While the scatter-plot is thinned due to the smaller number of individual distributions, the locations do not change compared to the original result (figure 3.17).

![Figure 4.3](image)

Figure 4.3— As figure 3.17 but for $N = 1000$.

4.4 Nonlinear error growth

Nonlinear error growth is reached when the perturbation can no longer be considered small with respect to the underlying process. However, as evident by the results in section 3.3 a different error growth pattern is not observed in PUMA even for large perturbations.

A study by Harlim et al. (2005) that has investigated growth rates of errors has found that for atmospheric processes there are three major regimes of growth. The slowest and least affected by non-linear interactions is identified as baroclinic instability. This type of error growth dominates after the initial small error has grown too far for the other processes. The fastest process which is on the time scale of up to an hour is identified with turbulence. Here initial errors grow very rapidly until non-linear interactions stop further error growth. From then onward on a time scale of hours up to one day a process identified as convection takes over and is the main driving process for error growth. Its growth rates are lower than for turbulence but non-linear interactions start to become important at far larger errors. From then onward on the time scale of days baroclinic instability has the
lowest error growth rates but is uninfluenced by non-linearities until the error gets even larger.

From this study it is probable that the error was still not large enough to be in the non-linear region for baroclinic instability. Since turbulence or convection are not simulated in PUMA, the growth rate of infinitesimal errors can only be influenced by baroclinic processes, so the error growth patterns do not differ even for large errors. In higher resolution models and especially in models that model convection, the infinitesimal error growth and error growth of the larger errors will almost certainly be different.

4.5 Error growth and Eady growth rate

The major aspect in this chapter is to link the instability assessed by error growth with traditional meteorological methods. In PUMA the sole unstable process that is a major part of the dynamics is baroclinic instability. It is therefore logical to believe that the regions with largest average error growth (and therefore largest average error or distance between the model instances) are the regions with the highest activity of baroclinic instability. Another often used tool to identify regions of large baroclinic instability is the Eady growth rate (Hoskins and Valdes, 1990). However, as seen in section 3.4 the regions of largest error growth and the regions of high values of Eady growth rate differ.

Eady growth rate mainly consists of two parts. One part is mainly the vertical wind gradient while the other part is dependent on the static stability of the atmosphere and therefore dependent on the vertical temperature gradient. Additionally Eady growth rate is often computed above the boundary layer (Hoskins and Valdes, 1990) since processes in the boundary layer can often have misleading influence on the Eady growth rate. In PUMA the boundary layer is disregarded as well even though it would not strictly be necessary since boundary layer processes are not resolved and the difference would be a larger wind gradient due to surface friction.

In contrast to more advanced models, the vertical stability of the atmosphere in PUMA is relatively homogeneous due to missing moist processes. The values are slightly higher at the equator than at the poles, but they differ far less than the total difference in the Eady growth rate. The vertical wind gradient, however, differs significantly between the jet regions around 40° north and south and the poles and equator. Both phenomenons can be seen in figure 4.4. There the Coriolis parameter $f$ and the the Brunt-Vaisala frequency $N$ are combined to $f/N$ and the zonal mean plotted. The same is done for the total Eady growth rate and the vertical wind gradient although they have been scaled to fit into one plot. It is evident that the Eady growth rate is primarily defined by the vertical wind gradient in PUMA, the part $f/N$ has minor influence since it is very homogeneous with the exception of the equator region. The main reason for this is once again the coarse resolution of PUMA. In this resolution no real fronts can develop since they are not resolved. But regions with highest Eady growth rates are typically the frontal zones (Hoskins and
4.6 Potential vorticity and error growth

Potential Vorticity as such is not useful to identify regions of baroclinicity as its values are dominated by the Coriolis parameter $f$. However, the deviations from the mean state contain some information. This is due to the definition of potential vorticity and the fact that it is a conserved quantity along a trajectory. This in turn mandates that in regions with developing cyclones the variability of the potential vorticity is largest. Since development of cyclones is directly related to baroclinic instability, regions of high error growth and large variability of potential vorticity are supposed to be the same. Indeed, the results from chapter 3.5 show a very good agreement between the error growth and potential vorticity variance. This would furthermore mean, that regions with large baroclinicity as assessed from the

Figure 4.4— Zonal mean values of the Eady growth rate, the vertical wind gradient $du/dz$ and the factor $f/N$. The Eady growth rate has been scaled down by a factor of 20, while the vertical wind gradient has been scaled up by a factor of 10 so that all three distributions can be plotted into one figure. The y-axis scale is therefore only correct for the factor $f/N$.


In conclusion it can be assumed that the Eady growth rate is not an efficient tool to assess regions of baroclinic instabilities in low resolution models, at least when moist processes are disregarded. In contrast to the Eady growth rate, the error growth analysis is more demanding as it can not be performed after the simulation by using the meteorological output of the model. As a first guess Eady growth rate still has some value in low resolution experiments.
Eady growth rate and regions of large baroclinicity as assessed by the potential vorticity are not the same. But since both are used to locate the regions of largest baroclinicity one has to settle for one of these indicators. The argument in favour of the Eady growth rate is that it is designed to locate atmospheric states with a high potential for instabilities to occur as either the vertical or horizontal setup is unstable. The potential vorticity on the other hand analyses regions where the developing and developed instabilities occur. The Eady growth rate has therefore some value for prediction as an instability may not yet exist, while the potential vorticity analysis will just pinpoint the current position of instabilities that have already developed.

In addition to the spatial distribution of error growth, Eady growth rate and potential vorticity deviations, the general distributions are investigated in the respective sections of the previous chapter (figures 3.13, 3.14 and 3.16). These results provide further evidence that error growth and potential vorticity deviations are more similar to each other than Eady growth rate. Both potential vorticity (figure 3.16) and error growth (figure 3.14) are alike in terms of general features of their distributions, the Eady growth rate however shows distinct differences as presented in chapter 3.4. In general, the Eady growth rate is distributed more uniformly, while error growth and potential vorticity deviations have rare peaks of very high values.

4.7 Blocking and stability

The results for blocking with regard to stability and predictability are not conclusive, however, but there are some hints as to why this is the case.

The simplest reason for these results is the model itself and the resolution that is used. T42 with 10 vertical layers is the absolute minimum that is required to get any blocking at all. If the modified Tibaldi-Molteni method from section 2.4.2 is used, the remaining blocking is extremely low, often not even 1%.

There are other reasons why the PUMA model is probably not very well suited for the task to simulate blocking. A study suggests that blocking, once it is formed, is maintained by transfer of angular momentum from smaller eddies to the blocking anticyclone (Shutts, 1983). However, T42 as a resolution is not sufficient enough to simulate these smaller eddies. This is probably the main reason, why blocking is far more realistic in T85 resolution (Schalge, 2010).

In addition to this there are even more phenomena that support blocking (e.g. (Tschuck, 1998; Palmer et al., 1986)), all of which are processes not resolved or regarded in PUMA.

4.8 Conclusions

In conclusion, many of the presented results are in agreement with similar studies. The most striking difference is the fact that negative local largest Lyapunov exponents were not previously observed for quasi-geostrophic experiments, even though
they are from a theoretical point of view simpler than the primitive equation model used here. It seems that the primitive equations have more potential to produce such behaviour.
Chapter 5

Summary and outlook

5.1 Summary

In this study, the dynamical systems theory is employed to assess predictability in the global atmospheric circulation Model PUMA. The general experiment setup features the model run in two parallel instances such that one of the instances serves as a reference run, while the other run is the main run that is used for the investigation. The focus of the predictability analysis lies on the assessment of the growth of errors. For this purpose the two model runs are initialised with slightly different initial conditions and the evolution of this difference is subsequently analysed. The mean rate with which this difference grows with time is the global Lyapunov exponent. Larger values for these exponents indicate lower predictability and fast error growth. In non-chaotic systems where errors are not amplified by the dynamics this exponent vanishes. A sensitivity study is conducted where the Lyapunov exponent is calculated for different values of the pole-equator temperature gradient that drives the model. Very low gradients result in vanishing Lyapunov exponents and consequently non-chaotic dynamics, while larger gradients show increasing Lyapunov exponents indicating a dependence of predictability on the temperature gradient. Furthermore, a clear dependence on the model resolution is found as Lyapunov exponents in the T42 resolutions were approximately twice as large as the corresponding exponents in the T21 case. In addition to the largest Lyapunov exponent, the Lyapunov spectrum provides further insight into the dynamics of the system. Since the spectrum is not available directly, an indirect method to approximate the number of positive Lyapunov exponents is applied. This method utilises the link between different attractor dimensions and the Lyapunov spectrum to give a first guess for the number of positive Lyapunov exponents.

This global assessment of predictability is supplemented by a local analysis. Here the growth rate of errors is analysed for shorter time intervals in the order of days. The result is a local largest Lyapunov exponent that is dependent on the state of the system. The mean value of the local largest Lyapunov exponent is identical to the global largest Lyapunov exponent, however, individual values fluctuate and there are periods found where the exponent becomes negative. These periods are
especially common for low resolution experiments. A statistical evaluation of these fluctuations shows that they were nearly Gaussian and that the probability to observe negative values decreases with the length of the time interval for which the growth is assessed. Negative values of error growth become increasingly unlikely with increasing horizontal resolution and therefore increasing degrees of freedom. The fluctuations are checked whether they obey the relations of the fluctuation theorem. Therefore a relation between error growth and the entropy production of the system is established and subsequently the growth rates are used as surrogates for the actual entropy production that is not available. Consequently the applicability of the fluctuation theorem can only be shown in an approximated way. The analysis confirms that the fluctuations are in accordance with the fluctuation theorem in this context. Additionally it is investigated whether larger initial errors show the same growth characteristics than the infinitesimal errors used before. According to theory the whole analysis is only valid for small errors, however, no different behaviour is found even for clearly non-infinitesimal errors. The deviations of the considered distributions from Gaussianity is assessed and skewness-kurtosis relations, common in many system, are investigated.

While these methods provide a unique insight into the model dynamics they provide very little information about the spatial distribution of error growth. For this reason the difference itself is analysed and its distribution evaluated. The mid-latitudes are identified as the regions with the largest mean error growth but also with the largest fluctuations. To put this result into perspective traditional methods to assess predictability are used for comparison. The Eady growth rate shows distinct differences as the region of largest growth rates is shifted equator-wards, while the analysis of the deviations of potential vorticity from the zonal mean show very similar distributions with regard to the error growth pattern. The reasons for the differences are discussed and most probably it is due to the different definitions of instability.

The study concludes with the attempt to find a link between the error growth rates and blocking. Blocking is of general importance due to its persistent nature. During a blocking period the atmospheric circulation is very stable in the vicinity of the block and it is theorised that this would be visible in low or even negative values of error growth. However, the link can not be established as the global analysis of the error growth shows no correlation with large, but on a global scale still local phenomena like blocking.

5.2 Outlook

This study has several areas where further research can be conducted. Calculating the Lyapunov spectrum for a primitive equation global circulation model is perhaps the most challenging task from a technical and computational perspective, but it opens up a large area to explore. The spectrum as such possesses some valuable information about the dynamics of the system that could only be crudely guessed in
5.2 Outlook

this study. Furthermore, a rigorous investigation whether the fluctuation theorem is valid for PUMA would become possible. The entropy could be calculated and would not have to be approximated and the Lyapunov dimension could be calculated directly and compared to the results of the correlation dimension as calculated.

5.2.1 Computational Restrictions

This work would need some serious advancement in most computational aspects. Calculating the Lyapunov spectrum requires either the recurring orthonormalisation of large sets (around $10^4$ for the lower resolutions) of vectors or the calculation of eigenvalues and eigenvectors for equally large matrices. Computers these days are not used to their full potential by existing subroutines or methods as they are either written for single-thread programs or they may even become numerically unstable for the large number of vectors and exponents. The latter phenomenon was experienced here first-hand with the attempt to orthogonalise a set of vectors that formed the basis of a T21L5 PUMA experiment. The method did successfully orthogonalise the first 9000 vectors, but any additional vectors were no longer orthogonal. The currently available software for extensive computation tasks such as these are not yet synchronised with the massively parallel computational background. Almost all software would have to be re-written and sometimes new numerical methods would certainly be necessary to close the current gap between the theoretical and actual potential to compute all the mentioned properties of a high-dimensional dynamical system.

Once these obstacles are overcome though, the whole analysis could be extended to more complex models with moist processes. However, much higher resolutions or far more complicated models would still be out of reach. Even though the models themselves often scale well with parallel setups it would still take too long to run these models for sufficiently long times needed by the methods presented in this study. Most methods require time series of considerable length to get meaningful statistics.

5.2.2 Relation to other meteorological analyses

One of the main items of this study was the investigation of the error growth from a dynamical systems perspective and its relation to other measures of predictability in general that have been used in meteorology. In addition to the Eady growth rate, potential vorticity and blocking there are other partly related analyses like wave-breaking, storm tracks or singular vector analysis that could complement the methods used in this study. Singular vectors, however, are closely related to Lyapunov vectors and their computation would be equally difficult than the computation of the Lyapunov spectrum.

One point that can be expanded is the relation between blocking and error growth. As seen in this study the relation at least on a global scale is very loose if there is any at all. However, a detailed study for regions with high blocking activity like the
Atlantic-European region could lead to better results and even a rigorous connection between the onset or decay of blocking and the error growth rate.

5.2.3 Subscale predictability and parametrisations

One speculative scope of application of the dynamical systems analysis regards the parametrisations of subscale processes in models. Different processes will have different error growth characteristics and subsequently will have varying impacts on the large scale evolution of errors. Most of the processes are parametrised and might therefore show very different error growth characteristics compared to the same process if it was resolved. An analysis of the resolved process in a separate model can give valuable information about error growth patterns and rates as well as constraints as to how large an error can become by the considered process. As a result, processes with a large possible impact on the large scale dynamics can be identified and possibly information about the error growth dynamics can be incorporated into the parametrisations to improve the whole model.
Appendix A

Appendix

The Appendix has a printed part and an electronic part.

A.1 Appendix Part A

This appendix consists of additional figures that supplement figures in other parts of the study.

![Graph showing log(ε) versus log(S(ε)) with curves labeled T21, T31, T42.]

Figure A.1 — As figure 3.3 but the whole range of $\log S(\epsilon)$ is shown rather than the linear regime.
Figure A.2— As figure 4.2 but for the absolute value of the difference.
A.2 Appendix Part B

This part of the appendix is available on the enclosed data storage device. It follows a List of contents.

- A MATLAB movie of the evolution of the difference between the two model instances for the surface pressure in T15L3 resolution. It shows the evolution of the difference over 2000 time steps. The rescaling after one day or 48 time steps become visible and it is evident if the total error grew or not. However the movie only shows the pressure part of the total error. The ’playmovie.m’ files need to be executed in MATLAB to view the video.

- The same movie as above but for the absolute value of the difference.

- The two movies above, converted into MPEG-4/AVC format.

- The source code of the Lyapunov subroutine and child subroutines that include the Eady growth rate and the potential vorticity.

- The source code of the blocking detection program.

- This document as a PDF file.
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Nomenclature

\((\Delta T_R)_{EP}\) Equator to Pole Temperature Gradient

\((\Delta T_R)_{NS}\) Pole to Pole Temperature Gradient

\(\bar{\Sigma}\) Mean Entropy Production Rate [1/day]

\(\dot{\sigma}\) Vertical Velocity in Sigma-System

\(\hat{\lambda}\) Largest Local Lyapunov Exponent [1/day]

\(\kappa\) Adiabatic Coefficient

\(\lambda\) Largest Lyapunov Exponent [1/day] or Longitude

\(\lambda_i\) i-th Lyapunov Exponent [1/day]

\(\omega\) Vertical Velocity in p-System

\(\Phi\) Geopotential

\(\rho\) Air Density [kg/m\(^3\)]

\(\Sigma\) Entropy Production Rate [1/day]

\(\sigma_{\text{tp}}\) Tropopause Level

\(\tau_F\) Friction Timescale

\(\tau_H\) Hyperdiffusion Timescale

\(\tau_R\) Heating Timescale

\(\Theta\) Potential Temperature

\(\zeta\) Relative Vorticity

\(a\) Planet Radius

\(D\) Divergence

\(d, d_0\) Distances
$D_1$ Information Dimension
$D_2$ Correlation Dimension
$D_L$ Lyapunov Dimension
$D_q$ Renyi Dimension
$E$ Eady Growth Rate
$f$ Coriolis Parameter
$g$ Gravitational Acceleration = 9.81 m/s$^2$
$H_B$ Hyperdiffusion of Variable B
$J$ Diabatic Heating Rate
$N^2$ Brundt-Vaissala Frequency
$p$ Atmospheric Pressure [Pa]
$P_B$ Parameterisation Concerning Variable B
$p_s$ Surface Pressure
$PV$ Potential Vorticity
$R$ Gas Constant
$T$ Temperature
$T'$ $T - T_0$
$T_0$ Heat Capacity of Dry Air at Constant Pressure
$T_0$ Reference Temperature
$u$ Zonal Wind
$v$ Meridional Wind or a Vector
$Y$ Spherical Harmonics
$z$ Height [m]
$z_{tp}$ Height of Tropopause
Bibliography


Publications derived from this dissertation