Gyrokinetic Large Eddy Simulations

Alejandro Bañón Navarro
Supervisor: Prof. Daniele Carati

Physique statistique et des plasmas

Université Libre de Bruxelles

A thesis submitted for the degree of

Philosophiæ Doctor (PhD) in Physics

2012 July
The Thesis Jury

Prof. Daniele Carati
Université Libre de Bruxelles

Prof. Pierre Gaspard
Université Libre de Bruxelles

Prof. Bernard Knaepen
Université Libre de Bruxelles

Prof. Frank Jenko
Max-Planck-Institut für Plasmaphysik

Dr. Özgür D. Gürcan
École Polytechnique

Defense date: 25th of October, 2012
ABSTRACT

Anomalous transport due to plasma micro-turbulence is known to play an important role in confinement properties of magnetically confined fusion plasma devices such as ITER. Indeed, plasma turbulence is strongly connected to the energy confinement time, a key issue in thermonuclear fusion research. Plasma turbulence is described by the gyrokinetic equations, a set of nonlinear partial differential equations. Due to the various scales characterizing the turbulent fluctuations in realistic experimental conditions, Direct Numerical Simulations (DNS) of gyrokinetic turbulence remain close to the computational limit of current supercomputers, so that any alternative is welcome to decrease the numerical effort. In particular, Large-Eddy Simulations (LES) are a good candidate for such a decrease. LES techniques have been devised for simulating turbulent fluids at high Reynolds number. In these simulations, the large scales are computed explicitly while the influence of the smallest scales is modeled.

In this thesis, we present for the first time the development of the LES for gyrokinetics (GyroLES). The modeling of the smallest scales is based on free energy diagnostics. Indeed, free energy plays an important role in gyrokinetic theory, since it is known to be a nonlinear invariant. It is shown that its dynamics share many properties with the energy transfer in fluid turbulence. In particular, one finds a (strongly) local, forward (from large to small scales) cascade of free energy in the plane perpendicular to the background magnetic field.

The GyroLES technique is implemented in the gyrokinetic code GENE and successfully tested for the ion temperature gradient instability (ITG), since ITG is suspected to play a crucial role in gyrokinetic micro-turbulence. Employing GyroLES, the heat flux spectra obtained from highly resolved direct numerical simulations are recovered. It is shown that the gain of GyroLES runs is 20 in terms of computational time. For this reason, Gyrokinetic Large Eddy Simulations can be considered a serious candidate to reduce the numerical cost of gyrokinetic simulations.
RÉSUMÉ DE LA THÈSE

Le transport anormal de l’énergie observé en régime turbulent joue un rôle majeur dans les propriétés de stabilité des plasmas de fusion par confinement magnétique, dans des machines comme ITER. En effet, la turbulence plasma est intimement corrélée au temps de confinement de l’énergie, un point clé des recherches en fusion thermonucléaire.

Du point de vue théorique, la turbulence plasma est décrite par les équations gyrocinétiques, un ensemble d’équations aux dérivées partielles non linéaires couplées. Par suite des très différentes échelles spatiales mises en œuvre dans des conditions expérimentales réelles, une simulation numérique directe et complète (DNS) de la turbulence gyrocinétique est totalement hors de portée des plus puissants calculateurs actuels, de sorte que démontrer la faisabilité d’une alternative permettant de réduire l’effort numérique est primordiale. En particulier, les simulations de grandes échelles (“Large-Eddy Simulations” - LES) constituent un candidat pertinent pour permettre une telle réduction. Les techniques LES ont initialement été développées pour les simulations de fluides turbulents à haut nombre de Reynolds. Dans ces simulations, les plus grandes échelles sont explicitement simulées numériquement, alors que l’influence des plus petites est prise en compte via un modèle implémenté dans le code.

Cette thèse présente les premiers développements de techniques LES dans le cadre des équations gyrocinétiques (GyroLES). La modélisation des plus petites échelles est basée sur des bilans d’énergie libre. En effet, l’énergie libre joue un rôle important dans la théorie gyrocinétique car elle en est un invariant non linéaire bien connu. Il est démontré que sa dynamique partage de nombreuses propriétés avec le transfert d’énergie dans la turbulence fluide. En particulier, il est montré l’existence d’une cascade d’énergie libre, fortement locale et dirigée des grandes échelles vers les petites, dans le plan perpendiculaire à celui du champ magnétique ambiant.

La technique GyroLES est aujourd’hui implantée dans le code GENE et a été testée avec succès pour les instabilités de gradient de température ionique (ITG), connues pour jouer un rôle crucial dans la micro-turbulence gyrocinétique. À l’aide des GyroLES, le spectre du flux de chaleur obtenu dans des simulations à très hautes résolutions est correctement reproduit, et ce avec un gain d’un facteur 20 en termes de coût numérique. Pour ces raisons, les simulations gyrocinétiques GyroLES sont potentiellement un excellent candidat pour réduire l’effort numérique des codes gyrocinétiques actuels.
# Table of Contents

1 Introduction
   1.1 Motivation .................................................. 1
   1.2 Nuclear Fusion ............................................... 1
   1.3 Plasma dynamics ............................................. 3
      1.3.1 Particle and fluid drifts ............................ 4
   1.4 Toroidal plasmas ............................................. 5
   1.5 Radial transport processes in plasmas .................... 8
   1.6 Turbulent transport ......................................... 9
   1.7 Plasma drift-wave micro-instability ..................... 11
      1.7.1 Ion temperature gradient mode (ITG) ............... 12
      1.7.2 Electron temperature gradient mode (ETG) ......... 13
      1.7.3 Trapped electron mode (TEM) ....................... 14
      1.7.4 Spatial scales of the turbulence ................... 14
   1.8 Simulation of drift-wave instabilities .................. 15
   1.9 Outline of the thesis ...................................... 17

2 Gyrokinetics and the GENE code
   2.1 The Vlasov-Maxwell system ............................... 19
   2.2 The gyrokinetic ordering .................................. 20
   2.3 Modern derivation of the gyrokinetic equation ........ 22
      2.3.1 The one-form guiding center Lagrangian .......... 23
      2.3.2 The one-form gyrokinetic Lagrangian .......... 25
   2.4 The gyrokinetic equation .................................. 28
   2.5 The gyrokinetic field equations ......................... 29
   2.6 Field aligned coordinate system ......................... 32
      2.6.1 Local flux-tube approximation ..................... 32
      2.6.2 Magnetic equilibrium geometry ................... 34
   2.7 The nonlinear gyrokinetic GENE code .................. 35
      2.7.1 Normalization ........................................ 35
      2.7.2 The gyrokinetic equation solved in GENE ........ 37
      2.7.3 The gyrokinetic field equations solved in GENE .. 39
      2.7.4 Adiabatic electron response ....................... 40
      2.7.5 Adiabatic ion response ............................ 41
      2.7.6 Transport quantities ............................... 41
# TABLE OF CONTENTS

3 Large-Eddy Simulations ........................................... 43
   3.1 Introduction to fluid turbulence .......................... 43
      3.1.1 The inertial range cascade ......................... 46
      3.1.2 The Kolmogorov spectrum ......................... 46
   3.2 Simulation of fluid turbulence ......................... 47
   3.3 Introduction to Large-Eddy Simulations ............... 49
      3.3.1 Sub-grid modeling .............................. 52
      3.3.2 The Smagorinsky model ......................... 53
      3.3.3 The dynamic procedure ......................... 55
   3.4 Extension of the LES approach to conductive fluids .. 57

4 Free energy cascade in gyrokinetic turbulence ............ 59
   4.1 Overview ........................................... 59
   4.2 Free energy in kinetic systems ........................ 60
   4.3 Derivation of the balance equation ................... 61
      4.3.1 Time derivative ................................ 61
         4.3.1.1 Kinetic term ............................ 62
         4.3.1.2 Electromagnetic terms .................... 63
         4.3.1.3 Total time derivative .................... 64
      4.3.2 Linear part .................................... 64
         4.3.2.1 Equilibrium density and temperature gradients . 65
         4.3.2.2 Magnetic curvature ....................... 66
         4.3.2.3 Parallel term ............................ 66
      4.3.3 Numerical dissipation ............................ 67
      4.3.4 Contribution of the nonlinear term ............... 68
   4.4 The free energy balance equation .................... 69
      4.4.1 Free energy balance: Adiabatic electrons .......... 69
      4.4.2 Free energy balance: Adiabatic ions ................ 70
   4.5 Simulation results: Cyclone Base Case ............... 70
      4.5.1 Free energy conservation by the nonlinear term . 71
      4.5.2 Time evolution of the free energy components .......... 71
      4.5.3 Free energy transfers .......................... 73
   4.6 Summary and conclusions .............................. 78

5 Free energy studies for gyrokinetics ....................... 81
   5.1 Entropy and electrostatic energy operators .......... 81
      5.1.1 Derivation of the entropy balance equation ........ 82
      5.1.2 Derivation of the electrostatic energy balance equation .. 83
      5.1.3 Final equations ................................ 84
   5.2 Simulation results: Cyclone Base Case ............... 85
      5.2.1 Entropy and electrostatic time evolution .......... 85
      5.2.2 The effect of the collision operator ............. 86
      5.2.3 Local free energy balance ........................ 87
   5.3 Summary and conclusions .............................. 89
## TABLE OF CONTENTS

6 Extension of the LES approach to gyrokinetics 93  
6.1 The filtered gyrokinetic equation 93  
6.2 The filtered free energy balance equation 96  
6.3 The physics of the sub-grid term 97  
6.3.1 The sub-grid term contribution 97  
6.3.2 Role of the sub-grid term 97  
6.3.3 Final remarks 98  
6.4 Developing a gyrokinetic LES model 99  
6.4.1 Calibration of the model 100  
6.5 Computational gain 101  
6.6 Accuracy of the GyroLES model 101  
6.7 Estimate for the global quantities 102  
6.8 Limitations of the GyroLES model 106  
6.8.1 Lower turbulent case 106  
6.8.2 Higher turbulent case 106  
6.9 Conclusions 108  

7 Dynamic procedure for GyroLES 109  
7.1 An improved model for the sub-grid term 109  
7.2 Dynamic procedure for gyrokinetics 111  
7.3 Numerical results: Cyclone Base Case 115  
7.4 Computational gain 117  
7.5 Robustness while varying the logarithmic temperature gradient 118  
7.6 Robustness while varying the magnetic shear 120  
7.7 Conclusions 123  

8 Conclusions 125  

A Generic derivation of a Poisson bracket integration 129  

B On the free energy 131  

C On hyperdiffusion and associated free energy 137  

Glossary 139  

Bibliography 143  

Acknowledgements 150  

Declaration 151  

Publications 152
Chapter 1

INTRODUCTION

1.1 Motivation

In many complex systems, simulating the entire dynamics is definitively out of reach of today’s computers. Examples of such complex systems can be found in geophysics, with the study of the dynamics of the atmosphere systems and the oceans; in astrophysics, with the study of the evolution of stars and galaxies; in aeronautics, with the study of airplanes; and of course in nuclear fusion, with the study of tokamak plasmas (see Fig. 1.1). There are several options that one can take instead of solving the entire dynamics (or the full set of first-principle equations) for the complete problem: one can simulate a simplified model using a transport code; one can simulate simpler problems, for example using a simplified geometry; one can simulate only a sub-domain of the problem, for example simulating the plasma core without plasma wall interactions, etc. These examples are taken from tokamak physics, but similar approaches have been developed in the simulation of geophysical, astrophysical, biological and industrial problems. Another option, which has been considered mainly in the simulation of turbulence in fluids, is to perform under-resolved simulations of the first-principle equation. The idea is to use much lower resolution than the one imposed by the physics of the problem. Here, the smallest scales are filtered out and their influence is modeled. In fluid turbulence, this approach is known as Large-Eddy Simulations (LES). The main objective of this thesis is to explore the advantages of transposing LES to the field of nuclear fusion and, in particular, to the modeling of the tokamak system. For this reason, a brief introduction to this field will be given in following sections before presenting the outline of the thesis.

1.2 Nuclear Fusion

The controlled nuclear fusion of hydrogen isotopes holds the promise of a practically inexhaustible source of energy. The most favorable fusion reaction is between deuterium (D) and tritium (T):

\[ \text{D} + \text{T} \rightarrow \text{He}^4 + \text{n} + 17.6 \text{MeV}. \]  

(1.1)

This reaction creates an Helium-4 (or \( \alpha \)-particle), releases a neutron (n) and produces 17.6 MeV of energy.
In order to get a sustainable fusion reaction and produce net energy, the mixture of deuterium and tritium must be heated to a temperature of at least 10 KeV (around 100 million degree Celsius) at a density of the order $10^{20}$ particles per cubic meter. At these temperatures the D – T mixture is a fully ionized gas. This ionized gas is called plasma and it consists of a large number of negatively and positively charged particles. In order for the fusion reaction to reach ignition (the heating of the plasma by the products of the fusion reactions is sufficient to maintain the temperature of the plasma against the energy losses) the plasma must be confined for sufficiently long time. This time is known as the confinement time and under the temperature and density above mentioned, must be of the order of one second. These conditions, known in the fusion community as the Lawson criterion, establish the minimum required values for temperature, density and confinement time in order to get a sustainable fusion reaction. The Lawson criterium has not been achieved yet in any fusion device, although the latest generations of machines have come close. These devices use magnetic fields to
confine the plasma. For this reason, the understanding of the behavior and the
dynamics of charged particles in magnetic fields is fundamental. This study is
necessary in order to minimize the losses of particles and energy in a reactor and
in this way, to reach the Lawson criterium and produce net energy.

1.3 Plasma dynamics

The dynamics of the plasma can be described by studying the motion of each
individual particle in the externally imposed electromagnetic field and the fields
generated by other particles in the plasma. However, this is too complex and it
has very little practical use. We have to make certain approximations to facili-
tate analytical and numerical manipulations and to get insight into the plasma
dynamics. In practice, there are three approaches widely used in the plasma
community that turn out to be the most useful:

a) Single particle description

In this approach, the dynamics of the plasma is simplified by considering
a single particle entering a region permeated by electromagnetic fields pro-
duced by some unspecified external force. Although this approach is very
limited since it is only applicable to very dilute plasmas, it explains one
of the most fundamental aspects of a magnetized plasma, the drifts. Here,
the motion of the charged particle is treated as the superposition of a fast
circular motion around the magnetic field line and a slow drift relative to
it.

b) Fluid description

Although a plasma represents an N-body problem, in many cases it is suf-
ficient to reduce the problem to a macroscopic fluid-like description. Here,
statistical averages over small volumes of the plasma give representative
results for the density, temperature and the mean velocity of the charged
particles. In the two-fluid model, the dynamics of the ions and electrons are
described separately, and coupled through electric and magnetic fields as
well as collisions. This model is capable of describing the dynamic evolution
of the plasma self-consistently and covers turbulence driving instabilities as,
e.g., drift-waves (see Section 1.7). Sometimes it is also convenient to treat
the dynamics of the electrons and ions jointly forming a single fluid. This
model, usually referred to as magnetohydrodynamics (MHD), provides the
simplest approach to analyze plasma instability.

c) Kinetic description

A kinetic description of a plasma involving a six-dimensional distribution
function plus time is the most general way to study the plasma dynamics.
Here, the Vlasov equation is used to describe the dynamics of this sys-
tem. This description is often necessary for high temperature (collisionless)
plasmas in order to accurately describe drift-wave type instabilities. However, considering the high dimensionality and complexity of this system, under some assumptions, a gyrokinetic approach may be applied to reduce the number of dimensions. This is the approach used in this work and a detailed description is given in chapter 2.

1.3.1 Particle and fluid drifts

Particle and fluid drifts are fundamental for the understanding of plasma dynamics. They are also crucial in the design and conception of fusion devices and magnetic field geometries. In the following, the most important drifts are discussed.

The interaction of a charged particle with the electric $E$ and magnetic $B$ field is given by the Lorentz force law:

$$m \frac{d\mathbf{v}}{dt} = q \mathbf{E} + q \mathbf{v} \times \mathbf{B}, \quad (1.2)$$

where $m$ and $q$ are the mass and the charge of the particle, respectively. When the Lorentz force reduces to a constant electric field, the particle will undergo a uniform acceleration in the direction of the field. On the contrary, if there is only a uniform and stationary magnetic field, the particle will perform a helical motion wrapping itself around the magnetic field line, with the cyclotron (or gyro) frequency $\Omega$ and an average gyro radius (or Larmor radius) $\rho$ given by:

$$\Omega = \frac{qB}{m}, \quad \rho = \frac{v_\perp}{\Omega} = \frac{mv_\perp}{qB}. \quad (1.3)$$

Here, $v_\perp$ is the velocity perpendicular to the magnetic field.

When the two fields are present simultaneously, the particle no longer remains attached to a single magnetic field line, but rather drifts through space in a direction perpendicular to both the electric and magnetic field. This drift is known as the $E \times B$ drift velocity and is given by:

$$\mathbf{V}_{E \times B} = \frac{\mathbf{E} \times \mathbf{B}}{B^2}. \quad (1.4)$$

It is independent of the charge and the mass of the particles. As a result, it is in the same direction for negatively and positively charged particle. Therefore, there is not electric current associated with this drift.

Particles moving along magnetic field lines in curved and inhomogeneous magnetic field also experience drifts, which are due to the centrifugal forces and gradients in the magnetic field, respectively. The curvature and the gradient drift velocities are given by

$$\mathbf{V}_c = \frac{2W_\parallel R_c}{qR_c^2} \frac{\mathbf{R}_c \times \mathbf{B}}{B^2}, \quad \mathbf{V}_\nabla B = -\frac{W_\perp \nabla B \times \mathbf{B}}{q \frac{B^3}{B^2}}. \quad (1.5)$$
1.4 Toroidal plasmas

Here, $W_\parallel$ and $W_\perp$ are the kinetic particle energy parallel and perpendicular to the magnetic field and $R_c$ is the curvature radius of the magnetic field line. These drifts depend on the charge of the particles. Consequently, they lead to charge separation and the creation of an electric current.

Another drift that only appears in the fluid description of the plasma and is related to gradients in the plasma pressure $p = nT$ is the diamagnetic drift velocity:

$$V_D = -\frac{\nabla p \times B}{nqB^2},$$  \hspace{1cm} (1.6)

where $n$ and $T$ are the plasma density and temperature, respectively. Fig. 1.2 shows the Larmor orbits of positively charged particles gyrating around a magnetic field directed into the paper. The contribution of particles in the presence of a density or temperature gradient produce a mean plasma flow when averaged within a volume element (there is a greater current going to the left than to the right, despite the fact that the guiding centers are stationary [1]).

Figure 1.2: Larmor orbits of ions in the presence of a density gradient. In the enclosed region there is a net current to the left. Adapted from [2].

1.4 Toroidal plasmas

As we mentioned in the previous section, charged particles moving in a homogeneous magnetic field are free to move in the direction parallel to the magnetic field. Hence, in order to confine a hot plasma of sufficiently high density for a sufficiently long time, the magnetic fields must be necessarily inhomogeneous and curved. In this case, the fact that $\nabla \cdot B = 0$ (from Maxwell’s equations) imposes conditions on the topology of the field lines; these fields lines must be either closed, or extend to infinity.

Magnetic fields of the latter type are used in the so-called open configuration fusion devices, the best known of which is the magnetic mirror device. These devices are based on the principle that if the magnetic field becomes stronger as the particle moves along the field, the particle feels a force in the direction away from the stronger field. If the increase in the magnetic field is sufficiently large
1. INTRODUCTION

this force will be able to reflect the particle back along its path. This force is known as the mirror force. However, these devices faced considerable problems in the 70’s and they are no longer used.

On the contrary, closed magnetic field lines are used to confine the plasma in the shape of a torus. The magnetic field lines form nested surfaces, known as magnetic flux surfaces. These surfaces provide the most natural magnetic field based coordinate because most plasma processes (charged particle motion and transport) are much more rapid along magnetic field lines and within flux surfaces than across them. Nevertheless, as a consequence of the magnetic field geometry, curvature and gradient drifts cause a vertical charge separation. Due to this vertical charge separation a vertical electric field is generated and the associated \( E \times B \) drift is always directed away from the torus centre and results in a continuous radial loss of electrons and ions. Fig. [1.3] sketches this effect. In addition, the magnetic geometry including the magnetic flux surfaces is also indicated. In toroidal coordinates, they are represented by the a radius \( r \), poloidal angle \( \theta \) and toroidal angle \( \phi \). Here, the size of the plasma is characterized by the major radius \( R \) and the minor radius \( a \).

Figure 1.3: Schematic of the magnetic field geometry. On left side of the torus the magnetic flux surfaces are indicated. On the right side of the torus the effect of the charge separation due to gradient and curvature drifts and the resulting radial \( E \times B \) drift is sketched.

An effective way to overcome this drift is to twist the magnetic field lines around the major circle of the torus so the drifts cancel out. This works mainly because the drift velocity is much smaller than the velocity along the magnetic field line and also because charged particles essentially remain tied to the magnetic field line. There are two ways to twist the magnetic field lines: by internal currents as in tokamak devices and by external coils as in stellarator devices.

The tokamak (Russian abbreviation for toroidal chamber with magnetic coils, see Fig. [1.4] (left)) is characterized by a large magnetic field in the toroidal direction (traveling around the torus in circles) and a smaller poloidal field (traveling in circles orthogonal to the toroidal field). The toroidal field is produced by external field coils and the poloidal field by a large toroidal current in the plasma.
1.4 Toroidal plasmas

Figure 1.4: A schematic cartoon of a tokamak (left) and a stellarator (right) with their major coils and the plasma shape (yellow). The tokamak is a two dimensional configuration while the stellarator is a three-dimensional configuration. Source: IPP.

The current is induced by a central transformer, being the plasma the secondary circuit. The plasma is limited by a vacuum vessel. In this configuration, the magnetic fields are axisymmetric (independent of the toroidal angle $\phi$). As a consequence, the magnetic fields are characterized by the radial coordinate $r$ and by the poloidal angle $\theta$. Therefore, the tokamak is a two-dimensional configuration.

In tokamaks, the twisting of the magnetic field lines is described by the safety factor $q$. The safety factor represents the number of toroidal rotations per $2\pi$ rotation in the poloidal angle $\theta$. The safety factor in cylindrical approximation is given by

$$q = \frac{r B_\phi}{R B_\theta},$$

where $B_\theta$ and $B_\phi$ are the poloidal and toroidal magnetic field components, respectively.

The stellarator (Fig. 1.4 (right)) is an inherently three-dimensional configuration best described as a helically symmetric system bent into a torus. In contrast to the tokamak, the twist of the magnetic field lines is achieved purely by external magnetic field coils without the use of a transformer. The advantage of this concept is a steady-state operation. The stellarator has one main disadvantage compared to the tokamak, the coil system needed to generate a stellarator magnetic field is more complicated technologically than the tokamak coil system.

In this work, we will focus on the tokamak device since it is considered the most promising way to achieve fusion energy. In particular, with the next stage tokamak ITER (see Fig. 1.5). ITER is a grand international project that aims to demonstrate that fusion is an energy source for the future. It is currently under construction in Cadarache (south of France) and it is expected to produce 500 Megawatts of output power for 50 Megawatts of input power.
1. INTRODUCTION

Figure 1.5: A cut-away view of the design of ITER Tokamak. It is currently under construction in the south of France. It is expected to produce ten times the amount of energy put in. Source: [http://www.iter.org/](http://www.iter.org/)

1.5 Radial transport processes in plasmas

In tokamaks, the confinement of particles and energy is limited by thermal conduction, convection processes and radiation. The simplest model to explain the confinement of the particles is the random walk model. In this model, the particle will diffuse across the magnetic field as consequence of the collisions with other particles. When a particle gyrating around a magnetic field line collides, the particle will move to another field line separated around a characteristic length of the order of the Larmor radius. These collisions are equally likely in the inward or outward direction. However, the fact that the particle density is higher at the centre of the device makes the resulting flow outward.

Including the effects of the toroidal geometry, one finds out that there is also a subset of particles which, in addition to their gyro-motion along the magnetic field line, move in a broader orbit. Therefore, they are subject to a higher outward transport. This subset of particles, known as trapped particles, arises from the variation of the magnetic field amplitude that the particles see as they follow their spiral orbits along the field (mirror effect). Hence, these trapped particles are prevented from performing a full poloidal turn. Their trajectory, as projected onto the poloidal cross-section, has the form of a banana, see Fig. 1.6.

The collisional transport of the particles which circulate freely around the torus (untrapped or passing particles) is called classical transport. The higher transport due to the trapped particles is called neoclassical transport. The neoclassical transport is around two orders of magnitude larger than the classical transport.

The random walk model contains the essential physics of these diffusion processes, although a more sophisticated kinetic theory is required to accurately
calculate the diffusion coefficients, see Ref. [2] for a comprehensive review of the classical and neoclassical theories in tokamaks.

1.6 Turbulent transport

The fundamental collisional diffusion processes explained in the previous section are not enough to explain the observations. In tokamak experiments the radial transport is much larger than the one predicted by collisional transport theory. This phenomenon was called anomalous transport or turbulent transport [3]. At present day, it is widely accepted that fluctuations in the plasma parameters (like electric and magnetic fields, density or temperature) are responsible for most of the transport. In particular, it is supposed that electrostatic turbulence transport caused by $E \times B$ drift is responsible for the bigger part of radial transport in experiments. The investigation of turbulent transport is a current topic in fusion science and the theoretical description and understanding is a quite challenging task. For this reason, a brief description of turbulent transport in tokamaks is given in this section.

In the study of turbulent transport, any plasma dynamical quantity is usually decomposed into a sum of two terms:

$$ Q(x, t) = Q_0(x) + \delta Q(x, t). \quad (1.8) $$

The first term $Q_0$ denotes a stationary equilibrium of $Q$ and the second term $\delta Q$ represents a small time-dependent fluctuation of $Q$.

The equation that describes the electrostatic turbulent transport averaged over a flux surface and over time is given by:

$$ \Gamma = \langle \hat{v}_r \hat{n} \rangle_{FS,t}, \quad (1.9) $$
where $\langle \cdot \rangle_{FS,t}$ denotes the flux surface and time average. Here, $\Gamma$ represents the radial particle flux and $\tilde{v}_r$ is the fluctuation of the radial component of the $E \times B$ drift which can be expressed in terms of the poloidal electric field fluctuations $\tilde{E}_\theta$ giving:

$$\tilde{v}_r = \frac{\tilde{E}_\theta}{B} \Rightarrow \Gamma = \frac{1}{B} \left\langle \tilde{E}_\theta \tilde{n} \right\rangle_{FS,t}.$$  

(1.10)

In order to calculate the turbulent transport, it is convenient to represent the fluctuation quantities $\tilde{E}_\theta(t)$ and $\tilde{n}(t)$ by their Fourier transform in space and time:

$$\tilde{n}(x,t) = \int dk \int d\omega \tilde{n}(k,\omega) e^{i(k \cdot x - \omega t)}, \quad \tilde{E}_\theta(x,t) = \int dk \int d\omega \tilde{E}_\theta(k,\omega) e^{i(k \cdot x - \omega t)}.$$  

(1.11, 1.12)

Taking that into account, the turbulent transport becomes:

$$\Gamma = \frac{1}{B} \int dk \int d\omega |\tilde{E}_\theta(k,\omega)||\tilde{n}(k,\omega)| \cos (\varphi(k,\omega)_E - \varphi(k,\omega)_n).$$  

(1.13)

Here, $\varphi(k,\omega)_E$ and $\varphi(k,\omega)_n$ are the phases of the poloidal electric field and the density fluctuations, respectively. In general, the density and the potential fluctuations are the measured quantities. For this reason, it is convenient to express the poloidal electric field in terms of the potential fluctuations via the relation $\tilde{E}_\theta(k,\omega) = -ik\tilde{\varphi}(k,\omega)$. Therefore, the turbulent transport becomes:

$$\Gamma = \frac{1}{B} \int dk \int d\omega k|\tilde{\varphi}(k,\omega)||\tilde{n}(k,\omega)| \sin (\varphi(k,\omega)_n - \varphi(k,\omega)_\phi),$$  

(1.14)

where $\varphi(\omega)_\phi$ is the phase of the potential fluctuations. According to this equation, the maximal outward transport is associated with $\varphi(k,\omega)_n - \varphi(k,\omega)_\phi = \pi/2$ and it vanishes when the quantities are in phase: $\varphi(k,\omega)_n - \varphi(k,\omega)_\phi = 0$.

An example of this process is illustrated in Fig. 1.7 (left) which shows a local potential fluctuation $\tilde{\varphi}$ on an unperturbed background density with a gradient in the radial direction. The resulting $E \times B$ drift creates a circular flow. This process does not create net particle transport, because the same amount of density is transported outward at the bottom as inward at the top of the potential perturbation \[4\]. This is also the case if a density perturbation in phase with respect to the potential perturbation is present (see Fig. 1.7 (middle)). Only if the density and potential perturbation are out of phase, Fig. 1.7 (right), the $E \times B$ drift causes a radial net transport.

In the following section, the plasma drift-wave micro-instability (instability of the order of the Larmor radius), which it is believed to be responsible for electrostatic fluctuations, is described.
1.7 Plasma drift-wave micro-instability

The mechanism for the development of a drift-wave micro-instability is illustrated in Fig. 1.8. Drift-wave occurs when there is a background density gradient and a three dimensional density perturbation with a finite parallel wavelength $k_{||} \neq 0$. The dynamic of the drift wave is governed by the high mobility of the electrons. The electrons react first to the parallel density gradient, which creates an increasing positive potential $\tilde{\phi}$ inside the regions of positive density perturbations and vice-versa. The resulting electric field leads to the $E \times B$ drift. If the parallel movement of the electrons is assumed to be instantaneous, the cross phase between the potential and the density perturbation will be zero. In this case, the resulting net transport is zero. The electrons with an instantaneous parallel response are called adiabatic. In this case, the $E \times B$ drift leads to a simple propagation of the density perturbation into the electron-diamagnetic direction ($\nabla p \times B$).

The drift wave becomes unstable if the parallel response of the electrons to the parallel density gradient is delayed. A non-adiabatic response of the electrons introduces a non-zero cross phase which leads to the destabilization of the drift wave. In this case, the potential perturbation lags behind the density perturbation and the region of the outward directed $E \times B$ drift shifts to the region of positive density perturbations, which are now amplified.

There are at least three types of plasma drift-waves micro-instabilities which are believed to be the responsible for the anomalous transport in tokamaks. These are the ion temperature gradient mode (ITG), the electron temperature gradient
1. INTRODUCTION

Figure 1.8: Drift-wave instability. Due to their higher mobility, the electrons move faster along the magnetic field than ions causing a charge separation. The drift-wave is stable if the parallel movement of the electron is instantaneous. In this case, the density perturbation propagates into the electron-diamagnetic direction.

mode (ETG) and the trapped electron mode (TEM). In the following a brief description of these instabilities is given based on a very simple fluid model.

1.7.1 Ion temperature gradient mode (ITG)

The ion temperature gradient mode (ITG) is a variation of the plasma drift-wave and it is believed to be the cause of the observed density and ion temperature fluctuations in experiments. ITG mode arises when the ion temperature gradient is parallel to the magnetic field gradient. This occurs in the outer part (or low-field side) of the torus. For this reason, this region is known as the bad curvature region. On the contrary, in the inner part (or high-field side) of the torus, the temperature gradient and the magnetic field gradient are in opposite directions. This region is called the good curvature region. Since ITG is primarily driven by bad curvature effects, the parallel dynamics are ignored in the following model.

Fig. 1.9 (right) shows the ITG instability in the region of bad curvature. Assuming an initial temperature perturbation, as a result of the kinetic energy dependence in the gradient-B drift, particles in hot plasma regions drift (upwards) faster than those in cold plasma region. This charge separation creates an electric field which results in a $E \times B$ drift that further amplifies the perturbation: the temperature perturbation grows and becomes unstable.

In the good curvature region (see Fig. 1.9 (left)), the gradient-B drift is upwards. Therefore, the resulting charge separation leads to an $E \times B$ drift which
reduces the initial temperature perturbation: the temperature perturbation decreases and becomes stable.

\[ \mathbf{E} \times \mathbf{B} \]

\[ \nabla B \]

\[ \nabla T \]

**Figure 1.9:** The ITG instability in a region of good curvature (left) and bad curvature (right). The gradient-B drift causes a charge separation in a temperature perturbation, which leads to an $\mathbf{E} \times \mathbf{B}$ drift. In the good curvature region, the magnetic field gradient is anti-parallel to the temperature gradient. The resulting $\mathbf{E} \times \mathbf{B}$ drifts reduces the perturbation. In the bad curvature region, the magnetic field gradient is parallel to the temperature gradient. The resulting $\mathbf{E} \times \mathbf{B}$ drifts amplifies the perturbation.

Due to the stabilization on the high-field and the destabilization on the low-field side, the amplitudes differ for both regions. This is one of the main characteristics of ITG modes in toroidal geometry. This feature can be observed in gyrokinetic simulations. For example, Fig.1.10 shows a simulation of ITG with the gyrokinetic code GENE (see Chapter 2 for a detailed description of the code). In the high-field side, the fluctuations are small, while in the low-field side, the fluctuations are bigger. Moreover, it is worth to point out the elongated structure of the fluctuations in the parallel direction. They are due to charged particles that quickly move along the field lines, thus making the temperature perturbation very extended along the field. It can also be observed how the twisting of the field lines is able to connect the unstable side to the stable side. This is another way to understand why the twisting of the magnetic field lines is good for the stabilization of the plasma.

### 1.7.2 Electron temperature gradient mode (ETG)

The turbulence mechanism of ETG is similar to that of ITG instability. However, ETG turbulence is driven by the gradient of the electron temperature and it is linked with transport at smaller scales. Recent numerical studies have shown
1. INTRODUCTION

Figure 1.10: Gyrokinetic simulation with the GENE code of the ion temperature gradient (ITG) mode. In this picture, the ion temperature fluctuations are shown (negative fluctuations in blue and positive fluctuations in red). The amplitude of the fluctuations is higher in the low-field side than in the high-field side. In addition, one can also appreciate the elongation of the fluctuations in the direction parallel to the magnetic field and how the twisting of the magnetic field is able to connect both regions.

that ETG could be responsible for the electron heat transport due to structures with high radial elongation \[5\]. However, the importance of ETG for turbulent transport is still disputed. Fig. 1.11 shows a simulation of ETG with the GENE code, where the formation of radially elongated structures (also called streamers) can be observed.

1.7.3 Trapped electron mode (TEM)

The trapped electron mode is believed to be the candidate for explaining the experimentally observed electron heat (and particle) transport in fusion plasmas \[7\]. This mode can be understood with the same model as in case of the temperature gradient modes, but taking into account that in a tokamak a significant fraction of the particles may be trapped in the low-field side (or bad curvature) due to the mirror force. Therefore, these trapped particles will not be stabilized via the twisting of the magnetic field lines.

1.7.4 Spatial scales of the turbulence

Before concluding this section, it is worth mentioning that ITG, TEM and ETG drive electrostatic turbulence at different scales. Fig. 1.12 shows an illustration of the linear growth ($\gamma$) of the different instabilities versus the perpendicular wavenumber ($k_y$) normalized to the ion Larmor radius ($\rho_i$). For ITG the max-
1.8 Simulation of drift-wave instabilities

In order to describe properly the different micro-instabilities, a kinetic approach should be used. Although the fairly well established kinetic equations that have been derived to describe these micro-instabilities, due to their complexity, the equations cannot generally be solved analytically, so that a numerical approach has to be taken. The emergence of massively parallel computers during the last two decades and the development of kinetic and, more specifically, gyrokinetic solvers (see Chapter 2) has however opened the road to more and more accurate simulations of magnetized plasmas in realistic conditions. Nevertheless, these simulations remain very expensive.

We have now reached the point that motivated this work: the need to introduce a different approach in order to reduce the computational cost of gyrokinetic simulations. The idea is to use a much lower resolution than the one imposed by

**Figure 1.11:** A numerical simulation of the electron temperature gradient (ETG) mode with the GENE code. It shows a contour plot of the electrostatic potential fluctuations (positive fluctuations in red and negative fluctuations in blue) in the direction perpendicular to the magnetic field \((x, y)\). The lengths are normalized to the electron Larmor radius \(\rho_e\). One can observe the elongated structures in the radial \((x)\) direction. Adapted from [6].

The maximum linear growth rate is at scales similar to the ion Larmor radius while for ETG the maximum linear growth rate is at smaller scales (of the order of the electron Larmor radius). For TEM the maximum linear growth rate is also at scales similar to the ion Larmor radius. This is due to the fact that TEM is driven by fluctuations in the electron temperature caused by trapped electrons performing a broad orbit.
1. INTRODUCTION

![Graph showing different modes of instabilities]

**Figure 1.12:** A schematic picture showing the different scales where the most important instabilities dominate. The vertical-axis represents the linear growth rate of the instability $\gamma$ normalized in units of $c_s/R$. Here, $R$ is the major radius of the tokamak and $c_s = \sqrt{T_e/m_i}$, with $T_e$ being the electron temperature and $m_i$ the mass of the ion species. The horizontal-axis represents the perpendicular wavenumber $k_y$ normalized to the ion Larmor radius $\rho_i$. The fact that the linear growth of ETG is larger than the one of ITG and TEM is due to the normalization used for this representation. Figure courtesy of F. Jenko.

The physics of the problem studied using the gyrokinetic codes. This is achieved by filtering out the smallest scales of motion and by modeling their effects on the largest scales. The main objective of this filtering strategy is to reduce the complexity of the fields and probability distributions that have to be computed. This scale separation has a theoretical motivation because the largest scales are usually very much dependent on the experimental conditions (boundary conditions, geometry). Their modeling is problem-dependent, which means that new models, or at least new model parameters, have to be chosen when a new situation is considered. On the other hand, the smallest scales have a more universal behavior. They are thus describable by models that could be almost problem independent and supported by theoretical approaches.

This scale separation strategy is usually referred to as *Large-Eddy Simulations* (LES), as it was first developed in the framework of fluid turbulence. The work that we present in this thesis is based on the idea to explore the advantages of transposing LES methods to gyrokinetic theory. The resulting gyrokinetic large eddy simulations (GyroLES) is of course much less expensive than the original simulation. This computational gain is one of the goals of this thesis. On a more theoretical viewpoint, developing the GyroLES approach is also useful in order to better understand the turbulent process in gyrokinetics. The description and implementation of these two goals will be discussed in detailed throughout the
thesis.

1.9 Outline of the thesis

The present thesis is structured as follows. Chapter 2 describes briefly the derivation of the gyrokinetic equations. These equations will be then presented in the normalized units of the GENE (Gyrokinetic Electromagnetic Numerical Experiment) code. GENE solves the equation numerically and it is the code used in this work to study the extension of the Large-Eddy Simulation approach to gyrokinetic simulations. In Chapter 3 a general overview of the Large-Eddy simulation approach for fluids and its extension to conductive fluids will be described. In Chapters 4 and 5 the free energy balance equation will be introduced. The underlying physics of this equation will be analyzed numerically for the ion temperature gradient mode. The results obtained in these chapters are used to the development of the LES approach to gyrokinetics in Chapters 6 and 7. Finally, in Chapter 8 the new contributions to the field are summarized, and a description of the latest results and future work planned are given.
1. INTRODUCTION
In this chapter, we will first derive the gyrokinetic-Maxwell system starting from the well-known Vlasov-Maxwell system of equations. Then we will describe the GENE [5] code, which is the numerical tool used in this work to solve this system of equations and to produce the data that will be analyzed in the thesis.

2.1 The Vlasov-Maxwell system

In the kinetic description of plasmas the state of the system is characterized by a six-dimensional distribution function \( f_j(x, v, t) \) per each species \( j \), which depends on position, velocity and time. The index \( j \) can take two values: \( j = e \) for the electrons and \( j = i \) for the ions. The distribution function represents the number density of particles (at a given time) found near a point in the six-dimensional phase space \( (x, v) \). Its evolution in time is given by the Vlasov equation:

\[
\frac{df_j}{dt} = \frac{\partial f_j}{\partial t} + v \frac{\partial f_j}{\partial x} + \frac{q_j}{m_j} \left( \mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \frac{\partial f_j}{\partial v} = 0, \tag{2.1}
\]

expressed in cgs units and \( c \) being the speed of light. Here, \( q_j \) and \( m_j \) are the charge and the mass of the \( j \) species, respectively. When collisions are important, an additional term must be included in the right hand side of this equation. However, for high temperature plasmas, as it is usually the case in magnetic confinement plasmas, the collision frequency is very small and allows us to neglect the collision term in the following.

The electromagnetic fields \( \mathbf{E} \) and \( \mathbf{B} \) obey the Maxwell’s equations:

\[
\nabla \cdot \mathbf{E} = \frac{4\pi}{c} \sum_j q_j n_j, \quad \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \tag{2.2}
\]

\[
\nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \sum_j j_j, \quad \nabla \cdot \mathbf{B} = 0, \tag{2.3}
\]

\(^1\)For simplicity, we will discuss in this work only plasmas which have a single species of ions.
2. GYROKINETICS AND THE GENE CODE

The particle density $n_j$ and the current density $j_j$ are obtained by the state of the plasma itself, that is, by taking the velocity moments of the distribution function $f_j$:

$$n_j = \int f_j \, d^3v, \quad j_j = q_j \int f_j \, v \, d^3v. \quad (2.4)$$

Consequently, $E$ and $B$ are functionals of $f_j$, and when substituted back into Eq. (2.1) make the last term nonlinear (quadratic) in $f_j$.

This system of equations is called the Vlasov-Maxwell system. It is a system of nonlinear integro-differential equations that cannot be solved analytically. This is why this system must be solved numerically with the help of a computer. However, for typical fusion plasmas the great variety of time and space scales present demands very high resolutions that cannot be achieved even with today’s supercomputers. Thus, we must develop specific approximations, which allow us to simplify the equations in order to be able to solve them numerically. One of the modern approaches is the gyrokinetic theory \[8\]. This approach to plasma turbulence is the one used in this work, and for this reason, the main steps towards the derivation of the so-called gyrokinetic-Maxwell system are given in the following sections.

2.2 The gyrokinetic ordering

The gyrokinetic-Maxwell system is a Vlasov-Maxwell system on which different approximations in the magnitude of various quantities are used. These approximations known as the gyrokinetic ordering, are not just used to derive the system of equations. They are motivated by experiments and years of theoretical analysis of various micro-instabilities in tokamak plasmas. More particularly, these plasmas are characterized as strongly turbulent systems driven by plasma drift-wave type instabilities with the following features:

a) Gyro-motion is much faster than the turbulent frequencies

Plasma drift-waves type instabilities have a typical frequency ($\omega$) of the order of the diamagnetic frequency. For tokamak plasmas, $\omega$ is much smaller than the gyro-frequency ($\Omega$). Introducing this simplification in the Vlasov-Maxwell system, allows us to eliminate the fast time scales from the system and approximate the gyro-motion of the charged particles by the dynamics of charged rings, i.e. instead of following the orbiting particles, one follows charged rings which move along the magnetic field lines and being subjected to drift effects. This approximation, reduces the problem from a six-dimensional to five-dimensional plus time distribution function. Three spatial coordinates representing the motion of the guiding centers of the charged rings and two velocity coordinates related to the equilibrium magnetic field.
2.2 The gyrokinetic ordering

b) Small amplitude perturbations

In a turbulent description of a plasma any fluctuation quantity \( Q \) like the electromagnetic fields, the density or the temperature can be decomposed into a sum of two terms:

\[
Q(\mathbf{x}, t) = Q_0(\mathbf{x}) + \delta Q(\mathbf{x}, t).
\]  

(2.5)

The first term \( Q_0 \) denotes the equilibrium part of \( Q \) (which can vary on the macroscopic scale of the system) and \( \delta Q \) represents a deviation from the equilibrium, i.e. the fluctuation of \( Q \). It has been observed experimentally that the relative fluctuation level \( \delta Q/Q_0 \) is very small for plasma micro-turbulence.

c) Strong spatial anisotropy of the turbulent fluctuations:

Turbulent structures are elongated in the direction parallel to the magnetic field, that is, they have very long parallel wavelength (or very short parallel wavenumber \( k_\parallel \)). On the other hand, turbulent fluctuations have short wavelength in the perpendicular direction (or large wavenumber \( k_\perp \)). This is due to the fact that the parallel velocity of the charged particles is much faster than the perpendicular one caused by the different drifts.

d) Macroscopic scale lengths are much larger than the Larmor radius:

The fluctuations in the direction perpendicular to the magnetic field \( k_\perp \) are of the order of the Larmor radius \( \rho \), that is, \( k_\perp \rho \sim 1 \). On the contrary, the spatial variations of the equilibrium quantities \( Q_0 = (T_0, n_0, ...) \), which can be expressed in logarithmic gradient length scales

\[
\frac{1}{L_{Q_0}} = \frac{\left| \nabla Q_0 \right|}{|Q_0|} = \left| \nabla \ln Q_0 \right|, 
\]  

(2.6)

are ordered to be on the scale of the tokamak major radius \( R \).

All the above simplifications define the gyrokinetic ordering. It can be expressed mathematically as:

\[
\frac{\omega}{\Omega} \sim \frac{\delta n}{n_0} \sim \frac{\delta T}{T_0} \sim \frac{k_\parallel}{k_\perp} \sim \frac{\rho}{L_{n_0}} \sim \frac{\rho}{L_T} \sim \frac{\rho}{R} \sim \epsilon \ll 1, 
\]  

(2.7)

\[
k_\perp \rho \sim 1. 
\]  

(2.8)

where \( \epsilon \) represents a very small parameter.

It is worth to remark that, although the perturbations have small amplitude, they have sharp gradients (short perpendicular wavelengths). Therefore, terms like \( \nabla \delta Q \) and \( \nabla Q_0 \) are of the same order of magnitude:

\[
\frac{\nabla \delta Q}{\nabla Q_0} \sim \frac{k_\perp \delta Q}{1/RQ_0} \sim k_\perp R \frac{\delta Q}{Q_0} \sim k_\perp \rho \frac{R \delta Q}{\rho Q_0} \sim 1 \epsilon^{-1} \epsilon \sim 1. 
\]  

(2.9)
2. GYROKINETICS AND THE GENE CODE

2.3 Modern derivation of the gyrokinetic equation

The modern gyrokinetic equations are based on the Lagrangian variational method together with the gyrokinetic ordering defined in the previous section. In the following, the most important steps needed to derive the gyrokinetic equation will be given following Scott [9] and the thesis of Püschel [10]. For more detailed information on the gyrokinetic theory, we refer to a recent review by Brizard and Hahm [11].

The Lagrangian of a particle of charge $q$ and mass $m$ in the non-canonical coordinates $(x, v)$ has the well-known form [12]:

$$L(x, v) = \left( \frac{q}{c} A(x) + m v \right) \cdot \dot{x} - H(x, v),$$  \hspace{1cm} (2.10)

$$H(x, v) = m \frac{v^2}{2} + q \phi(x),$$  \hspace{1cm} (2.11)

where $H$ is the Hamiltonian of the system, and the potentials ($\phi$ and $A$) give us the electromagnetic fields via

$$B = \nabla \times A, \quad E = -\nabla \phi - \frac{1}{c} \frac{\partial A}{\partial t}.$$  \hspace{1cm} (2.12)

The equations of motion of this dynamical system are obtained by minimizing the action given by the time integral along the particle trajectory of this Lagrangian:

$$\delta \int dt L = 0.$$  \hspace{1cm} (2.13)

The result gives the Euler-Lagrange equation:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{z}_i} - \frac{\partial L}{\partial z_i} = 0 \quad \text{with} \quad i = 1, 2, ..., 6,$$  \hspace{1cm} (2.14)

where $\{z^i\}$ represents $z^1 = x, z^2 = y, z^3 = z, z^4 = v_x, z^5 = v_y$ and $z^6 = v_z$.

Using the Euler-Lagrange equation and the Lagrangian defined in Eq. (2.10), the Lorentz force can be easily obtained:

$$\dot{x} = v, \quad \dot{v} = \frac{q}{m} \left( E + \frac{v}{c} \times B \right).$$  \hspace{1cm} (2.15)

In order to derive the gyrokinetic equation it turns out that it is more convenient to convert the Lagrangian into a six-dimensional phase space Lagrangian. This is done by absorbing the $dt$ factor into $L$. The result is an one-form Lagrangian:

$$\gamma(x, v) = \left( \frac{q}{c} A(x) + m v \right) \cdot dx - H(x, v) dt = \gamma_\alpha dz^\alpha - H dt = \gamma_\alpha dz^\alpha,$$  \hspace{1cm} (2.17)

$$H = m \frac{v^2}{2} + q \phi(x),$$  \hspace{1cm} (2.18)
2.3 Modern derivation of the gyrokinetic equation

where the first element of \( \{ z^a \} \) represents the time \( (z^0 = t) \), and the others \( \{ z^i \} \) represent the spatial and velocity coordinates as before. Here, the Einstein notation with respect to the summation over repeated index is also assumed.

The principle of minimum action of the one-form Lagrangian just is then expressed as:

\[
\delta \int \gamma = \delta \int (\gamma + ds) = 0, \tag{2.19}
\]

where in the last step, we have used the property that the variation of the action is invariant under the addition of an exact differential \( ds \). The function \( ds \) is known as a gauge function.

2.3.1 The one-form guiding center Lagrangian

In the way towards the derivation of the gyrokinetic equation, the first step is to assumed that there are not electric and magnetic field perturbations, \( \delta E = \delta B = 0 \), and that there is only an equilibrium magnetic field:

\[
E(x) = 0, \quad \phi(x) = 0, \quad B(x) = B_0(x), \quad B(x) = \nabla \times A_0(x). \tag{2.20}
\]

The equilibrium one-form Lagrangian is now:

\[
\gamma_0(x, v) = \left( \frac{q}{c} A_0(x) + m v \right) \cdot dx - H(x, v) dt, \tag{2.22}
\]

\[
H = m \frac{v^2}{2}. \tag{2.23}
\]

We would like now to remove the fast gyro-motion from this system. This can be done by introducing a change of coordinates, from the particle coordinates to the guiding center coordinates, given by the following transformation: \( (x, v) \rightarrow (X, v\parallel, \mu, \theta) \):

\[
X = x - \rho a(\theta), \tag{2.24}
\]

\[
\mu = \frac{mv^2}{2B_0} \quad \text{with} \quad v_\perp = v\perp c(\theta), \tag{2.25}
\]

\[
v\parallel = v \cdot b_0, \tag{2.26}
\]

\[
\theta = \tan^{-1} \left( \frac{v \cdot e_1}{v \cdot e_2} \right). \tag{2.27}
\]

where \( X \) is the guiding center position, \( \mu \) is the magnetic moment and \( \theta \) is the gyro-angle coordinate. Here also, \( \Omega = \frac{qB_0}{mc} \) is the gyro-frequency, \( \rho a(\theta) = \rho (\cos \theta e_1 - \sin \theta e_2) \) is the instantaneous gyro-radius and \( c(\theta) = \partial a(\theta) / \partial \theta \). Moreover, \( e_1 \) and \( e_2 \) are orthogonal unit vectors in the plane perpendicular to the magnetic field unit vector \( b_0 \).
2. GYROKINETICS AND THE GENE CODE

The fast gyro-motion in the system is represented by the gyro-angle coordinate \( \theta \). It can be eliminated from the Lagrangian taking into account the slow spatial and temporal variation of the equilibrium quantities. Therefore, we can replace the particle position by the guiding center by doing an expansion in the parameter \( \epsilon \). In this way we can approximate:

\[
A_0(x) = A_0(X + \rho a(\theta)) = A_0(X) + \rho a(\theta) \cdot \nabla A_0(X) + O(\epsilon^2) + \ldots \tag{2.28}
\]

The new one-form Lagrangian in the guiding center coordinates represented by \( \{Z^\alpha\} \), where \( Z^0 = t, Z^1 = X, Z^2 = Y, Z^3 = Z, Z^4 = v||, Z^5 = \mu \) and \( Z^6 = \theta \), reads up to \( O(\epsilon) \):

\[
\Gamma_0 = \left( q/c A_0 + \rho a(\theta) \cdot \nabla A_0 + m v|| b_0 + m v_\perp c(\theta) \right) \cdot (dX + d(\rho a)) - H dt = \Gamma_0 \alpha dZ^\alpha, \tag{2.29}
\]

As we can observe, this guiding center one-form Lagrangian still depends on the gyro-phase. Nevertheless, it can be eliminated from this system in two equivalent ways:

1) By applying to the one-form Lagrangian a gyro-average operator:

\[
\langle G(\theta) \rangle = \frac{1}{2\pi} \int G(\theta) d\theta, \quad \forall G(\theta), \tag{2.30}
\]

which will cancel all terms either proportional to \( a(\theta) \) or \( c(\theta) \) due to periodicity. We thus have:

\[
\langle (\rho a(\theta) \cdot \nabla A_0) \cdot dX \rangle = 0, \tag{2.31}
\]

\[
\langle A_0 \cdot dX \rangle = A_0 \cdot dX, \tag{2.32}
\]

\[
\langle A_0 \cdot d(\rho a) \rangle = 0, \tag{2.33}
\]

\[
\ldots
\]

2) Through a suitable choice of a gauge function \( S \) such that the gyro-phase dependent terms are cancelled order by order in the transformation \( \Gamma_0 \rightarrow \Gamma_0 + dS \). For instance, at lowest order \( (\epsilon^{-1}) \), there are not gyro-phase dependent terms, thus \( S_0 = 0 \). At the next order \( (\epsilon^0) \), there are three terms which depends on the gyro-phase:

\[
\Gamma_0(\epsilon^0) = \frac{q}{c} \rho a(\theta) \cdot \nabla A_0 \cdot dX + \frac{q}{c} A_0 \cdot d(\rho a) + m v_\perp c(\theta) \cdot dX, \tag{2.34}
\]

\[
\Gamma_0(\epsilon^0) \rightarrow \Gamma_0(\epsilon^0) + dS_1. \tag{2.35}
\]

If we choose \( S_1 = -\frac{q}{c} \rho a(\theta) \cdot A_0 \), given \( dS_1 = -\frac{q}{c} d(\rho a) \cdot A_0 - \frac{q}{c} \rho a(\theta) \cdot (dX \cdot \nabla A_0) \), after some manipulation is easy to show that both contributions cancel. The same procedure can be applied to the higher order terms to eliminate rest of the gyro-phase dependent terms.
2.3 Modern derivation of the gyrokinetic equation

After performing all the operations needed by either one of the methods mentioned above, the following one-form Lagrangian remains:

\[ \Gamma_0 = \left( \frac{q}{c} A_0 + m v_\parallel b_0 \right) \cdot dX + \frac{\mu B_0}{\Omega} d\theta - H dt, \]  
\[ H = m \frac{v_\parallel^2}{2} + \mu B_0. \]  

This Lagrangian is known as the guiding-center Lagrangian and was given by Littlejohn in 1983 [13] in terms of the one-form representation.

2.3.2 The one-form gyrokinetic Lagrangian

In a second step we introduce the perturbed electric and magnetic fields to deal with plasma turbulence:

\[ E(x, t) = \delta E(x, t), \quad \phi(x, t) = \delta \phi(x, t), \]  
\[ B(x, t) = B_0(x) + \delta B(x, t), \quad A(x, t) = A_0(x) + \delta A_\parallel(x, t). \]  

In the following we will assume for simplicity that the perpendicular fluctuations in the vector potential \( \delta A_\perp(x, t) \) are negligibly small. Furthermore, for a given quantity \( Q \) we will use either a \( \delta Q \) or \( Q_1 \) to represent its fluctuation in order to remark that it is first order in \( \epsilon \).

Taking that into account, the perturbed guiding center Lagrangian reads:

\[ \Gamma_1 = \frac{q}{c} A_\parallel b_0 \cdot dX - q \phi_1 dt. \]  

Now the fluctuations depend on the spatial position \( x \). As a result, the fast gyro-motion has been re-introduced in the system. The fact that the potentials are now strongly spatial-temporarily fluctuating fields prohibits us from replacing the particle position by the guiding center position. Therefore, we cannot replace the particle positions by the guiding center position and we are not able to remove the fast gyro-motion with any of the two methods mentioned in the previous section.

In order to solve this issue the Lie-transformation method is introduced. The Lie transform is a near identity transformation with the form:

\[ T = e^{\epsilon L_G}, \quad T^{-1} = e^{-\epsilon L_G}, \]  

where \( L_G \) is the Lie derivative and \( \epsilon \) is the small parameter of our problem. In gyrokinetic theory, \( T^{-1} \) is known as the push-forward operator. It represents a transformation of coordinates. In our case, a transformation from a guiding-center coordinates to a new coordinate system, the gyro-center coordinates, whose resulting one-form Lagrangian does not depend on the gyro-phase. The inverse transformation, which will be needed in the next section, is represented by the so-called pull-back operator \( T \). In addition, the Lie derivative is expressed in terms
of generating vector field $G$, and its operation on a scalar $F$ and on an one-form \( \Gamma \) are:

\[
L_G F = G^\alpha \frac{\partial F}{\partial Z^\alpha}, \quad (L_G \Gamma)_\alpha = G^\beta \left( \frac{\partial \Gamma_\alpha}{\partial Z^\beta} - \frac{\partial \Gamma_\beta}{\partial Z^\alpha} \right).
\] (2.42)

The actual operation on the Lie-transform on the one-form guiding center Lagrangian $\Gamma$ up to first order in $\epsilon$ is given by:

\[
\overline{\Gamma} = T^{-1} \Gamma + dS \approx (1 - \epsilon L_{G1}) \Gamma + dS,
\] (2.43)

where $\overline{\Gamma}$ is the one-form Lagrangian in the gyro-center coordinates and $dS$ is the gauge function as before. In addition, we can now expand the Lagrangian into an equilibrium (represented by the subscript 0) and a fluctuating part (represented by the subscript 1):

\[
\Gamma_0 = \Gamma_0 + dS_0, \\
\Gamma_1 = \Gamma_1 - L_{G1} \Gamma_0 + dS_1.
\] (2.44, 2.45)

Here, $\Gamma_0$ is the equilibrium (unperturbed) guiding center one-form Lagrangian, which was obtained in the previous section and from which it follows immediately that $dS_0 = 0$.

The $\alpha$ component of the (perturbed) one-form gyro-center Lagrangian is:

\[
\Gamma_{1\alpha} = \Gamma_{1\alpha} - G^\beta_1 \left( \frac{\partial \Gamma_{0\alpha}}{\partial Z^\beta} - \frac{\partial \Gamma_{0\beta}}{\partial Z^\alpha} \right) + \frac{\partial S_1}{\partial Z^\alpha}.
\] (2.46)

The fast gyro-motion can now be eliminated for the perturbed one-form Lagrangian through a corresponding choice of the generator fields $G^\alpha_1$ and the gauge function $S_1$. Furthermore, the gauge function and the field generators are chosen to satisfy also

\[
\Gamma_{1v_1} = \Gamma_{1\mu} = \Gamma_{1\theta} = 0,
\] (2.47)

in order to obtain a simple one-form Lagrangian.

The above conditions constraint the value of the field generators and the gauge function, that up to first order in $\epsilon$ are expressed as:

\[
G^X_1 = C^\alpha_1 = 0,
\]

\[
G^\mu_1 = \frac{q}{mc} \frac{\partial S_1}{\partial \theta},
\]

\[
G^{v_1}_1 = \frac{q}{mc} A^{v_1}_1,
\]

and the gauge function is simply given by

\[
\frac{\partial S_1}{\partial \theta} = \frac{mc}{B_0} \left( \tilde{\phi}_1 - \frac{v_{1\parallel}}{c} \tilde{A}_{1\parallel} \right).
\] (2.51)
In Eq. (2.51), the fluctuating quantities \( Q_1 \) are divided into a gyro-phase independent part \( \langle Q_1 \rangle \) and a gyro-phase dependent part \( \tilde{Q}_1 \) defined by:

\[
\langle Q_1 \rangle = \frac{1}{2\pi} \int d\theta Q_1(x) = \frac{1}{2\pi} \int d\theta Q_1(X + \rho a(\theta)),
\]

\[
\tilde{Q}_1 = Q_1 - \langle Q_1 \rangle.
\]

The resulting one-form Lagrangian is now independent of the gyro-phase coordinate and its components are given by:

\[
\Gamma_{1X} = \Gamma_{0X} - \frac{G_0}{\mu} \left( \frac{\partial \Gamma_{0X}}{\partial \mu} - \frac{\partial \Gamma_{0\mu}}{\partial X} \right) - \frac{G_1}{v_\parallel} \left( \frac{\partial \Gamma_{0X}}{\partial v_\parallel} - \frac{\partial \Gamma_{0v}}{\partial X} \right),
\]

\[
\Gamma_{1t} = \Gamma_{0t} - \frac{G_0}{\mu} \left( \frac{\partial \Gamma_{0t}}{\partial \mu} - \frac{\partial \Gamma_{0\mu}}{\partial X} \right) - \frac{G_1}{v_\parallel} \left( \frac{\partial \Gamma_{0t}}{\partial v_\parallel} - \frac{\partial \Gamma_{0v}}{\partial t} \right).
\]

Thus, taking into account that \( \Gamma_{0\mu} = \Gamma_{0v} = 0 \) and that

\[
\frac{\partial \Gamma_{0X}}{\partial \mu} = 0, \quad \frac{\partial \Gamma_{0X}}{\partial v_\parallel} = m b_0,
\]

\[
\frac{\partial \Gamma_{0t}}{\partial \mu} = B_0, \quad \frac{\partial \Gamma_{0t}}{\partial v_\parallel} = m v_\parallel,
\]

we have:

\[
\Gamma_{1X} = \frac{q}{c} \mathbf{A}_1 \cdot \mathbf{v} - \frac{q}{m c} \mathbf{A}_1 \cdot \mathbf{b}_0 = \frac{q}{c} \langle \mathbf{A}_1 \rangle,
\]

\[
\Gamma_{1t} = q \phi - B_0 \frac{q}{B_0} \left( \phi - \frac{v_\parallel}{c} \mathbf{A}_1 \right) - \frac{q}{m c} \mathbf{A}_1 \cdot \mathbf{v} = q \langle \phi \rangle.
\]

Hence, the perturbed one-form Lagrangian is

\[
\Gamma_1 = \frac{q}{c} \langle \mathbf{A}_1 \rangle \cdot d\mathbf{X} - q \langle \phi \rangle \cdot dt.
\]

Together with the equilibrium one-form Lagrangian \( \Gamma_0 \), gives the total gyro-center Lagrangian:

\[
\Gamma = \Gamma_0 + \Gamma_1 = \left( \frac{q}{c} \mathbf{A}_0 + m v_\parallel \mathbf{b}_0 + \frac{q}{c} \langle \mathbf{A}_1 \rangle \right) \cdot d\mathbf{X} + \frac{\mu B_0}{\Omega} \cdot d\theta - \left( \frac{m v_\parallel^2}{2} + \mu B_0 + q \langle \phi \rangle \right) \cdot dt.
\]

From this Lagrangian, using the Euler-Lagrange equation, the resulting gyro-center equations of motion can be obtained up to first order in \( \epsilon \):

\[
\dot{\mathbf{X}} = v_\parallel \mathbf{b}_0 + \frac{B_0}{B_0^\parallel} \left( \mathbf{v}_\times + \mathbf{v} v_\parallel \mathbf{b}_0 + \mathbf{v}_c \right),
\]

\[
\dot{v}_\parallel = \frac{\dot{\mathbf{X}}}{m v_\parallel} \cdot \left( -q \nabla \langle \phi \rangle - \frac{q}{c} \frac{\partial}{\partial t} \langle \mathbf{A}_1 \rangle - \mu \nabla B_0 \right),
\]

\[
\dot{\phi} = \Omega,
\]

\[
\dot{\mu} = 0,
\]
with the (modified) $E \times B$ drift
\begin{equation}
\mathbf{v}_\chi = -\frac{c}{B_0^2} \nabla \chi_1 \times \mathbf{B}_0,
\end{equation}
the gradient-$B$ drift
\begin{equation}
\mathbf{v} \nabla B_0 = \frac{\mu}{m\Omega} \mathbf{b}_0 \times \nabla B_0,
\end{equation}
and the curvature drift
\begin{equation}
\mathbf{v}_c = \frac{v_\parallel^2}{\Omega} (\nabla \times \mathbf{b}_0)_\perp.
\end{equation}
Here, the modified potential $\chi_1$ is given by
\begin{equation}
\chi_1 = \phi_1 - \frac{v_\parallel}{c} \langle A_1 \parallel \rangle,
\end{equation}
and also, $\mathbf{B}_0^\ast = \nabla \times \mathbf{A}_0^\ast$ with $\mathbf{A}_0^\ast = \mathbf{A}_0 + mc/qv_\parallel \mathbf{b}_0$. It is worth to mention that in this approximation the magnetic moment is an invariant of the motion.

### 2.4 The gyrokinetic equation

The equations derived in the previous section are the equations of motion for the individual gyro-centers. In order to obtain the equation for the gyro-center distribution function per each species $f_j(X, v_\parallel, \mu, t)$, i.e. the gyrokinetic equation, we need to take into account that the phase space volume of the distribution function is also conserved in the gyro-center coordinates:
\begin{equation}
\frac{df_j}{dt} = 0 \Rightarrow \frac{\partial f_j}{\partial t} + \dot{X} \cdot \nabla f_j + v_\parallel \frac{\partial f_j}{\partial v_\parallel} = 0,
\end{equation}
where $\dot{X}$ and $v_\parallel$ are given by Eqs. (2.62) and (2.63), respectively.

It is convenient to split the gyro-center distribution function $f_j$ into a Maxwellian distribution function $F_{0j}$ defined as
\begin{equation}
F_{0j} = \left( \frac{m_j}{2\pi T_{0j}} \right)^{3/2} n_{0j} e^{-\frac{mv_\parallel^2/2 + \mu B_0}{T_{0j}}},
\end{equation}
and a first order fluctuation part $f_{1j}$:
\begin{equation}
f_j = F_{0j} + f_{1j} \quad \text{satisfying} \quad \frac{f_{1j}}{F_{0j}} \sim \epsilon \ll 1.
\end{equation}
Here, $T_{0j}$ is the equilibrium temperature (in units where the Boltzmann’s constant is set to one) and $n_{0j}$ is the equilibrium density of the species. This splitting
2.5 The gyrokinetic field equations

separates the macroscopic evolution of the plasma (contained in $F_{0j}$) from the micro-turbulence. Additionally, it reduces the computational effort of the simulations.

Introducing the modified distribution function

$$g_{1j} := f_{1j} + v_{\parallel} \frac{q_j T_{0j}}{c} F_{0j} \langle A_{1\parallel} \rangle,$$

(2.73)

and the so-called non-adiabatic part of the distribution function

$$h_{1j} := f_{1j} + \frac{q_j}{T_{0j}} F_{0j} \langle \phi_1 \rangle = g_{1j} + \frac{q_j}{T_{0j}} F_{0j} \chi_{1j}.$$  

(2.74)

The perturbed gyrokinetic equation can be expressed as

$$\frac{\partial g_{1j}}{\partial t} = \frac{B_0}{B_{0\parallel}} v_x \cdot \left( \nabla F_{0j} + \frac{F_{0j}}{T_{0j}} \mu \nabla B_0 \right) + \frac{B_0}{B_{0\parallel}} \left( v_x + v \nabla B_0 + v_c \right) \cdot \nabla h_{1j}$$

$$+ v_{\parallel} b_0 \cdot h_{1j} - \left( \frac{1}{m_j} b_0 + \frac{B_0}{m_j v_{\parallel} B_{0\parallel}} v_c \right) \cdot \left( -q \nabla \langle \phi_1 \rangle - \frac{q}{c} \frac{\partial}{\partial t} \langle A_{1\parallel} \rangle - \mu \nabla B_0 \right) \frac{\partial f_{1j}}{\partial v_{\parallel}}.$$  

(2.75)

Remark that the nonlinear term is this equation is the product of $v_x \cdot \nabla h_{1j}$.

2.5 The gyrokinetic field equations

In order to solve the gyrokinetic equation, the fluctuating potentials ($\phi_1, A_{1\parallel}$) entering in the equation must be determined in terms of the gyro-center distribution function. This is done using the Maxwell’s equations. In the case of a non-relativistic plasma the displacement current can be neglected. The resulting Maxwell’s equations are then expressed as:

$$\nabla \cdot E_1 = \frac{4\pi}{c} \sum_j q_j n_j, \quad \nabla \times E_1 = -\frac{1}{c} \frac{\partial B_1}{\partial t},$$

(2.76)

$$\nabla \times B_1 = \frac{4\pi}{c} \sum_j j_j, \quad \nabla \cdot B_1 = 0.$$  

(2.77)

Taking into account that the fields derive from potentials:

$$E_1 = -\nabla \phi_1 - \frac{1}{c} \frac{\partial A_{1\parallel}}{\partial t}, \quad B_1 = \nabla \times A_{1\parallel},$$

(2.78)

we can define the Poisson’s and (parallel) Ampère’s law:

$$\nabla^2 \phi_1 \approx \nabla^2 \phi_1 = -\frac{4\pi}{c} \sum_j q_j n_j \quad \nabla^2 A_{1\parallel} \approx \nabla^2 A_{1\parallel} = -\frac{4\pi}{c} \sum_j j_{\parallel}.$$  

(2.79)
where we have used the Coulomb gauge $\nabla \cdot A_1 = 0$ and the gyrokinetic ordering to neglect the parallel fluctuations.

We recall that the potential fluctuations are evaluated at the particle position $\mathbf{x}$ and not in the gyro-center coordinates $\mathbf{X}$. We thus must specify the particle and current density in the same way, that is, they must be related to the particle distribution function $\tilde{f}_j(x, v, t)$ (hereafter defined with a tilde not to be confused with the gyro-center distribution function $f_j(X, v_\parallel, \mu, t)$):

$$n_j(x, t) = \int \tilde{f}_j(x, v, t) d^3v, \quad j_{\parallel}(x, t) = q_j \int \tilde{f}_j(x, v, t) v_\parallel d^3v. \quad (2.80)$$

To get the particle distribution function $\tilde{f}_j(x, v, t)$, we must first transform back the gyro-center distribution function $f_j$ to the guiding center distribution function $F_j$. This is done by the pull-back operator $T$. For a scalar it is defined as:

$$F_j(X, \mu, v_\parallel, \theta, t) = T f_j(X, \mu, v_\parallel, \theta, t) \approx (1 + \epsilon L_{G1}) f_j = f_j + \epsilon G_{1\alpha} \frac{\partial f_j}{\partial Z^\alpha}, \quad (2.81)$$

up to first order in $\epsilon$. Finally, we have to do a transformation from the guiding center to the particle position.

Doing this procedure for the particle density, we find:

$$n_j = \int \tilde{f}_j d^3v = \frac{B_0}{m_j} \int d\theta d\mu d\mu_{\parallel} d^3X \delta^3(X + \rho_j a(\theta) - x) F_j$$

$$= \frac{B_0}{m_j} \int d\theta d\mu d\mu_{\parallel} d^3X \delta^3(X + \rho_j a(\theta) - x) T f_j, \quad (2.82)$$

where $B_0/m_j$ is the Jacobian of the transformation. At this point it is convenient to split again the gyro-center distribution function $f_j$ into a Maxwellian distribution function $F_{0j}$ and a first order fluctuation part $f_{1j}$. Therefore, the action of the Lie derivative on a scalar up to first order is then expressed as

$$F_j = T f_j = F_0 + f_{1j} + G_{1\nu} \frac{\partial F_{0j}}{\partial v_\parallel} + G_{1\mu} \frac{\partial F_{0j}}{\partial \mu} = f_j - q_j \frac{F_{0j}}{T_{0j}} \tilde{\phi}_1, \quad (2.83)$$

where we have used:

$$\frac{\partial F_{0j}}{\partial v_\parallel} = -\frac{m_{\parallel}}{T_{0j}} F_{0j}, \quad \frac{\partial F_{0j}}{\partial \mu} = -\frac{B_0}{T_{0j}} F_{0j}. \quad (2.84)$$

Then, the equation for the particle density can be written as

$$n_j = \frac{B_0}{m_j} \int d\theta d\mu d\mu_{\parallel} d^3X \delta^3(X + \rho_j a(\theta) - x) \left( f_j - q_j \frac{F_{0j}}{T_{0j}} \tilde{\phi}_1 \right). \quad (2.85)$$
2.5 The gyrokinetic field equations

The first term gives the density of the gyro-centers \( \vec{\pi}_j \), and it is due to the gyro-phase independent part \( f_j \). Thus it requires only the gyro-average operator:

\[
\vec{\pi}_j = \frac{B_0}{m_j} \int d\theta d\mu dv_\parallel d^3 \mathbf{x} \delta^3(\mathbf{x} + \rho_j \mathbf{a}(\theta) - \mathbf{x}) f_j
\]

\[
= \frac{2\pi B_0}{m_j} \int d\mu dv_\parallel \langle f_j(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \rangle. \tag{2.86}
\]

Here, for clarity of the presentation, we have omitted the most obvious dependencies of the distribution function, i.e., \( f_j(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \) means \( f_j(\mathbf{x} - \rho_j \mathbf{a}(\theta), v_\parallel, \mu, \theta, t) \).

The second term of Eq. (2.85) can be split into two parts taking into account that:

\[
\tilde{\phi}_1 = \phi_1 - \langle \phi_1 \rangle. \tag{2.87}
\]

The first part \( \langle \phi_1 \rangle \) does not depend on the velocity variables nor on the guiding center coordinate. Hence, it can be taken out from the integral. This yields,

\[
- \frac{q_j}{T_{0j}} \frac{B_0}{m_j} \int d\theta d\mu dv_\parallel d^3 \mathbf{x} \delta^3(\mathbf{x} + \rho_j \mathbf{a}(\theta) - \mathbf{x}) F_{0j} = - \frac{q_j}{T_{0j}} \phi_1 n_{0j}. \tag{2.88}
\]

The second part \( \langle \phi_1 \rangle \) depends on \( \mathbf{X} \) and \( \mu \) through the gyro-average. Hence, it gets gyro-averaged again:

\[
\frac{B_0}{m_j} \int d\theta d\mu dv_\parallel d^3 \mathbf{x} \delta^3(\mathbf{x} + \rho_j \mathbf{a}(\theta) - \mathbf{x}) F_{0j} \langle \phi_1 \rangle = \frac{2\pi B_0 q_j}{T_{0j} m_j} \int d\mu dv_\parallel F_{0j} \langle \langle \phi_1(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \rangle \rangle. \tag{2.89}
\]

In addition, we have used the fact that the equilibrium distribution function varies only on the macroscopic length scales and can be extracted from the gyro-average. Therefore, Poisson’s law can be expressed as

\[
\nabla_\perp^2 \phi_1 = - \frac{4\pi}{c} \sum_j q_j \left( \frac{2\pi B_0}{m_j} \int d\mu dv_\parallel \langle f_j(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \rangle \right)
\]

\[
- \frac{q_j}{T_{0j}} \phi_1 n_{0j} + \frac{2\pi B_0 q_j}{T_{0j} m_j} \int d\mu dv_\parallel F_{0j} \langle \langle \phi_1(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \rangle \rangle. \tag{2.90}
\]

For the current density, applying the same procedure, we obtain:

\[
j_{\parallel j} = \frac{B_0}{m_j} \int d\theta d\mu dv_\parallel d^3 \mathbf{x} \delta^3(\mathbf{x} + \rho_j \mathbf{a}(\theta) - \mathbf{x}) v_\parallel \left( f_j - q_j \frac{F_{0j}}{T_{0j}} \tilde{\phi}_1 \right). \tag{2.91}
\]

The first term gives again the gyro-center contribution of the parallel current density. Since it is independent of the gyro-phase requires only gyro-average:

\[
\tilde{j}_{\parallel j} = \frac{B_0}{m_j} \int d\theta d\mu dv_\parallel d^3 \mathbf{x} \delta^3(\mathbf{x} + \rho_j \mathbf{a}(\theta) - \mathbf{x}) v_\parallel f_j
\]

\[
= \frac{2\pi B_0}{m_j} \int d\mu dv_\parallel v_\parallel \langle f_j(\mathbf{x} - \rho_j \mathbf{a}(\theta)) \rangle. \tag{2.92}
\]
2. GYROKINETICS AND THE GENE CODE

On the contrary, in this case the second term cancels since the \( v_\parallel \) dependence is only contained in the \( v_\parallel F_{0j} \) term. Due to the fact that \( F_{0j} \) is an even function of \( v_\parallel \) it cancels after integration. Thus, in this case the particle current density is just the current density of the gyro-centers:

\[
\mathbf{j}_{\parallel \jmath} = \mathbf{J}_{\parallel \jmath}.
\]  

(2.93)

Thus, Ampère’s law writes:

\[
\nabla_{\perp}^2 A_{1\parallel} = -\frac{4\pi}{c} \sum_{\jmath} \frac{2\pi B_0}{m_{\jmath}} \int d\mu \, dv_\parallel \, v_\parallel \, \langle f_{\jmath}(x - \rho_{\jmath} a(\theta)) \rangle.
\]  

(2.94)

The gyrokinetic equation (2.75) together with the Poisson’s (2.92) and (parallel) Ampère’s (2.94) law are known as the gyrokinetic-Maxwell system. However, the system is not yet self-contained, since it depends also on the equilibrium magnetic field \( B_0 \). This is why we need to specify the magnetic equilibrium geometry. In addition, the latter can be further simplified using a coordinate system that takes into account that the plasma micro-turbulence is extended along the magnetic field lines while it is much smaller in the perpendicular direction. This coordinate system is known as the field aligned coordinate system. For this reason, before describing the magnetic equilibrium geometry used in this work, the most important features of the field aligned coordinate system will be briefly described in the following section.

2.6 Field aligned coordinate system

The field aligned coordinate system exploits the scale separation between the perpendicular and parallel directions in order to save several order of magnitudes in computational effort compared with a traditional Cartesian coordinate system. It is represented by the coordinates \( \{x, y, z\} \), where \( z \) is the coordinate along the magnetic field line and the other two non-orthogonal coordinates are perpendicular to the magnetic field with \( x \) being a radial coordinate and \( y \) being a toroidal coordinate. We can further approximate the field-aligned coordinate system by considering a domain in the vicinity of the magnetic field line. This approximation is known as the local flux-tube approximation (in contrast to global or full torus, see picture 2.1).

2.6.1 Local flux-tube approximation

Here, all the coefficients can be expanded up to first order in \( x \) about the central flux surface with radial coordinate \( x_0 \). For instance, the safety factor can be expressed as

\[
q(x) \approx q_0 + \frac{dq}{dx} \bigg|_{x_0} (x - x_0) = q_0 \left( 1 + \frac{s(x - x_0)}{x_0} \right),
\]  

(2.95)
2.6 Field aligned coordinate system

![Figure 2.1](image)

**Figure 2.1:** Local (left) versus global (right) coordinate representation. Figure courtesy of T. Görler.

where we have defined the dimensionless magnetic shear parameter as:

$$\hat{s} = \frac{x_0 \frac{dq}{dq} |_{x_0}}{q_0 \frac{dq}{dq} |_{x_0} \xi}. \quad (2.96)$$

In addition, since the flux-tube is so narrow in the directions across the magnetic field line, we can ignore the equilibrium variations of all the fields. Therefore, all the equilibrium quantities and also their logarithmic gradient length scales are assumed to be constant (density, temperature, ...):

$$T_0 = T_0(x_0), \quad L_T = L_T(x_0), \quad (2.97)$$
$$n_0 = n_0(x_0), \quad L_n = L_n(x_0). \quad (2.98)$$

**Boundary conditions**

One of the main advantages of this local flux-tube approximation is that it allows us to use periodic boundary conditions in the perpendicular directions \(x\) and \(y\):

$$f(x + L_x, y, z) = f(x, y, z), \quad f(x, y + L_y, z) = f(x, y, z) \quad (2.99)$$

for any function \(f\). Here, \(L_x\) and \(L_y\) are the length of the simulation domain in the corresponding perpendicular directions. Furthermore, a Fourier decomposition in the directions \(x\) and \(y\) can be used:

$$f(k_x, k_y) = \frac{1}{L_x L_y} \int_0^{L_x} \int_0^{L_y} dx \, dy \, e^{-i(k_x x + k_y y)} f(x, y) \quad (2.100)$$

However, in the parallel direction \(z\) the situation is different. Due to the twisting of the flux-tube (represented by the safety factor \(q\)), the parallel ends of the flux-tube are not connected. The parallel condition, which takes into account the twisting of the magnetic field lines is:

$$f(k_x, k_y, z + L_z) = f(k_x + 2\pi \hat{s} k_y, k_y, z) e^{2\pi i k_y \hat{s} x_0} \quad (2.101)$$

33
where $L_z$ being the parallel flux-tube domain.

For more details on field aligned coordinates, and in particular, to the local flux-tube approximation, we refer to the reader to the thesis of Beer \[14\] and references therein.

**The gyroaverage**

In the flux-tube approximation it is possible to use the Fourier representation in the directions perpendicular to the magnetic field. As a result, the gyro-averages have a simpler form (for details, see Ref. \[15\]):

\[
\langle \phi_1(k_\perp) \rangle := J_0(k_\perp \rho_j) \phi_1(k_\perp), \quad \langle \langle \phi_1(k_\perp) \rangle \rangle := \Gamma_0(b_j) \phi_1(k_\perp),
\]

(2.102)

where $k_\perp = (k_x, k_y)$ is the perpendicular wave vector. Here also, $J_0$ is the Bessel function, $\Gamma_0(b_j) := e^{-b_j} I_0(b_j)$ where $I_0$ is the modified Bessel function and $b_j = k_\perp^2 \rho_j^2$.

Therefore, in this representation, we can express the following terms that appear in the Poisson’s and Ampère’s law as

\[
\frac{2\pi B_0}{m_j} \int d\mu d\nu \langle f_j(x - \rho_j a(\theta)) \rangle \to \frac{2\pi B_0}{m_j} \int d\mu d\nu J_0(k_\perp \rho_j) f(k_\perp),
\]

(2.103)

\[
\frac{2\pi B_0 q_j}{T_0 j m_j} \int d\mu d\nu F_{0j} \langle \langle \phi_1(x - \rho_j a(\theta)) \rangle \rangle \to n_{0j} \left( \frac{q_j}{T_0 j} \right) \Gamma_0(b_j) \phi_1(k_\perp),
\]

(2.104)

\[
\frac{2\pi B_0}{m_j} \int d\mu d\nu \langle f(x - \rho_j a(\theta)) \rangle \to \frac{2\pi B_0}{m_j} \int d\mu d\nu J_0(k_\perp \rho_j) f_j(k_\perp),
\]

(2.105)

where the density $n_{0j}$ and the temperature $T_{0j}$ are evaluated at a reference point $x_0$, and in the second identity the velocity integration has been also performed.

**2.6.2 Magnetic equilibrium geometry**

In this work the equilibrium magnetic field is obtained by a simple concentric circular model. The equilibrium magnetic field in the local flux-tube coordinates is represented by

\[
B_0 = B_{\text{ref}} \nabla x \times \nabla y.
\]

(2.106)

Here $B_{\text{ref}}$ is a reference magnetic field. In addition, the magnetic field amplitude $B_0 = |B_0|$ in terms of the $z$ coordinate is simply

\[
B_0(z) = \frac{B_{\text{ref}}}{1 + \epsilon_t \cos z},
\]

(2.107)

where $\epsilon_t = x_0/R$ is the aspect ratio.
Moreover, the Jacobian of this transformation (from Cartesian coordinates to flux-tube coordinates) $J(z)$ is then expressed as

$$J(z) = \frac{1}{(\nabla x \times \nabla y) \cdot \nabla z} = \frac{B_{\text{ref}}}{B_0} \cdot \nabla z.$$  

(2.108)

Finally, due to the non-orthogonality of this system of coordinates, the several differential and integral operators that appear in the gyrokinetic equations have to be expressed in terms of the metric coefficients (see Ref. [16]). Up to first order in $\epsilon_t$ the metric coefficients are:

$$g^{xx}(z) = 1,$$

(2.109)

$$g^{zy}(z) = g^{yz}(z) = \hat{s}z - \epsilon_t \sin z,$$

(2.110)

$$g^{yy}(z) = 1 + (\hat{s}z)^2 - 2\epsilon_t \cos z - 2\hat{s}z \epsilon_t \sin z,$$

(2.111)

$$g^{xz}(z) = g^{zx}(z) = \frac{-\epsilon_t \sin z}{x_0},$$

(2.112)

$$g^{yz}(z) = g^{zy}(z) = \frac{1 - 2\epsilon_t \cos z - \hat{s}z \epsilon_t \sin z}{x_0},$$

(2.113)

$$g^{zz}(z) = \frac{1 - 2\epsilon_t \cos z}{x_0^2}.$$  

(2.114)

Note that in the local flux-tube approximation and the axisymmetry of the equilibria considered here, all the coefficients depend only on the $z$ coordinate.

### 2.7 The nonlinear gyrokinetic GENE code

Solving the gyrokinetic-Maxwell system is a formidable task and for this reason a numerical approach has to be taken. In this work, the gyrokinetic GENE (Gyrokinetic Electromagnetic Numerical Experiment) code is the numerical tool used to solve the gyrokinetic-Maxwell system and to produce the turbulence data. A brief description of the code is given in this section.

GENE has been developed over the last years by a team led by Prof. Frank Jenko and is freely available. It solves the nonlinear gyrokinetic equations on a fixed grid in five dimensional phase space (plus time): two velocity coordinates related to the equilibrium magnetic field $(v_\parallel, \mu)$, and three field aligned coordinates $(x, y, z)$. It has the possibility to simulate a flux-tube (local simulations), or the full torus (global simulations, see Fig.2.2). The code runs very efficiently because it is parallelized over all phase space coordinates and it adapts to the given hardware and problem size. It also chooses the time step in an optimal way. For this reason, GENE runs on a large number of computer architectures.

#### 2.7.1 Normalization

In order to avoid the appearance of very large or very small numbers when solving numerically the equations, all the quantities have to be appropriately made
2. GYROKINETICS AND THE GENE CODE

Figure 2.2: Snapshot of a tokamak simulation with the GENE code. Image: [Link](http://gene.rzg.mpg.de).

dimensionless by means of normalization with respect to reference quantities. We define a reference mass $m_{\text{ref}}$, a reference temperature $T_{\text{ref}}$, a reference density $n_{\text{ref}}$ and a reference magnetic field evaluated on the magnetic axis $B_{\text{ref}}$. The resulting normalizations go as follows:

$$
B_0 \rightarrow B_{\text{ref}} B_0, \quad n_{0j} \rightarrow n_{\text{ref}} n_{0j}, \quad m_j \rightarrow m_{\text{ref}} m_j, \quad T_{0j} \rightarrow T_{\text{ref}} T_{0j}. \quad (2.115)
$$

In the local version the code, the one used in this work, the perpendicular directions $x$ and $y$ are represented by their respective Fourier components $k_x$ and $k_y$. Now taking into account the gyrokinetic ordering, the spatial coordinates are normalized to the microscopic scales of the problem

$$
k_x \rightarrow \frac{1}{\rho_{\text{ref}}} k_x, \quad k_y \rightarrow \frac{1}{\rho_{\text{ref}}} k_y, \quad z \rightarrow z, \quad (2.116)
$$

where $\rho_{\text{ref}}$ is a reference Larmor radius given by:

$$
\rho_{\text{ref}} = \frac{c_{\text{ref}}}{\Omega_{\text{ref}}} \quad \text{with} \quad c_{\text{ref}} = \sqrt{\frac{T_{\text{ref}}}{m_{\text{ref}}}} \quad \text{and} \quad \Omega_{\text{ref}} = \frac{e B_{\text{ref}}}{m_{\text{ref}} c} \quad \text{with} \quad q_j \rightarrow e q_j. \quad (2.117)
$$

The velocity coordinates are also normalized accordingly:

$$
v_\parallel \rightarrow c_{\text{ref}} v_{Tj} v_\parallel, \quad \mu \rightarrow \frac{T_{\text{ref}}}{B_{\text{ref}}} T_{0j} \mu. \quad (2.118)
$$

Here, $v_{Tj}$ is the thermal speed of the specie $j$:

$$
v_{Tj} = \sqrt{\frac{2 T_{0j}}{m_j}}. \quad (2.119)
$$
2.7 The nonlinear gyrokinetic GENE code

The time and the gyro-frequency are normalized to:

\[ t \rightarrow \frac{L_{\text{ref}}}{e_{\text{ref}}} t, \quad \Omega_j \rightarrow \Omega_{\text{ref}} \Omega_j, \]  \hspace{1cm} (2.120)

where \( L_{\text{ref}} \) is the macroscopic scale of the problem (generally the major radius \( R \) of the tokamak device).

The logarithmic density and temperature gradient scale lengths are also normalized using the reference macroscopic of the problem

\[ \frac{1}{L_{n_{0j}}} \rightarrow \frac{L_{\text{ref}}}{L_{n_{0j}}} = -\frac{L_{\text{ref}}}{\partial x} \frac{\partial \ln n_{0j}}{\partial x} = \omega_{nj}, \]  \hspace{1cm} (2.121)

\[ \frac{1}{L_{T_{0j}}} \rightarrow \frac{L_{\text{ref}}}{L_{T_{0j}}} = -\frac{L_{\text{ref}}}{\partial x} \frac{\partial \ln T_{0j}}{\partial x} = \omega_{Tj}. \]  \hspace{1cm} (2.122)

Here, the derivatives are still in real space assuming that their gradients are constant over a flux-tube simulation box. In the last term we used \( \omega_{Tj} \) and \( \omega_{nj} \) to represent the normalized temperature and density gradients, since it is the nomenclature used in the literature.

Finally, the fields and the distribution functions are normalized as well:

\[ \left\{ f_{1j}, g_{1j}, h_{1j} \right\} \rightarrow \frac{\rho_{\text{ref}} n_{\text{ref}} n_{0j}}{L_{\text{ref}}^3} \left\{ f_{1j}, g_{1j}, h_{1j} \right\}, \quad F_{0j} \rightarrow \frac{n_{\text{ref}} n_{0j}}{e_{\text{ref}}^3 v_{Tj}^3} F_{0j}, \]  \hspace{1cm} (2.123)

\[ \left\{ \phi_1, \chi_1 \right\} \rightarrow \frac{\rho_{\text{ref}} T_{\text{ref}}}{L_{\text{ref}}^3} e \left\{ \phi_1, \chi_1 \right\}, \quad A_{1||} \rightarrow \frac{\rho_{\text{ref}} B_{\text{ref}}}{L_{\text{ref}}} \rho_{\text{ref}} A_{1||}. \]  \hspace{1cm} (2.124)

As a result, the normalized local equilibrium (Maxwellian) distribution function \( F_{0j} \) is expressed as

\[ F_{0j} = \pi^{-3/2} e^{-(v_{Tj}^2 + \mu B_0)}. \]  \hspace{1cm} (2.125)

2.7.2 The gyrokinetic equation solved in GENE

Taking into account the flux-tube approximation and the normalizations used in GENE, the gyrokinetic equation governing the dynamics of a given species \( j \) can be written formally as follows:

\[ \frac{\partial g_{kj}}{\partial t} = L[g_{kj}] + D[g_{kj}] + N[g_{kj}, g_{kj}], \]  \hspace{1cm} (2.126)

where \( g_{kj} = g_{kj}(k_x, k_y, z, v_\parallel, \mu) \) is the modified distribution function for the species considered\(^1\)

\[ g_{kj} = f_{kj} + v_{Tj} v_\parallel \frac{q_j F_{0j}}{T_{0j} j_{0kj} A_{1||k}}. \]  \hspace{1cm} (2.127)

\(^1\)In the following, the subscript 1 is dropped from the distribution functions \( g_{kj}, f_{kj}, h_{kj} \) as well as for the modified field \( \chi_{kj} \) for clarity of the presentation.
2. GYROKINETICS AND THE GENE CODE

The linear term $L[g_{kj}]$ can be split into three contributions:

$$L[g_{kj}] = L_G[g_{kj}] + L_K[g_{kj}] + L_{\parallel}[g_{kj}].$$  \hfill (2.128)

The first term $L_G$ represents the influence of the density ($\omega_{nj}$) and temperature ($\omega_{Tj}$) gradients

$$L_G[g_{kj}] = -\left(\omega_{nj} + \left(v^2 + \mu B_0 - 3/2\right) \omega_{Tj}\right) F_{0j} k_y \chi_{kj},$$  \hfill (2.129)

Here, $\chi_{kj}$ is the modified electromagnetic term

$$\chi_{kj} = J_{0kj} \phi_{1k} - v_{Tj} v_{\parallel} J_{0kj} A_{1\parallel k}.$$  \hfill (2.130)

The second linear term $L_K$ describes effects due to magnetic curvature,

$$L_K[g_{kj}] = -\frac{T_{0j} (2v^2 + \mu B_0)}{q_j B_0} \left( K_x k_x + K_y k_y \right) h_{kj}.$$  \hfill (2.131)

In the above expression, the non-adiabatic part of the distribution function $h_{kj}$ is defined as:

$$h_{kj} = f_{kj} + \frac{q_j F_{0j} J_{0kj} \phi_{1k}}{T_{0j}} = g_{kj} + \frac{q_j F_{0j}}{T_{0j}} \chi_{kj}.$$  \hfill (2.132)

Moreover, we have introduced the normalized geometrical quantities:

$$K_x = -\frac{L_{\text{ref}} g^{xx} g^{yz} - g^{yx} g^{xz}}{B_{\text{ref}} B_0^2} \frac{\partial B_0}{\partial z},$$ \hfill (2.133)

$$K_y = -\frac{L_{\text{ref}} g^{xy} g^{yz} - g^{yx} g^{xz}}{B_{\text{ref}} B_0^2} \frac{\partial B_0}{\partial z}.$$ \hfill (2.134)

The equilibrium magnetic field $B_0$, the metric coefficients $g^{ij}$ and the Jacobian $J(z)$ come from the magnetic equilibrium chosen (see Sec. 2.6.2). The third linear term $L_{\parallel}$ contains the parallel dynamics involving magnetic trapping as well as the linear Landau damping. It can be expressed in terms of Poisson brackets as

$$L_{\parallel}[g_{kj}] = \frac{v_{Tj}}{2B_0 J(z)} \left[ \frac{h_{kj}}{F_{0j}}, F_{0j} \right]_{\parallel},$$ \hfill (2.135)

where the Poisson brackets are defined as usual

$$[f, g]_{ab} = \frac{\partial f}{\partial a} \frac{\partial g}{\partial b} - \frac{\partial f}{\partial b} \frac{\partial g}{\partial a}.$$ \hfill (2.136)

The next term in the GK equation (2.126) is the dissipation term $D[g_{kj}]$. The dissipation is ensured by hyper diffusion operators in the collisionless case:

$$D[g_{kj}] = \left( a_{z} \partial_z^2 + a_{v_{\parallel}} \partial_{v_{\parallel}} + a_{x} k_x^2 + a_{y} k_y^2 \right) h_{kj},$$ \hfill (2.137)
where typically \( n = 4 \) is used, and the coefficients \( a_x, a_y, a_z, \) and \( a_v \) can be adapted to a specific class of physical problems (for details, see Ref \([17]\)).

The nonlinear term \( N[g_{kj}, g_{kj}] \) arises from the \( \mathbf{E} \times \mathbf{B} \) drift velocity. In particular it comes from the term \( \mathbf{v}_\chi \cdot \nabla h_j \) of the gyrokinetic equation (2.75):

\[
N[g_{kj}, g_{kj}] = \sum_{k'} \sum_{k''} \left( k_x' k_x' - k_x k_y' \right) \chi_{k'j} h_{k''j} \delta_{k-k'-k''} \\
= \sum_{k'} \left( k_x' k_y - k_x k_y' \right) \chi_{k'j} h_{(k-k')j} \\
= \sum_{k'} \left( k_x' k_y - k_x k_y' \right) \chi_{k'j} g_{(k-k')j}.
\]

The nonlinear term can be expressed in several equivalent ways, and in the rest of the work we will use the most convenient representation in each case. For instance, it can be expressed as:

\[
N[g_{kj}, g_{kj}] = \sum_{k'} \left[ (k_x - k_x') \chi_{(k-k')j} k_y' g_{k'j} - (k_y - k_y') \chi_{(k-k')j} k_x' g_{k'j} \right].
\]

(2.139)

Also, it can be expressed in real space \((x, y)\) in terms of Poisson brackets:

\[
N[g_{kj}, g_{kj}] = - \left[ \chi_{j}, g_{j} \right]_{x,y}.
\]

(2.140)

### 2.7.3 The gyrokinetic field equations solved in Gene

The electrostatic potential \( \phi_{1k} \) is given by Poisson’s equation in Fourier space:

\[
\left[ k_x^2 \lambda_D^2 + \sum_j \frac{q_j^2 n_{0j}}{T_{0j}} [1 - \Gamma_0(b_j)] \right] \phi_{1k} = \pi B_0 \sum_j n_{0j} q_j \int J_{0kj} g_{kj} d\mu \, dv||
\]

(2.141)

and the magnetic vector potential \( A_{1||k} \) is given by the parallel Ampère’s Law:

\[
\left[ 2 k_x^2 / \beta + \pi B_0 \sum_j \frac{q_j^2 n_{0j} v_{Tj}^2}{T_{0j}} \int v_{||}^2 J_{0kj} F_{0j} d\mu \, dv|| \right] A_{1||k} = \pi B_0 \sum_j n_{0j} q_j v_{Tj} \int v_{||} J_{0kj} g_{kj} d\mu \, dv||,
\]

(2.142)

where \( \beta \) is the ratio of the plasma pressure to the magnetic pressure and \( \lambda_D \) is the Debye length:

\[
\beta = \frac{8\pi n_{ref} T_{ref}}{B_{ref}^2}, \quad \lambda_D^2 = \frac{B_{ref}^2}{4\pi^2 n_{ref} m_{ref}}.
\]
Here, the Bessel functions appropriately normalized are defined as follows:

\[
J_{0kj} = J_0(k_{\perp}\rho_j) = J_0\left(\frac{v_{Tj}}{\Omega_j}k_{\perp}\sqrt{B_0\mu}\right),
\]

(2.143)

\[
\Gamma_0(b_j) = \Gamma_0\left(\frac{v_{Tj}^2k_{\perp}}{\Omega_j}\right),
\]

(2.144)

where the amplitude of the perpendicular wave vector is given by

\[
k_{\perp}^2 = g_{xx}k_x^2 + 2g_{xy}k_xk_y + g_{yy}k_y^2,
\]

(2.145)

and depends on \(z\) through the metric coefficients.

Finally, we will mention that for low \(\beta\) plasmas it can be shown (see Ref. [15]) that the magnetic fluctuations can also be neglected. Consequently, the fluctuations are only electrostatic and there is not need of parallel Ampère’s law. Note that in this case, the following relations are trivially fulfilled:

\[
h_{kj} = f_{kj} + q_j F_{0j} J_{0kj} \phi_{1k},
\]

(2.146)

\[
f_{1kj} = g_{kj},
\]

(2.147)

\[
\chi_{kj} = J_{0kj} \phi_{1k}.
\]

(2.148)

### 2.7.4 Adiabatic electron response

The assumption of adiabatic electrons is commonly used in the literature. It is based on the fact that the electron response could be approximated as instantaneous in the case of sufficiently low frequency phenomena [18]. In this model, the magnetic fluctuations are also neglected. Here, the electron population is then described by its perturbed density \(n_{1e}\):

\[
q_en_{1e} = q_en_{0e} \pi B_0 \int d\mu dv_{||} J_{0ke} g_{ke} = \frac{q_e^2 n_{0e}}{T_{0e}} (\langle \phi_1 \rangle_{FS} - \phi_{1k}).
\]

(2.149)

We have also used the definition of the integration over a given flux surface

\[
\langle A \rangle_{FS} = \frac{\int J(z) A(k_x, k_y = 0, z) \, dz}{\int J(z) \, dz}.
\]

(2.150)

Therefore using Eq. (2.149), the resulting modified Poisson’s equation is:

\[
\pi B_0 q_i n_{0i} \int d\mu dv_{||} J_{0ki} g_{ki} = \frac{q_i^2 n_{0i}}{T_{0i}} (\phi_{1k} - \langle \phi_1 \rangle_{FS}) + \frac{q_i^2 n_{0i}}{T_{0i}} [1 - \Gamma_0(b_i)] \phi_{1k},
\]

(2.151)

where \(\chi_D^2 \to 0\) has been assumed, since generally the Debye length is much smaller than the typical Larmor radius of the species considered, thus being a higher order term.
2.7.5 Adiabatic ion response

A similar assumption can be done for the ion distribution function. In this case, a short-wavelength approximation is applied. All terms containing averaged over the ion gyro-motion vanish and the Poisson’s equation writes:

$$\pi B_0 q_e n_{0e} \int d\mu \, dv_\parallel \, J_{0ke,ke} = \left( \sum_i \frac{q_i^2 n_{0i}}{T_{0i}} + \frac{q_e^2 n_{0e}}{T_{0e}} \left[ 1 - \Gamma_0(b_e) \right] \right) \phi_{1k}, \quad (2.152)$$

where $$\lambda_D^2 \to 0$$ is also assumed and magnetic fluctuations have been neglected.

2.7.6 Transport quantities

As it was mentioned in Chapter 1, understanding the radial transport mechanisms that take place in tokamaks remains one of the key challenges for nuclear fusion devices. Therefore, the final goal of any gyrokinetic simulation is to predict and optimize the radial transport of particles and heat in tokamak plasmas. They are characterized through their respective particle and heat fluxes. In GENE they are calculated for each species $$j$$ as follows

$$\Gamma_j = - \frac{n_{0j}}{J(z)} \int d\mu \pi B_0 i k_y \chi_{kj} f_{-kj}, \quad (2.153)$$

$$Q_j = - \frac{n_{0j} T_{0j}}{J(z)} \int d\mu \pi B_0 i k_y \chi_{kj} \left( v_{\parallel}^2 + \mu B_0 \right) f_{-kj}, \quad (2.154)$$

Here, the particle flux $$\Gamma_j$$ is expressed in units of $$n_{\text{ref}} c_{\text{ref}} L_y^2$$ and the heat flux $$Q_j$$ is expressed in $$n_{\text{ref}} T_{\text{ref}} c_{\text{ref}} L_y^2$$ units. Finally, spatial average of a product of two fields $$A(x)$$ and $$B(x)$$ has been also assumed in the definitions:

$$\langle A(x)B(x) \rangle_V = \frac{\int J(z) A(x) B(x) dxdydz}{\int J(z) dxdydz}$$

$$= \frac{\int J(z) \sum_{k,k'} e^{i(k+k') \cdot x} A(k,z) B(k',z) dx dy dz}{L_x L_y \int J(z) dz}$$

$$= \frac{\int J(z) dz \sum_{k,k'} \delta_{k+k'} A(k,z) B(k',z)}{\int J(z) dz}$$

$$= \frac{\int J(z) dz \sum_k A(k,z) B(-k,z)}{\int J(z) dz}. \quad (2.155)$$
2. GYROKINETICS AND THE GENE CODE
Chapter 3

LARGE-EDDY SIMULATIONS

This work deals with the simulation of plasma turbulence. Plasma turbulence is an interdisciplinary field in which fluid dynamics, electromagnetism and kinetic theory play a fundamental role. This chapter introduces the basic concepts in fluid dynamics that we have applied to gyrokinetic theory. These concepts are necessary to understand the techniques developed in this thesis.

In Sec. 3.1 and 3.2, an introduction to fluid turbulence and its numerical simulation are given. Sec 3.3 introduces the Large-Eddy Simulation (LES) technique for fluid turbulence. Furthermore, the Smagorinsky model and the dynamic procedure are briefly explained. Finally, in Sec 3.4 we show how the LES approach has been extended to conductive fluids.

3.1 Introduction to fluid turbulence

Following Carati [19], an introduction to fluid turbulence and Large-Eddy Simulations is given below.

The most fundamental equation in fluid mechanics, which expresses the momentum balance of a fluid element, is the Navier-Stokes (N-S) equation:

\[
\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{\rho} \mathbf{f}^{\text{ext}} - \frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v},
\]

where \( \mathbf{v} = \mathbf{v}(\mathbf{x}, t) \) is the velocity of the fluid element at every point in space \( \mathbf{x} \) and time \( t \). Here, \( \rho \) is the mass density, \( p \) is the pressure and \( \nu \) is the kinematic viscosity. The external forces applied to the fluid element are represented by \( \mathbf{f}^{\text{ext}} \). We will also assume incompressible flow \( \nabla \cdot \mathbf{v} = 0 \), and work in units where \( \rho = 1 \). In this case, the pressure is related to the divergence of the advective term \( (\mathbf{v} \cdot \nabla)\mathbf{v} \):

\[
-\nabla^2 p = \nabla \cdot [(\mathbf{v} \cdot \nabla) \mathbf{v}],
\]

and can be treated as a modification of the advective derivative. Note that the advective term is a quadratic (nonlinear) term, since it involves the square of the velocity field.
3. LARGE-EDDY SIMULATIONS

For simplicity, let us now rewrite the N-S equation and the incompressibility condition in tensorial form:

\[ \frac{\partial}{\partial t} v_i + v_j \frac{\partial}{\partial x_j} v_i = f_i^{\text{ext}} - \frac{\partial}{\partial x_i} p + \nu \frac{\partial^2}{\partial x_i \partial x_j} v_i, \]
\[ \frac{\partial}{\partial t} v_i = 0, \]
where in addition to the Einstein’s convention of implicit summation over repeated indices, we use the notation:

\[ \frac{\partial}{\partial t} \equiv \frac{\partial}{\partial t}, \quad \frac{\partial}{\partial x_j} \equiv \frac{\partial}{\partial x_j}, \quad \frac{\partial^2}{\partial x_i \partial x_j} \equiv \frac{\partial^2}{\partial x_i \partial x_j}. \]

(3.5)

At this point, we would like to remark that although the Navier-Stokes equation is a fundamental equation of nature, it is a model: the motion is represented by macroscopic fluid elements defined on a continuum, even though the fluid is made up of discrete molecules. The dissipation due to molecular collisions is modeled by the smooth and continuous process of viscous diffusion.

In addition to the external forces applied to the system, the evolution of the flow is governed by two forces. These are the inertial force, represented by the advective term \( v_j \frac{\partial}{\partial x_j} v_i \), with the pressure included through the identity (3.2) and the dissipative force, represented by the viscous force \( \nu \frac{\partial^2}{\partial x_i \partial x_j} v_i \). We can characterize the relative strength of the forces defining a dimensionless number known as the Reynolds number \( Re \). It measures the ratio between the inertial force and the viscous force:

\[ Re = \frac{v_j \frac{\partial}{\partial x_j} v_i}{\nu \frac{\partial^2}{\partial x_i \partial x_j} v_i} \sim \frac{VL}{\nu}, \]

(3.6)

where \( L \) and \( V \) are the characteristic scale and velocity of the flow, respectively. Depending on the value of the Reynolds number, different regimes are defined. The so-called laminar regime is defined for low Reynolds numbers. In this regime, the dynamics of the system is dominated by the viscous term, making the system dissipative. In other words, the energy injected into the system is dissipated rapidly into heat. On the other hand, turbulent regimes are defined for sufficiently large Reynolds numbers. Here, the dissipation is weak and the motion is dominated by the inertial force term, causing the formation of eddies of many different length scales. In the following, we will focus on the study of turbulent regimes.

In order to understand the turbulent dynamics, it is recommended to look for quantities that are conserved by the nonlinear term. These quantities are known as nonlinear or ideal invariants. For Navier-Stokes equation, the kinetic energy is such an invariant.

The kinetic energy equation can be obtained by multiplying the N-S equation by \( \rho v \) (which in our notation translates to a multiplication by \( v_i \)) and by integrating over total the volume of the flow. This operation can be symbolized by applying a kinetic energy operator \( \mathcal{K}_v \) to the N-S equation (3.3):

\[ \mathcal{K}_v[\text{eq: N-S}] := \int_V \rho v_i [\text{eq: N-S}] = \langle v_i [\text{eq: N-S}] \rangle_V, \]

(3.7)
3.1 Introduction to fluid turbulence

where in the last step the integration over the volume of flow is represented by \( \langle \cdot \rangle_V \). In the following, we will restrict ourselves to the study of the flow in a periodic box. This will allow us to use periodic boundary conditions and simplify the problem. Regarding the time derivative term in the N-S equation, we have:

\[
K_v[\partial_t v_i] = \langle v_i \partial_t v_i \rangle_V = \left\langle \partial_t \frac{v_i^2}{2} \right\rangle_V = \frac{d}{dt} \left\langle \frac{v_i^2}{2} \right\rangle_V = \frac{dE_v}{dt}, \tag{3.8}
\]

where we have defined the mean kinetic energy of the flow as usual:

\[
E_v = \left\langle \frac{v_i^2}{2} \right\rangle_V = \int_V d^3r \frac{v_i^2}{2}. \tag{3.9}
\]

As we have just mentioned, the nonlinear term is conserved by the kinetic energy:

\[
K_v[v_j \partial_j v_i] = \langle v_i v_j \partial_j v_i \rangle_V = \left\langle \partial_j \frac{v_j v_i^2}{2} \right\rangle_V = \left\langle \partial_j \frac{v_j v_i v_i}{2} \right\rangle_V = 0, \tag{3.10}
\]

where we have used the incompressibility condition (3.4) and the fact that for any periodic function \( f \), \( \langle \partial_i f \rangle_V = 0 \).

For the terms in the right hand side of the N-S equation, the pressure term vanishes:

\[
K_v[\partial_i p] = -\langle v_i \partial_i p \rangle_V = -\langle \partial_i v_i p \rangle_V = 0, \tag{3.11}
\]

for the same reasons as in the case of the nonlinear term.

The external force gives a contribution to the kinetic energy balance equation:

\[
K_v[f_{ext}^{ext}] = \langle v_i f_{ext}^{ext} \rangle_V = \epsilon_i, \tag{3.12}
\]

where \( \epsilon_i \) is defined as the injection rate (energy injected per unit of time).

The viscous term also contributes to the kinetic energy balance equation:

\[
K_v[\nu \partial_{ij} v_i] = \langle \nu v_i \partial_{ij} v_i \rangle_V = -\nu \frac{1}{2} \langle (\partial_i v_j + \partial_j v_i)^2 \rangle_V = -\nu \langle 2S_{ij} S_{ij} \rangle_V = -\epsilon_d, \tag{3.13}
\]

where \( S_{ij} = (\partial_i v_j + \partial_j v_i)/2 \) is the strain-stress tensor and \( \epsilon_d \) is defined as the dissipation rate (energy dissipated per unit of time).

We group all terms playing a role in the kinetic energy balance equation and we obtain:

\[
\frac{dE_v}{dt} = \epsilon_i - \epsilon_d. \tag{3.14}
\]

If the flow is in a stationary state, the total energy of the system should remain constant. Thus, the injection rate \( \epsilon_i \) (due to external forces) and the dissipation rate \( \epsilon_d \) (due to viscous forces) balance:

\[
0 = \epsilon_i - \epsilon_d \Rightarrow \epsilon_i = \epsilon_d = \epsilon, \tag{3.15}
\]

where \( \epsilon \) is called the energy flux and has units of length squared \([L^2]\) per unit of time cubed \([T]^3\).
3. LARGE-EDDY SIMULATIONS

3.1.1 The inertial range cascade

In a turbulent system the energy is generally injected at large scales at a rate $\epsilon$ by external forces. On the other hand, this flux of energy can be only dissipated at small (collisional) scales. This leads to the existence of a range of scales where the energy is neither injected nor dissipated. This range, dominated by the inertial force, is known as the **inertial range**. Here, under inertial interactions the energy injected at the large scales is passed without dissipation to successively smaller scales in a so-called **cascade** process. At some sufficiently small scale the viscous dissipation becomes important and the kinetic energy injected into the system at the **forcing range** is converted into heat. The scale which mark the end of inertial range and the beginning of the dissipative range is known as the Kolmogorov scale and in the following will be labeled by $l_\nu$. This scale obviously depends on the viscosity. Generally, the smaller viscosity, the smaller the Kolmogorov scale. It also depends on the rate at which the energy is injected into the system. Assuming that the Kolmogorov scale is determined only by these two quantities, dimensional analysis leads to:

$$l_\nu \sim \nu^{\alpha} \epsilon^{\beta}.$$  \hspace{1cm} (3.16)

Since the viscosity $\nu$ has units of length squared per unit of time, $[\nu] = [L^2]/[T]$, we have:

$$[l_\nu] = \left[ \frac{L^2}{T} \right]^\alpha \left[ \frac{L^2}{T^3} \right]^\beta = [L].$$  \hspace{1cm} (3.17)

Solving $2\alpha + 2\beta = 1$ and $-\alpha - 3\beta = 0$ yields $\alpha = 3/4$ and $\beta = -1/4$, from which:

$$l_\nu \sim \left( \frac{\nu^3}{\epsilon} \right)^{1/4}.$$  \hspace{1cm} (3.18)

This cascade process can be visualized graphically in Fig. 3.1, where the turbulent eddies of different scales are represented by blobs of different sizes. This cascade is also known as a **forward** or **direct cascade** because the kinetic energy goes from large scales to small ones.

3.1.2 The Kolmogorov spectrum

Based on the notion of a cascade in the inertial range, Kolmogorov in 1941 derived his celebrated spectrum. It can be obtained by written the total energy as:

$$E_v = \left\langle \frac{v^2}{2} \right\rangle_v = \int dk E(k).$$  \hspace{1cm} (3.19)

Here, $E(k)$ is the spectral energy density and has units of $[L^3]/[T^2]$. It corresponds to the energy associated to turbulent structures with a characteristic length scale
3.2 Simulation of fluid turbulence

Figure 3.1: Energy introduced at the top at a rate $\epsilon$ is cascading down this hierarchy of eddies at the same rate and is eventually removed by dissipation at the bottom, still at the same rate $\epsilon$.

$\epsilon \propto k^{-1}$. Kolmogorov also assumed that in the inertial range the spectral energy density only depends on the scale $k$ and in the energy flux $\epsilon$. In other words, he assumed that in the inertial range the physics of the turbulent system is independent of the forcing and dissipation mechanisms:

$$E(k) \sim k^\alpha \epsilon^\beta. \quad (3.20)$$

Using dimensional analysis:

$$[E(k)] = \left[ \frac{1}{L} \right]^\alpha \left[ \frac{L^2}{T^3} \right]^\beta = \left[ \frac{L^3}{T^2} \right]. \quad (3.21)$$

Solving for $-3\beta = -2$ and for $-\alpha + 2\beta = 3$, we find $\beta = 2/3$ and $\alpha = -5/3$, and the energy scaling law is:

$$E(k) \sim k^{-5/3} \epsilon^{2/3}. \quad (3.22)$$

This expression describes the famous Kolmogorov $-5/3$ spectrum. It is one of the most important results of Kolmogorov theory [20, 21], and there are experimental evidences that support it [22]. The energy spectrum with the different regimes is presented schematically in Fig. 3.2.

3.2 Simulation of fluid turbulence

We have just shown how Kolmogorov was able to derive certain scaling laws for turbulent flows using some plausible hypotheses. However, Navier-Stokes equation is a very complex equation, which has been studied for more than hundred years, and scientists are unable to obtain exact or even approximate analytical
3. LARGE-EDDY SIMULATIONS

Figure 3.2: An illustration showing the different scales in a turbulent system. The energy injected in the forcing range is cascaded to the smallest scales where it will be dissipated. In the inertial range, the kinetic energy spectrum is proportional to $k^{-5/3}$.

solutions of the equation in a turbulent regime. For this reason, the simulation of the equation by computers is a very important tool to study turbulent flows. However, there are also limitations even with today’s computers. This can be understood using the following arguments. In order to simulate the N-S equation we need to discretize it and, in particular, the velocity field $\mathbf{v}(\mathbf{x}, t)$ must be discretized in space and time. In fluid turbulence, it is called a Direct Numerical Simulation (DNS) a simulation that retains all the active scales in the system, that is, from the injection range down to the dissipation range. This is why scales smaller than the dissipation (Kolmogorov) scale can be neglected, since those scales do not contain energy. Consequently, for three dimensional flows, the number of points in space for the discretization of the velocity goes as

$$N_{\text{space}} \sim \left( \frac{L}{l_\nu} \right)^3,$$

(3.23)

where $L$ is the largest scale in the system. Taking into account the definition of energy flux $\epsilon$ and the Reynolds number $Re$:

$$\epsilon = \frac{V^2}{T} = \frac{V^3}{L}, \quad Re = \frac{LV}{\nu},$$

(3.24)

where $V$ and $T$ are the characteristic velocity and time of the flow, we can express the Kolmogorov scale $l_\nu$, as

$$l_\nu = \left( \frac{\nu^3}{\epsilon} \right)^{1/4} = \left( \frac{\nu^3 L}{V^3} \right)^{1/4} = \left( \frac{\nu^3}{V^3 L^3} \right)^{1/4} L = Re^{-3/4} L,$$

(3.25)

and we find that:

$$N_{\text{space}} \sim \left( \frac{L}{l_\nu} \right)^3 \sim Re^{9/4}.$$

(3.26)
In addition, the velocity field must be known for every time step \( t_\nu \), where \( t_\nu \) is the time associated with the smallest scale of the system (the Kolmogorov scale). Thus, we need a total number of time steps that goes as

\[
N_{\text{time}} = \frac{T}{t_\nu}. \tag{3.27}
\]

The characteristic time \( (t_\nu) \) it is normally calculated as the time needed for convecting small scale structures on a distance \( l_\nu \) by large velocity flow \( V \). Taking that into account, we find:

\[
t_\nu = \frac{l_\nu}{V} = \frac{l_\nu L}{L V} = Re^{-3/4}T, \tag{3.28}
\]

and we have that the total number of time steps is given by

\[
N_{\text{time}} = \frac{T}{t_\nu} \sim Re^{3/4}. \tag{3.29}
\]

Hence, the total number of numerical operations for describing the experiment in a turbulent regime scales as:

\[
N_{\text{total}} = N_{\text{space}}N_{\text{time}} \sim Re^3. \tag{3.30}
\]

This number is huge for almost any turbulent flow in nature, where \( Re \sim 10^5 \) or even higher Reynolds numbers can be found. This is the reason why alternative approaches are needed for studying fully developed turbulence. This has prompted the development of Large-Eddy simulations (LES) for which the direct numerical computation is limited to the large scales of turbulence (under-resolved simulations) while a model is added to account for the effects of the small scale motions.

### 3.3 Introduction to Large-Eddy Simulations

Large-Eddy simulations assume an arbitrary scale separation between the large scales structures that are computed directly and the small scale phenomena that are not captured by the numerical grid and must be modeled. It should be pointed out that LES is not justified by the existence of a scale separation between large eddies and small scale structures. The coexistence of structures with various characteristics lengths is indeed ubiquitous in fluid turbulence, see Fig. 3.3. LES is rather based on an artificial separation mainly driven by computer simulations. This scale separation is introduced by a filtering operator that smoothes out all the scales smaller than a given scale \( \Delta \). In the following, the filtering operation is denoted by the symbol \( \cdots \) and is represented by a filter operator \( F_{\Delta} \) acting on the velocity field \( v_i \):

\[
\overline{v}_i(x) = F_{\Delta}[v_i] := \int G(x, y; \Delta) v_i(y) \, dy, \tag{3.31}
\]
3. LARGE-EDDY SIMULATIONS

Figure 3.3: Different scales can be found in a flow at the same time. Top: Homogenous turbulence behind a grid. Photo: M. Van Dyke. *An Album of Fluid Motion*. Left: Cigarette smoke makes the turbulent motion of rising heated air visible. Right: The image credited to Professor Y. Kaneda illustrates the small scales of turbulence obtained with an direct numerical simulation performed on the "Earth Simulator" used for weather and seismological simulations.

where $G(x, y; \Delta)$ is any kernel that serves to damp spatial fluctuations shorter than $\Delta$, and satisfying $\Delta > \Delta_{DNS}$. Here, $\Delta_{DNS}$ represents the smallest scale required for describing the flow. For instance, Fig. 3.4 shows the effect of the filter operation on the velocity field $v_i$.

Figure 3.4: The filter smoothes out the smallest scales of the system [19].

In the following, we will restrict ourselves to a common class of operators
defined as follows:

\[
\overline{v}_i(x) = \mathcal{F}_\Delta[v_i] := \int G(x - y; \Delta) v_i(y) \, dy.
\]

(3.32)

Here, the kernel only depends on the position difference \((x - y)\). Consequently, the same operator is used in the whole domain. These operators are known as **homogeneous operators**. Their main advantage is that they commute with the spatial (and also time) derivatives:

\[
[\partial_i, \mathcal{F}_\Delta] = 0 \Rightarrow (\partial_i \mathcal{F}_\Delta - \mathcal{F}_\Delta \partial_i) [v_i] = \mathcal{F}_\Delta \partial_i [v_i] = \partial_i \overline{v}_i = \overline{\partial_i v}_i.
\]

(3.33)

Therefore, if we apply now the filter operation \(\cdots\) to the N-S (3.3), we obtain the following equation:

\[
\overline{\partial_t v}_i + \overline{v}_j \partial_j v_i = \overline{f^\text{ext}}_i - \overline{\partial_i p} + \nu \partial_{jj} \overline{v}_i.
\]

(3.34)

Using the commutation property with the time and spatial derivatives of the filter operator, we have:

\[
\partial_t \overline{v}_i + \overline{v}_j \partial_j v_i = \overline{f^\text{ext}}_i - \overline{\partial_i p} + \nu \partial_{jj} \overline{v}_i.
\]

(3.35)

The nonlinear term is treated in a different way. Using the filtered incompressibility condition \(\partial_i \overline{v}_i = 0\), we can rewrite it as:

\[
\overline{v}_j \partial_j \overline{v}_i = \partial_j \overline{v}_j v_i = \partial_j \overline{v}_j \overline{v}_i.
\]

(3.36)

However, this term is unknown since it depends on the complete velocity field \(v_i\). For this reason, it is customary to express it in the following way:

\[
\partial_j \overline{v}_j \overline{v}_i = \partial_j \overline{v}_j \overline{v}_i + \partial_j \overline{\overline{v}_j v}_i - \partial_j \overline{\overline{v}_j v}_i = \partial_j \overline{v}_j \overline{v}_i + \partial_j \tau_{ij},
\]

where \(\partial_j \tau_{ij} = \partial_j (\overline{v}_j \overline{v}_i - \overline{\overline{v}_j v}_i)\).

(3.37)

(3.38)

Here, \(\tau_{ij}\) contains now the unknown term. Substituting the above expression in the filtered N-S equation (3.35), we have the so-called LES equation:

\[
\overline{\partial_t v}_i + \overline{v}_j \partial_j \overline{v}_i = \overline{f^\text{ext}}_i - \overline{\partial_i p} + \nu \partial_{jj} \overline{v}_i - \partial_j \tau_{ij}.
\]

(3.39)

This equations looks exactly the same as the Navier-Stokes equation but acting on the filtered velocity field \(\overline{v}_i\). However, it has one new term, which represents the effect of the **under-resolved** (small) scales on the **resolved** (large) scales and it is given by:

\[
\tau_{ij} = \overline{\overline{v}_i v}_j - \overline{v}_i \overline{v}_j.
\]

(3.40)

This term is known as the **sub-grid stress tensor**, and depends on both the resolved velocity field \(\overline{v}_i\) and the unknown complete velocity field \(v_i\). Therefore, this term
must be modeled. The LES technique consists in finding models $M$ to represent the sub-grid term that only depends on the filtered velocity field $\overline{v}_i$:

$$\tau_{ij} \approx \tau_{ij}^{\text{model}}[\overline{v}_i].$$  (3.41)

In this context, a DNS can be defined as a simulation where the filter operator $F_{\Delta \text{DNS}}$ (damping scales shorter than $\Delta \text{DNS}$) is applied to the N-S equation:

$$\partial_t \overline{v}_i + \partial_j \overline{v}_i \overline{v}_j = \overline{F}^i - \partial_i p + \nu \partial_j \overline{v}_i - \partial_j \tau_{ij},$$  (3.42)

and the sub-grid contribution can be neglected.

### 3.3.1 Sub-grid modeling

In order to correctly model the sub-grid term, we need to understand its role in the LES equation. For this purpose it is convenient to look at the filtered kinetic energy equation which can be obtained by applying the filtered kinetic energy operator $K_{\overline{v}}$ to the LES equation:

$$K_{\overline{v}} \{\text{eq : LES}\} := \langle \overline{v}_i \{\text{eq : LES}\} \rangle_V.$$  (3.43)

Following similar steps as we did to obtain the kinetic energy balance equation, we obtain the filtered kinetic energy equation:

$$\frac{d \overline{E}_v}{dt} = \langle \overline{F}_i \overline{v}_i \rangle_V - 2\nu \langle \overline{S}_{ij}^2 \rangle_V - \langle \overline{v}_i \partial_j \tau_{ij} \rangle_V.$$  (3.44)

Here, $\overline{E}_v = \frac{\overline{v}_i^2}{2}$ represents the filtered kinetic energy and $\overline{S}_{ij} = (\partial_i \overline{v}_j + \partial_j \overline{v}_i)/2$ is the filtered strain-stress tensor. As in the kinetic energy case, the contributions of the nonlinear term and the pressure term vanish. However, we have now a contribution due to the sub-grid term $\tau_{ij}$ that can be expressed as:

$$\langle \overline{v}_i \partial_j \tau_{ij} \rangle_V = -\langle \tau_{ij} \frac{1}{2} (\partial_i \overline{v}_j + \partial_j \overline{v}_i) \rangle_V = -\langle \tau_{ij} \overline{S}_{ij} \rangle_V.$$  (3.45)

Finally, if we consider a stationary flow $\frac{d \overline{E}_v}{dt} = 0$ we find

$$\langle \overline{F}_i \overline{v}_i \rangle_V - 2\nu \langle \overline{S}_{ij}^2 \rangle_V + \langle \tau_{ij} \overline{S}_{ij} \rangle_V = 0.$$  (3.46)

This expression can be further approximated if we take into account the following considerations. First, the external forces act on the large scales, thus the effect of the filter operator on them should be negligible:

$$\langle \overline{F}_i \overline{v}_i \rangle_V \sim \langle f_{\text{ext}}^i \overline{v}_i \rangle_V = \epsilon_i.$$  (3.47)
Second, the viscous term acts only at small scales. Thus, the effect of the filter in this term cancels it:

\[ 2\nu \left \langle \overline{S}^2_{ij} \right \rangle_V = \tau_d \sim 0. \]  

(3.48)

Finally, we end up with the following balance equation:

\[ \epsilon_i \sim \left \langle \tau_{ij} \overline{S}_{ij} \right \rangle_V, \]

(3.49)

which tells us that the sub-grid term should dissipate the kinetic energy injected into the system by some external forces at large scales. If we want to model this term, it must dissipate the correct amount of the kinetic energy from the system. This can be visualized in the schematic representation of Fig. 3.5 where the physics of the sub-grid term can be seen as a cascade process studied in the previous section:

(a) The kinetic energy is injected at the large scales through some mechanical forcing and dissipated into heat in the small scales through viscous effects. For high Reynolds numbers, the forcing range and the dissipation range are well separated by an inertial range dominated by the nonlinear dynamics (purple line).

(b) If the small scales are not resolved and the sub-grid scale term is not modeled, the balance between injection and dissipation of kinetic energy cannot be reached and the kinetic energy will be accumulated in the inertial range (red line).

(c) Therefore, a model for the sub-grid term is expected to drain energy from the large scales in order to mimic the effects of the dissipation range (blue line).

### 3.3.2 The Smagorinsky model

Several models have been proposed for the sub-grid term for Navier-Stokes turbulence. However, the simplest and most widely used models are based on the eddy viscosity concept:

\[ \tau_{ij} \approx \tau_{ij}^{\text{model}} = -2\nu_e \overline{S}_{ij}, \]

(3.50)

where \( \nu_e \) is called the *eddy viscosity* and \( \overline{S}_{ij} \) is the filtered strain-stress tensor.

In the Smagorinsky model, the expression for the eddy viscosity can be obtained considering the following. First, if the filter \( F_\Delta \) acts in the inertial range, by the same arguments used by Kolmogorov to predict the energy spectrum, the eddy viscosity should depend only on the energy flux \( \epsilon \) and on the scale \( \Delta \):

\[ \nu_e \sim \overline{S}^\epsilon \Delta^\gamma. \]

(3.51)
3. LARGE-EDDY SIMULATIONS

Figure 3.5: A schematic picture representing the effect of the small scales. Top: The kinetic energy injected into the system at the large scales is transferred to the small ones where it is dissipated (purple line). Middle: The small scales are not resolved and the sub-grid term is not modeled. Therefore, the kinetic energy transferred from the large scales is accumulated in the inertial range (red line). Bottom: As a consequence, a model for the sub-grid term has to dissipate the energy accumulated in the inertial range in order to mimic the effects of the dissipation range (blue line).
3.3 Introduction to Large-Eddy Simulations

Using dimensional analysis we find that:

$$\nu_e \sim \Delta^{4/3} \epsilon^{1/3}. \quad (3.52)$$

However, in numerical simulations of N-S the energy flux is not computed. For solving this issue Smagorinsky proposed to approximate the energy flux by (see (Eq. (3.49))) :

$$\epsilon \sim -\tau_{ij}\overline{S}_{ij}. \quad (3.53)$$

Substituting the expression for $\tau_{ij}$ (see Eq. (3.50)) leads to

$$\epsilon \sim \nu_e \overline{S}^2, \quad (3.54)$$

where $\overline{S} = (2\overline{S}_{ij}\overline{S}_{ij})^{1/2}$. Therefore, Eq. (3.52) can be rewritten as:

$$\nu_e \sim \Delta^{4/3} \epsilon^{1/3} \sim \Delta^{4/3} \left(\nu_e \overline{S}^2\right)^{1/3} \Rightarrow \nu_e = C\Delta^2 \overline{S} \quad (3.55)$$

and the Smagorinsky model reads

$$\tau_{ij}^{\text{model}} = -2\nu_e \overline{S}_{ij}, \quad (3.56)$$

with $\nu_e$ given by

$$\nu_e = C\Delta^2 \overline{S}. \quad (3.57)$$

The proportionality constant $C$ is a free parameter and must be calibrated for each flow. A dynamic procedure was proposed to calculate $C$ at each time-step during the course of a simulation. This method was introduced by Germano in 1991 [23], later improved by Lilly in 1992 [24] and finally, some mathematical inconsistencies were removed by Ghosal in 1995 [25]. The dynamic procedure will be explained in detailed in the following section.

3.3.3 The dynamic procedure

The basic formalism behind the method proposed by Germano is summarized below.

1) We start from the LES equation:

$$\partial_t \overline{\nu}_i + \partial_j \overline{\nu}_i \overline{\nu}_j = \overline{f_i^{\text{ext}}} - \partial_i \overline{p} + \nu \partial_j \overline{\nu}_i - \partial_j \tau_{ij}. \quad (3.58)$$

2) We apply to the LES equation a filter operation denoted by the symbol $\overline{}$ and defined by:

$$\overline{\nu}_i(x) = \mathcal{F}_\Delta[\nu_i] := \int G(x - y; \Delta) \nu_i(y) dy. \quad (3.59)$$
3. LARGE-EDDY SIMULATIONS

Here, the kernel $G(x - y; \Delta)$ is defined in such a way that it damps fluctuations shorter than $\Delta$, and satisfying $\Delta > \overline{\Delta}$. This filter is often referred to as a test filter. The resulting LES equation is:

$$\partial_t \tilde{v}_i + \partial_j \tilde{v}_i \tilde{v}_j = \tilde{f}_i^\text{ext} - \partial_i \tilde{p} + \nu \partial_{jj} \tilde{v}_i - \partial_j \tilde{\tau}_{ij} - \partial_j L_{ij},$$

(3.60)

where the sub-grid term is given by

$$\tilde{\tau}_{ij} = \tilde{v}_i \tilde{v}_j - \tilde{v}_i \tilde{v}_j,$$

(3.61)

and

$$L_{ij} = \tilde{v}_i \tilde{v}_j - \tilde{v}_i \tilde{v}_j,$$

(3.62)

is known as the Leonard term. It can be explicitly calculated because it depends on the filtered velocity field $\tilde{v}_i$, which is known during a LES. On the other hand, $\tilde{\tau}_{ij}$ cannot be calculated because it depends on the complete velocity field $v_i$.

3) If we now apply the filter operation $\tilde{\cdots}$ to the N-S (3.3), we find:

$$\partial_t \tilde{v}_i + \partial_j \tilde{v}_i \tilde{v}_j = \tilde{f}_i^\text{ext} - \partial_i \tilde{p} + \nu \partial_{jj} \tilde{v}_i - \partial_j \tilde{\tau}_{ij}^2,$$

(3.63)

with

$$\tilde{\tau}_{ij}^2 = \tilde{v}_i \tilde{v}_j - \tilde{v}_i \tilde{v}_j.$$

(3.64)

4) The comparison between equations (3.60) and (3.63) leads to the property [23, 26]:

$$L_{ij} + \tilde{\tau}_{ij} - \tilde{\tau}_{ij}^2 = 0,$$

(3.65)

which is known as the Germano identity and it is a relation between two unknowns ($\tilde{\tau}_{ij}$ and $\tilde{\tau}_{ij}^2$) and the Leonard tensor $L_{ij}$.

5) If we consider now the Smagorinsky model we can approximate:

$$\tau_{ij} \approx -2\nu \overline{S}_{ij} = -2C(t)\overline{S}\overline{\Delta}^2\overline{S}_{ij},$$

(3.66)

$$\tau_{ij}^2 \approx -2\nu \overline{S}_{ij} = -2C(t)\overline{S}\overline{\Delta}^2\overline{S}_{ij},$$

(3.67)

where by the same arguments that lead the derivation of the Smagorinsky model, we have assumed that $C(t)$ is constant in space but depends on time and is the same in $\tau_{ij}$ and $\tau_{ij}^2$. This fact allows us to take it out of the filter operation in $\tilde{\tau}_{ij}$. Therefore, the Germano identity can be expressed as

$$L_{ij} - C(t) \left(2\overline{\Delta}^2\overline{S}\overline{S}_{ij} - 2\overline{\Delta}^2\overline{S}\overline{S}_{ij}\right) = 0$$

$$\Rightarrow L_{ij} - C(t) M_{ij} = 0,$$

(3.68)

with

$$M_{ij} = \left(2\overline{\Delta}^2\overline{S}\overline{S}_{ij} - 2\overline{\Delta}^2\overline{S}\overline{S}_{ij}\right).$$

(3.69)
3.4 Extension of the LES approach to conductive fluids

Finally, the square of Eq. (3.68) can be minimize respect to $C(t)$. This yields to

$$C(t) = \left\langle \frac{M_{ij} L_{ij}}{M_{kl} M_{kl}} \right\rangle_v .$$  \hfill (3.70)

Therefore, the parameter $C(t)$ can be calculated at each time-step during a LES.

3.4 Extension of the LES approach to conductive fluids

Many electrically conductive fluids – including plasmas – can be described within the framework of the magnetohydrodynamics (MHD) [27]. MHD is basically classical fluid dynamics, but the fluid is capable of generating and interacting with magnetic fields. Their balance equations read:

$$\partial_t v_i = - \partial_j (v_i v_j - b_i b_j) + \nu \partial_{jj} v_i - \partial_i p ,$$ \hfill (3.71)

$$\partial_t b_i = - \partial_j (v_i b_j - b_i v_j) + \eta \partial_{jj} b_i ,$$ \hfill (3.72)

$$\partial_i v_i = \partial_i b_i = 0 .$$ \hfill (3.73)

These equations are written here with the fluid velocity $v_i$ and the magnetic field $b_i$ both expressed in Alfvén speed units (the constant mass density is rescaled to unity). The total pressure $p$ can also be obtained by imposing the incompressibility of $v_i$ as in the N-S case. The dissipation coefficients are the viscosity $\nu$ and the magnetic diffusivity $\eta$. The balance between the linear and the nonlinear term in the induction equation (3.72) defines the magnetic Reynolds number $Rm = V L / \eta$ ($V$ and $L$ being a characteristic flow velocity and length scale, respectively). Simulation of MHD processes are thus not only limited by the grid requirement related to the velocity field but also by the necessity to properly capture the magnetic field. For instance, direct numerical simulations of three-dimensional MHD turbulence on today’s supercomputers [28, 29, 30] are limited to values of $Rm$ that are still several orders of magnitude lower than the ones found in nature, e.g., in the solar convection zone. Thus, there is a double motivation for developing LES techniques for this type of problem.

As usual, the large scale fields that will be directly computed in LES for MHD are assumed to be obtained from the complete field by means of a filtering operator that will be noted by $\overline{\cdots}$. The filtered equations for $\overline{v}$ and $\overline{b}$ thus read:

$$\partial_t \overline{v}_i = - \partial_j (\overline{v}_i \overline{v}_j - \overline{b}_i \overline{b}_j) + \nu \partial_{jj} \overline{v}_i - \partial_i \overline{p} - \partial_j \tau^\nu_{ij} ,$$ \hfill (3.74)

$$\partial_t \overline{b}_i = - \partial_j (\overline{v}_i \overline{b}_j - \overline{b}_i \overline{v}_j) + \eta \partial_{jj} \overline{b}_i - \partial_j \tau^b_{ij} ,$$ \hfill (3.75)

$$\partial_i \overline{v}_i = \partial_i \overline{b}_i = 0 ,$$ \hfill (3.76)
3. LARGE-EDDY SIMULATIONS

where two unknown terms, the sub-grid scale stress tensors, are introduced by the filtering operations:

$$\tau_{ij}^v = (v_i v_j - \bar{v}_i \bar{v}_j) - (b_i b_j - \bar{b}_i \bar{b}_j)$$  \hspace{1cm} (3.77)

and

$$\tau_{ij}^b = (v_i b_j - \bar{v}_i \bar{b}_j) - (b_i v_j - \bar{b}_i \bar{v}_j).$$  \hspace{1cm} (3.78)

These tensors have to be modeled. Therefore, we have to study their effect in the kinetic $E_v = \langle v^2/2 \rangle_V$ and magnetic $E_b = \langle b^2/2 \rangle_V$ energy balance equations, which can easily be derived and are expressed as follows:

$$\frac{\partial}{\partial t} E_v = D_v - T_{vb} - D_{v-sgs},$$  \hspace{1cm} (3.79)

$$\frac{\partial}{\partial t} E_b = D_\eta - T_{bv} - D_{b-sgs},$$  \hspace{1cm} (3.80)

where $T_{vb}$ represents the transfer of energy from $v_i$ to $b_i$ in the large scales. Because the total energy is conserved by the nonlinearities, this term is exactly the opposite of the transfer of energy from $b_i$ to $v_i$: $T_{vb} = - T_{bv}$. The other terms represent the viscous dissipation $D_v$, the Joule dissipation $D_\eta$ and the sub-grid scale dissipation of kinetic energy $D_{v-sgs}$ and of magnetic energy $D_{b-sgs}$. Like in Navier-Stokes turbulence, the main effect of the sub-grid scales in MHD has been assumed to dissipate the correct amount of energy and the sub-grid scale tensor can be modeled using eddy viscosity and eddy magnetic diffusivity terms:

$$\tau_{ij}^v = -\nu_e (\partial_j \bar{v}_i + \partial_i \bar{v}_j),$$  \hspace{1cm} (3.81)

$$\tau_{ij}^b = -\eta_e (\partial_j \bar{b}_i - \partial_i \bar{b}_j).$$  \hspace{1cm} (3.82)

Smagorinsky eddy viscosity models have been tested for $\nu_e$ and extended to the eddy magnetic resistivity $\eta_e$. In addition, the constant that appears in $-\nu_e$ and $-\eta_e$ have been derived using the dynamic procedure. This approach has been successfully tested for both forced and decaying MHD homogenous turbulence [31, 32, 33].
Chapter 4

FREE ENERGY CASCADE IN
GYROKINETIC TURBULENCE

4.1 Overview

Let us first briefly summarize what we have discussed in the previous chapter. In fluid turbulence, the kinetic energy is conserved by the advective nonlinearity. It is usually assumed to be injected into the system at the largest scales through mechanical forcing, and to be dissipated at the smallest scales by viscous effects. The role of the nonlinearity is then to transfer the kinetic energy from the large scales to the small ones in what is usually referred to as a cascade process. Based on the physics of the cascade process, sub-grid models for LES in fluid turbulence were developed.

For Gyrokinetic Large Eddy Simulations, the design of models should, like in fluid equations, be influenced by their expected role on the invariant balance. The difficulty is to identify which ideal invariant has to be considered. Recently, there has been a lot of effort devoted to the derivation of conservation laws in gyrokinetic equations. Independently of the present approach, the existence of conserved quantities by the gyrokinetic equations is very important in assessing the accuracy of the numerical solvers [34, 35].

In a recent paper [36], Schekochihin et al. have discussed in detail the energy balance in kinetic and gyrokinetic theory. They pointed out that, although conservation of energy is indeed important, the conservation of the free energy in gyrokinetics presents much more similarities with kinetic energy conservation in fluid equations. In addition, for two-dimensional gyrokinetic turbulence, it was shown [37, 38] that the free energy is indeed injected into the system at macroscopic scales via the equilibrium density and temperature gradients, and expected to be dissipated at small (space and/or velocity space) scales. Therefore, one role of the nonlinear term in gyrokinetic turbulence is to transfer the free energy from the largest perpendicular scales to the smallest ones. However, a definitive investigation of the free energy transfer dynamics in a self-driven, three-dimensional system (which is the standard case for magnetically confined plasmas) was still lacking. These facts motivated the new studies carried out in the present chapter.

This chapter is organized as follows. In Section 4.2, we introduce the general expression of the free energy in kinetic systems. In Sec 4.3, we derive the free
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

energy balance equation for gyrokinetics, in particular, within the framework of the formalism used in Gene. Then, in Sec 4.4 the resulting free energy balance equation is presented. It will be also shown in the case of adiabatic electrons and in the case of adiabatic ions. In Section 4.5, the numerical results are presented. Finally, the conclusions and the chapter summary are given in Sec. 4.6.

4.2 Free energy in kinetic systems

Let us first introduce the general expression of the free energy $E$ for kinetic systems:

$$E = U - T_0 S = K + E_E + E_M - T_0 S. \quad (4.1)$$

Here, $U$ is the total energy of the system, which it is composed of the kinetic $K$, the electric $E_E$ and magnetic $E_M$ energy. They are given by:

$$K = \sum_j \int d^3x \int d^3v \tilde{f}_j(x, v) m v^2, \quad E_E = \int d^3x \frac{E^2}{8\pi}, \quad \text{and} \quad E_M = \int d^3x \frac{B^2}{8\pi}. \quad (4.2)$$

where $\tilde{f}_j(x, v)$ is the particle distribution function and the integration is performed over the whole six-dimensional phase space $d^3x d^3v$. Moreover, $T_0$ represents the total temperature of the species considered. Finally, $S$ corresponds to the entropy of the system:

$$S = -\sum_j \int d^3x d^3v \tilde{f}_j \ln \tilde{f}_j. \quad (4.3)$$

If we split the distribution function $\tilde{f}_j$ into a Maxwellian distribution function $F_{0j}$ and a first order fluctuation part $\tilde{f}_{1j}$, the entropy part in the free energy equation can be re-expressed as:

$$-T_0 S = \sum_j T_{0j} \int d^3x \int d^3v \left[ \ln F_{0j} + \tilde{f}_{1j} + \tilde{f}_{1j}^2 \frac{2}{F_{0j}} \right], \quad (4.4)$$

by keeping only terms up to order two in $\tilde{f}_{1j}$.

The first term in the above equation

$$\sum_j T_{0j} \int d^3x \int d^3v \left( F_{0j} + \tilde{f}_{1j} \right) \ln F_{0j} = -\sum_j \int d^3x d^3v \left( F_{0j} + \tilde{f}_{1j} \right) m \frac{v^2}{2} = -K, \quad (4.5)$$

exactly cancels the kinetic energy $K$ in the expression for $E$. The second term in Eq. (4.4) simply represents the normalization of the fluctuating distribution.
4.3 Derivation of the balance equation

function and is assumed to be a constant that will disappear from the free energy balance equation. Only the last term contributes to the entropy part:

\[-T_0 S = \sum_j T_{0j} \int d^3x d^3v \frac{\tilde{f}_{lj}^2}{2 F_{0j}}.\] (4.6)

Grouping all the terms together, the free energy for kinetic systems can then be re-written as:

\[\mathcal{E} = -T_0 S + \mathcal{E}_E + \mathcal{E}_M\]

\[= \sum_j T_{0j} \int d^3x d^3v \frac{\tilde{f}_{lj}^2}{2 F_{0j}} + \int d^3x \frac{E^2}{8\pi} + \int d^3x \frac{B^2}{8\pi}.\] (4.7)

4.3 Derivation of the balance equation

In gyrokinetics, the free energy balance equation can be obtained by applying a free energy operator denoted by \(\Xi_h\) to the gyrokinetic equation (GK) (2.126) and adding its complex conjugate part (cc):

\[\Xi_h [\text{eq : GK}] + cc := \sum_{j,k} \left\langle \int d\mu dv_\parallel \frac{\pi}{2} B_0 n_{0j} \left( \frac{T_{0j} g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) [\text{eq : GK}] \right\rangle_z + cc,\] (4.8)

where we have used the following definition for the z-average:

\[\langle A(z) \rangle_z = \frac{\int J(z) A(z) dz}{\int J(z) dz}, \quad \forall A(z).\] (4.9)

Also, for simplicity of the presentation we use the notation

\[\sum_{j,k} = \sum_j \sum_k,\] (4.10)

where \(j\) labels the species (electron or ion) and \(k = (k_x, k_y)\) denotes the Fourier components in the perpendicular directions. The summation is performed over all \(k\) values, from \(-k_{\text{max}}\) to \(+k_{\text{max}}\) where the minus \(k\) index denotes the complex conjugate part of the unknown quantities. Furthermore, the summation over repeated \(k\) index is not assumed in the following.

4.3.1 Time derivative

Regarding the part of the time derivative we have to compute:

\[\Xi_h [\partial_t g_{kj}] + cc = \sum_{j,k} \left\langle \int d\mu dv_\parallel \frac{\pi}{2} B_0 n_{0j} \left( \frac{T_{0j} g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) [\partial_t g_{kj}] \right\rangle_z + cc.\] (4.11)
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

We can now to distinguish between the kinetic term (\( g - g \) coupling) and the electromagnetic term (\( \chi - g \) coupling).

4.3.1.1 Kinetic term

The kinetic term can be expressed as:

\[
\sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \frac{\pi}{2} B_0 n_{0j} T_{0j} \frac{g_{kj}}{F_{0j}} \partial_t g_{kj} \right\rangle_z + c.c = \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} T_{0j} \frac{|g_{kj}|^2}{2F_{0j}} \right\rangle_z.
\]  

(4.12)

The modified distribution function is defined as \( g_{kj} = f_{kj} + v_{Tj} q_j F_{0j} J_{0kj} A_{1||k} \), so Eq. (4.12) contains the following terms:

\[
|g_{kj}|^2 = \left| f_{kj} + v_{Tj} q_j F_{0j} J_{0kj} A_{1||k} \right|^2 
= |f_{kj}|^2 + v_{Tj}^2 q_j^2 F_{0j}^2 J_{0kj} A_{1||k}^2 + v_{Tj} q_j F_{0j} J_{0kj} (f_{-kj} J_{0kj} A_{1||k} + f_{kj} J_{0-kj} A_{1||-k})
\]  

(4.13)

Inserting this into Eq (4.12) yields

\[
\partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} T_{0j} \frac{|g_{kj}|^2}{2F_{0j}} \right\rangle_z = \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} T_{0j} \frac{|f_{kj}|^2}{2F_{0j}} \right\rangle_z
+ \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} v_{Tj}^2 v_{\perp j}^2 q_j \left( f_{-kj} J_{0kj} A_{1||k} + f_{kj} J_{0-kj} A_{1||-k} \right) \right\rangle_z
+ \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \frac{\pi}{2} B_0 n_{0j} v_{Tj} v_{\perp j} q_j (f_{-kj} J_{0kj} A_{1||k} + f_{kj} J_{0-kj} A_{1||-k}) \right\rangle_z.
\]  

(4.14)

Using the Ampère’s law written in terms of \( f_{-kj} \):

\[
2 \frac{k^2}{\beta} A_{1||-k} = \sum_j \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} v_{Tj} v_{\perp j} q_j J_{0kj} f_{-kj},
\]  

(4.15)

where we have used the property of the Bessel function \( J_{0-kj} = J_{0kj} \). Then, it is possible to re-write the last term of Eq. (4.14) as:

\[
\partial_t \sum_{j,k} \left\langle \int d\mu \, dv_{\parallel} \pi B_0 n_{0j} v_{Tj} v_{\perp j} \frac{1}{2} f_{-kj} J_{0kj} A_{1||k} + f_{kj} J_{0-kj} A_{1||-k} \right\rangle_z = \partial_t \sum_{k} \left\langle 2 \frac{k^2}{\beta} |A_{1||k}|^2 \right\rangle_z,
\]  

(4.16)
4.3 Derivation of the balance equation

and putting all the terms together, we finally get for that part of the time derivative

\[ \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_\parallel \pi B_0 n_{0j} T_{0j} \frac{|g_{kj}|^2}{2 F_{0j}} \right\rangle_z = \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_\parallel \pi B_0 n_{0j} T_{0j} \frac{|f_{kj}|^2}{2 F_{0j}} \right\rangle_z \]

\[ + \partial_t \sum_{j,k} \left\langle \int d\mu \, dv_\parallel \pi B_0 n_{0j} v_j^2 \frac{q_j^2 F_{0j}}{2 T_{0j}} |J_{0kj} A_{1||k}|^2 \right\rangle_z + \partial_t \sum_{k} \left\langle \frac{k^2}{\beta} |A_{1||k}|^2 \right\rangle_z. \]

(4.17)

4.3.1.2 Electromagnetic terms

The coupling term between \( g \) and \( \chi \), can be re-written using the definition of the modified field \( \chi_{kj} = J_{0kj} \phi_1k - v_{Tj} v_\parallel J_{0kj} A_{1||k} \) in its complex conjugate form:

\[ \sum_{j,k} \left\langle \int d\mu \, dv_\parallel \pi B_0 n_{0j} q_j \chi_{kj} \partial_t g_{kj} \right\rangle_z + \text{cc} = \sum_{j,k} \left\langle \int d\mu \, dv_\parallel \pi \frac{B_0 n_{0j} q_j J_{0kj}}{2} \left[ \phi_{1-k} - v_{Tj} v_\parallel A_{1||-k} \right] \partial_t g_{kj} \right\rangle_z + \text{cc}. \]

(4.18)

The right hand side (rhs) of Eq. (4.18) can be re-written in the form:

\[ \sum_{k} \left\langle \phi_{1-k} \partial_t \sum_{j} \int d\mu \, dv_\parallel \pi \frac{B_0 n_{0j} q_j J_{0kj} g_{kj}}{2} \right\rangle_z - \sum_{k} \left\langle A_{1||-k} \partial_t \sum_{j} \int d\mu \, dv_\parallel \pi \frac{B_0 n_{0j} q_j v_{Tj} v_\parallel J_{0kj} g_{kj}}{2} \right\rangle_z + \text{cc}. \]

(4.19)

Now we can use the Poisson’s law (2.141) (to replace \( g_{kj} \) by \( \phi_{1k} \)) and the Ampère’s law (2.142) (to replace the \( g_{kj} \) term for a \( A_{1||k} \)) and we finally get:

\[ \partial_t \sum_{k} \left\langle \left[ \frac{1}{2} \lambda_0^2 k_\parallel^2 |\phi_{1k}|^2 - \frac{k_\parallel^2}{\beta} |A_{1||k}|^2 + \sum_{j} \frac{n_{0j} q_j^2}{2 T_{0j}} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right. \right. \]

\[ - \left. \left. \sum_{j} \int d\mu \, dv_\parallel \pi B_0 n_{0j} v_j^2 \frac{q_j^2 F_{0j}}{2 T_{0j}} |J_{0kj} A_{1||k}|^2 \right]\right\rangle_z. \]

(4.20)
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

4.3.1.3 Total time derivative

Grouping all terms together, the time derivative part in the free energy balance equation is:

\[
\frac{\partial}{\partial t} E = \frac{\partial}{\partial t} \left[ E_f + E_\phi + E_A \right] = \partial_t \sum_k \left\langle \pi B_0 \sum_j n_{0j} T_{0j} \int d\mu \, dv \frac{f_{jk}}{2 T_{0j}} \right\rangle_z \\
+ \partial_t \sum_k \left\langle \frac{1}{2} \lambda_D^2 k_1^2 |\phi_{1k}|^2 \right\rangle_z + \sum_j \frac{n_{0j} q_j^2}{2 T_{0j}} \left[ 1 - \Gamma_0(b_j) \right] |\phi_{1k}|^2 \\
+ \partial_t \sum_k \left\langle \frac{k_1^2}{\beta} |A_1||k| \right\rangle_z , \quad (4.21)
\]

where the free energy \( E \) has been split into an entropy term \( E_f \) defined as:

\[
E_f = \sum_k \left\langle \pi B_0 \sum_j n_{0j} T_{0j} \int d\mu \, dv \frac{f_{jk}}{2 T_{0j}} \right\rangle_z \\
, \quad (4.22)
\]

an electrostatic term \( E_\phi \):

\[
E_\phi = \sum_k \left\langle \frac{1}{2} \lambda_D^2 k_1^2 |\phi_{1k}|^2 \right\rangle_z + \sum_j \frac{n_{0j} q_j^2}{2 T_{0j}} \left[ 1 - \Gamma_0(b_j) \right] |\phi_{1k}|^2 \\
, \quad (4.23)
\]

and a magnetic term \( E_A \) defined as:

\[
E_A = \sum_k \left\langle \frac{k_1^2}{\beta} |A_1||k| \right\rangle_z . \quad (4.24)
\]

4.3.2 Linear part

Regarding the terms on the right hand side of the gyrokinetic equation, we will focus first on the linear term. For this term, we have to compute:

\[
\Xi_h[L|g_{kj}|] + cc = \sum_{j,k} \left\langle \int d\mu \, dv \frac{\pi}{2} B_0 n_{0j} \left( \frac{T_{0j} g_{kj} - q_j \chi_{-k_j}}{F_{0j}} \right) |L|g_{kj}| \right\rangle_z + cc. \quad (4.25)
\]

Since the linear term contains three different contributions (due to the equilibrium density and temperature gradients, due to the magnetic curvature effects and due to the parallel effects), in the following we will analyze their contributions to the free energy balance equation separately.
4.3 Derivation of the balance equation

4.3.2.1 Equilibrium density and temperature gradients

We start first calculating the free energy contribution due to the equilibrium density and temperature gradient terms:

\[ G := \Xi_b[L_G(g_{k_j})] + \text{cc} = -\sum_{j,k} \left( \int d\mu d\nu \right) \frac{\pi}{2} B_0 n_{0j} \left( T_{0j} \frac{g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) F_{0j} i k_y \chi_{kj} \left( x, y \right) \]

We can find that the electromagnetic part (coupling between \( \chi \) and \( \chi \)) vanishes:

\[ -\sum_j \left( \int d\mu d\nu \right) \pi B_0 n_{0j} \omega_{nj} \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} F_{0j} \sum_k i k_y \chi_{kj}^2 \left( x, y \right) \]

due to the fact that the summation over all \( k \) space of any quantity proportional to \( \propto \sum_k k_x v_\parallel \chi_{kj} \chi_{kj} \) is zero due to the symmetry of the modes.

Second, the term coupling \( g_{kj} \) and \( \chi_{kj} \) under the integral does not vanish:

\[ -\sum_{j,k} \left( \int d\mu d\nu \right) \pi B_0 n_{0j} T_{0j} \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) g_{-kj} i k_y \chi_{kj} \left( x, y \right) \]

This term can be split into four pieces (using the definitions of \( g \) and \( \chi \)):

I) \(-\sum_{j,k} \left( \int d\mu d\nu \right) \pi B_0 n_{0j} T_{0j} \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) f_{-kj} i k_y J_{0kj} \phi_{1k} \left( x, y \right) \)

II) \(+\sum_{j,k} \left( \int d\mu d\nu \right) \pi B_0 n_{0j} T_{0j} \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) f_{-kj} i k_y v_{Tj} v_i J_{0kj} A_{1||k} \left( x, y \right) \)

III) \(-\sum_{j,k} \left( \int d\mu d\nu \right) \pi B_0 n_{0j} T_{0j} \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) v_{Tj} v_i \frac{q_j F_{0j}}{T_{0j}} A_{1||k} i k_y |J_{0kj}|^2 \phi_{1k} \left( x, y \right) \)

IV) \(-\sum_{j,k} \left( \int d\mu d\nu \right) \pi B_0 n_{0j} T_{0j} \left( \omega_{nj} + \left( v_\parallel^2 + \mu B_0 - \frac{3}{2} \right) \omega_{Tj} \right) v_{Tj}^2 v_i^2 \frac{q_j F_{0j}}{T_{0j}} A_{1||k} i k_y |J_{0kj} A_{1||k}|^2 \left( x, y \right) \)

We observe that the fourth term in Eq. (4.28) cancels since \( \sum_k k_y |J_{0kj} A_{1||k}|^2 = 0 \). The third term, which couples \( \phi_{1k} \) and \( A_{1||k} \), also cancels since it involves odd moments of the equilibrium distribution function \( F_{0j} \) that are zero by definition.
Finally, only couplings between the distribution function and the potentials remain. One can re-express the two terms as linear combinations of species radial fluxes:

\[ G = \sum_j \left[ T_{0j} \left( \omega_{nj} - \frac{3}{2} \omega_T j \right) \Gamma_j + \omega_T j Q_j \right], \]

where we have used the definitions of the particle \( \Gamma_j \) and heat \( Q_j \) fluxes given by Eq. (2.153) and (2.154), respectively.

### 4.3.2.2 Magnetic curvature

Regarding the linear term that contains the curvature effects we have to compute:

\[ \mathcal{L}_K := \Xi_h [L_K [g_{kj}]] + cc = - \sum_{j,k} \left\langle \int \mu \nu \pi B_0 n_{0j} \left( T_{0j} \frac{g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) \right\rangle + cc. \]

Now, if we take into account that

\[ T_{0j} \frac{g_{-kj}}{F_{0j}} + q_j \chi_{-kj} = T_{0j} \frac{h_{-kj}}{h_{0j}}, \]

we can rewrite that term as follows:

\[ \mathcal{L}_K = - \sum_j \left\langle \int \mu \nu \pi B_0 n_{0j} \frac{T_{0j}^2 (2v_x^2 + \mu B_0)}{q_j B_0} \sum_k [K_x i k_x + K_y i k_y] |h_{kj}|^2 \right\rangle. \]

Since the \( K \)'s do not depend on perpendicular variables, the curvature contribution completely vanishes under summation with respect to the perpendicular wave vectors through the Fourier space symmetry.

### 4.3.2.3 Parallel term

Concerning the linear parallel term, we start from its general form expressed in terms of Poisson brackets:

\[ \mathcal{L}_|| := \Xi_h [L|| [g_{kj}]] + cc = \sum_{j,k} \left\langle \int \mu \nu \pi B_0 n_{0j} \left( T_{0j} \frac{g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) \right\rangle + cc. \]

\[ \left\langle \frac{v_T j}{2B_0 J(z)} \left[ \frac{h_{kj}}{F_{0j}} \right] \right\rangle z + cc. \]

---

This is the main reason we represent the free energy operator as \( \Xi_h \), to show explicitly the dependence of this operator on the \( h \) term.
4.3 Derivation of the balance equation

It can be re-written as follows:

$$\mathcal{L}_\parallel = \sum_{j,k} \left< \int \frac{d\mu}{2} n_0 j \frac{v_{Tj}}{2J(z)} T_{0j} \frac{h_{kj}}{F_{0j}} \left[ \frac{h_{kj}}{F_{0j}} \right]_{z_{\parallel}} \right> + \text{cc.} \quad (4.34)$$

In order to analyze this term, we will use the fact that an integration of a Poisson bracket for two given functions $f(a,b)$ and $g(a,b)$ of the form:

$$\int_a^b f[g]_{ab} \, da \, db = \int_a^b \left[ f_a^b \frac{\partial g}{\partial a} - f_a^b \frac{\partial g}{\partial b} \right] \, da \, db,$$

(4.35)
cancels upon the fulfillment of the following condition,

$$\int_a^b f_a^b \frac{\partial g}{\partial b} \, da - \int_a^b f_a^b \frac{\partial g}{\partial a} \, db = 0.$$

(4.36)

For details, see Appendix A.

Now, for our particular case, substituting $f = \frac{h_{kj}}{F_{0j}}$ and $g = F_{0j}$ and taking into account the first derivatives of the equilibrium distribution are $\frac{\partial F_{0j}}{\partial v_\parallel} = -2v_\parallel F_{0j}$, and $\frac{\partial F_{0j}}{\partial z} = -\mu \frac{\partial B_0}{\partial z} F_{0j}$, we end up with the following expression:

$$\sum_{j,k} \int \frac{d\mu}{2} n_0 j v_{Tj} T_{0j} \left\{ \int v_\parallel \left[ \frac{|h_{kj}|^2}{F_{0j}} \right]_{z_{\parallel}} \, dv_\parallel \right\}$$

(4.37)

This term requires two conditions to actually vanish. The (second) $v_\parallel$ part cancellation relies on a proper decaying of $|h_{kj}|^2/F_{0j}$ at the $v_\parallel$ boundaries. Taking into account that the $v_\parallel$ boundaries are between $v_{-\infty}$ and $v_\infty$ and since the Maxwellian distribution $F_{0j}$ decays to 0 for high $|v_\parallel|$, by the gyrokinetic ordering, also the $h_{kj}$ (or $h_{kj}^2$) term must decay to 0. The (first) $z$ part cancellation, on the contrary, requires a complementary summation over $k_x$, due to the flux-tube parallel boundary condition. The $z$ boundaries are between $-\pi$ and $\pi$, and one might expect the term $h_{kj}^2/F_{0j}$ would be symmetric with respect to these boundaries and this contribution should vanish. However, due to the flux-tube parallel boundary condition, a $-\pi$ boundary connects with $\pi$ but with a different $k_x$. Therefore, in order to cancel the boundaries, in addition we need to sum over the all $k_x$ modes to compensate this effect.

4.3.3 Numerical dissipation

In practice, our simulations will be done without collision operator. For such simulations, in order to achieve a turbulent steady state, the system must include some finite dissipation [39]. This is done in GENE with artificial diffusion.
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

These terms are proportional to $\frac{\partial^{n}}{\partial a_{\mu}^{n}}$ with $n \geq 2$ and $a = x, y, z, v_{i}, \mu$. When $n \geq 4$, they are known as hyperdiffusion terms. These terms must act as a sink of free energy in order to satisfy Boltmann’s H-theorem. In this sense, they mimic the effect of collisions. In Appendix C, we show which functional dependences of $D[g_{kj}]$ satisfy this property. In the following we just represent its contribution to the free energy balance equation as:

$$D := \Xi_{h}[D[g_{kj}]] + cc = \sum_{j,k} \left\langle \int d\mu d\nu \frac{\pi}{2} B_{0} n_{0j} \left( \frac{T_{0j}}{F_{0j}} g_{-kj} + q_{j} \chi_{-kj} \right) D[g_{kj}] \right\rangle_{z} + cc.$$  (4.38)

4.3.4 Contribution of the nonlinear term

In the gyrokinetic formalism the free energy acts as a nonlinear conserved quantity. It means that the following contribution to the free energy balance equation vanishes

$$N := \Xi_{h}[N[g_{kj}, g_{kj}]] + cc = \sum_{j,k} \left\langle \int d\mu d\nu \frac{\pi}{2} B_{0} n_{0j} \left( T_{0j} \frac{g_{-kj}}{F_{0j}} + q_{j} \chi_{-kj} \right) \right\rangle_{z} + cc.$$  (4.39)

This term can be written in real space in terms of Poisson brackets (see Eq. 2.140) in the perpendicular space directions $x, y$:

$$N = \sum_{j} \left\langle \int d\mu d\nu dx dy \pi B_{0} n_{0j} \left( T_{0j} \frac{g_{j}}{F_{0j}} + q_{j} \chi_{j} \right) [\chi_{j}, g_{j}]_{x,y} \right\rangle_{z}.$$  (4.40)

The easiest proof that this contribution vanishes comes from the property of the Poisson bracket:

$$\int da db (for g)[f, g]_{a,b} = 0.$$  (4.42)

For example, if we choose $f = g_{j}$ and $g = \chi_{j}$ we have:

$$\sum_{j} \left\langle \int d\mu d\nu \pi B_{0} n_{0j} \frac{T_{0j}}{F_{0j}} \int dx dy g_{j} [\chi_{j}, g_{j}]_{x,y} \right\rangle_{z} = 0,$$  (4.43)

since in the flux-tube approximation there are no dependencies on $x$ or $y$ in the prefactors $(T_{0j}, F_{0j} \ldots)$. The same arguments can be applied to the other term. Choosing now $f = \chi_{kj}$ and $g = g_{kj}$, we have a term:

$$\sum_{j} \left\langle \int d\mu d\nu \pi B_{0} n_{0j} T_{0j} q_{j} \int dx dy \chi_{j} [\chi_{j}, g_{j}]_{x,y} \right\rangle_{z}$$  (4.44)

that vanishes.
4.4 The free energy balance equation

We group all terms playing a role on the free energy balance and we obtain:

\[ \frac{\partial}{\partial t} \mathcal{E} = \frac{\partial}{\partial t} (\mathcal{E}_f + \mathcal{E}_\phi + \mathcal{E}_A) = \mathcal{G} + \mathcal{D}. \]  
(4.45)

and

\[ \mathcal{L}_K = \mathcal{L}_\parallel = N = 0. \]  
(4.46)

The entropic \( \mathcal{E}_f \), electrostatic \( \mathcal{E}_\phi \) and magnetic \( \mathcal{E}_A \) contributions are given by:

\[ \mathcal{E}_f = \sum_{j,k} \left\langle \pi B_0 n_{0j} T_{0j} \int d\mu d\nu \frac{|f_{jk}|^2}{2 F_{0j}} \right\rangle, \]  
(4.47)

\[ \mathcal{E}_\phi = \sum_k \frac{1}{2} k_\perp^2 \lambda_D^2 \left\langle |\phi_{1k}|^2 \right\rangle_z + \sum_{j,k} \frac{n_{0j} q_j^2}{2 T_{0j}} \left\langle [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z, \]  
(4.48)

\[ \mathcal{E}_A = \sum_k \left\langle \frac{k_\perp^2}{\beta} |A_{1||k}|^2 \right\rangle_z. \]  
(4.49)

The sources are due the equilibrium gradients \( \mathcal{G} \) and the sinks are the due to hyperdiffusions \( \mathcal{D} \):

\[ \mathcal{G} = \sum_j \left[ T_{0j} \left( \omega_{nj} - \frac{3}{2} \omega_{Tj} \right) \Gamma_j + \omega_{Tj} Q_j \right], \]  
(4.50)

\[ \mathcal{D} = \sum_{j,k} \left\langle \int d\mu d\nu \pi B_0 n_{0j} \left( \frac{T_{0j}}{F_{0j}} g_{-kj} + q_j \chi_{-kj} \right) D[g_{kj}] \right\rangle_z. \]  
(4.51)

Here, the free energy is given in units of \( n_{\text{ref}} T_{\text{ref}} \pi^2 / L_{\text{ref}}^2 \). We would like to remark that \( \mathcal{E} \) is the same quantity that was obtained for kinetic systems in the previous section (see Eq. 4.7) but expressed in terms of the gyro-center distribution function \( f_{kj} \), the potentials \( \phi_{1k}, A_{1||k} \), and properly normalized in the GENE units. For a detailed calculation see Appendix B.

4.4.1 Free energy balance: Adiabatic electrons

We will consider now a simplified case of adiabatic electrons response. In this model, the magnetic fluctuations are neglected as well as the factor \( \lambda_D^2 \). Therefore, the general form remains the same, except now there is not a magnetic fluctuation term:

\[ \frac{\partial}{\partial t} (\mathcal{E}_f + \mathcal{E}_\phi) = \mathcal{G} + \mathcal{D}. \]  
(4.52)
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

Recall that in the electrostatic case $g_{kj} = f_{kj}$ and $\chi_{kj} = J_{0kj}\phi_{1k}$. Therefore, the different terms can be simplified as follows:

\[
E_f = \sum_k \left\langle \pi B_0 n_0 T_{0i} \int d\mu d\nu || f_{ki} ||^2 \right\rangle_z \left/ \frac{2F_{0i}}{F_{0e}^2} \right.,
\]

\[
E_\phi = \frac{n_0 q_i^2}{2T_{0e}} \sum_k \left[ \langle |\phi_{1k}|^2 \rangle_z - \langle |\phi_1^f \rangle^2 \right]_{FS} + \frac{n_0 q_i^2}{2T_{0i}} \sum_k \langle [1 - \Gamma_0(b_i)] |\phi_{1k}|^2 \rangle_z,
\]

and

\[
\mathcal{G} = \omega_{T_i} Q_i,
\]

\[
\mathcal{D} = \sum_k \left\langle \int d\mu d\nu || B_0 n_0 \left( \frac{T_{0i}}{T_{0e}} g_{-ki} + q_i \chi_{-ki} \right) D[g_{ki}] \right\rangle_z.
\]

In the adiabatic approximation, it can be shown that due to the ambipolar diffusion, the ion particle flux vanish identically, $\Gamma_i = 0$, giving a simplified expression of the source term.

4.4.2 Free energy balance: Adiabatic ions

Taking into account the adiabatic ion response, the electrostatic free energy balance equation reads:

\[
\partial_t (E_f + E_\phi) = \mathcal{G} + \mathcal{D}
\]

where the different contributions are defined as follows:

\[
E_f = \sum_k \left\langle \pi B_0 n_0 T_{0e} \int d\mu d\nu || f_{ke} ||^2 \right\rangle_z \left/ \frac{2F_{0e}}{F_{0e}^2} \right.,
\]

\[
E_\phi = \frac{n_0 q_i^2}{2T_{0i}} \sum_k \langle |\phi_{1k}|^2 \rangle_z + \frac{n_0 q_e^2}{2T_{0e}} \sum_k \langle [1 - \Gamma_0(b_e)] |\phi_{1k}|^2 \rangle_z,
\]

and

\[
\mathcal{G} = \omega_{T_e} Q_e,
\]

\[
\mathcal{D} = \sum_k \left\langle \int d\mu d\nu || B_0 n_0 \left( \frac{T_{0e}}{T_{0e}} g_{-ke} + q_e \chi_{-ke} \right) D[g_{ke}] \right\rangle_z.
\]

4.5 Simulation results: Cyclone Base Case

The free energy balance equations defined in the preceding section have been evaluated from a numerical simulation using GENE. The physical parameters used in the following corresponds to the standard case of collisionless ion temperature.
4.5 Simulation results: Cyclone Base Case

Gradient (ITG) drive turbulence known as the Cyclone Base Case (CBC) \[40\]. The Cyclone Base Case values have served as a reference for many gyrokinetic codes in order to study ITG turbulence. The corresponding set of parameters extracted from the tokamak DIII-D shot number 81499 are the following: \(n_e = 4.5 \times 10^{19} \text{ m}^{-3} \), \(T_e = T_i = 2 \times 10^3 \text{ eV} \), \(B_{\text{ref}} = 1.91 \text{ T} \), \(a = 0.625 \text{ m} \), \(R = 1.71 \text{ m} \), \(q = 1.4 \), \(\delta = 0.78 \), \(w_n = 2.22 \) and \(w_{Ti} = 6.96 \).

All the results shown below are obtained from simulations with box size \(L_x \times L_y = 125\rho_s \times 125\rho_s \) in the perpendicular directions. The three-dimensional spatial simulation domain is represented by \(256 \times 64 \times 64 \) grid points. The velocity space variables \(v_i \) and \(\mu \) run from \(-3v_{Ti}\) to \(3v_{Ti}\) and from 0 to \(9 T_0/B_{\text{ref}} \), respectively.

For the velocity space discretization, \(32 \times 8 \) grid points are typically used. Finally, electrostatic fluctuations and a large aspect-ratio, circular cross section model equilibrium \[16\] as described in Chapter 2 is used.

4.5.1 Free energy conservation by the nonlinear term

Before analyzing the free energy balance equations in detail, the numerical accuracy of the code has been checked by considering two simple tests.

First, the impact of the nonlinear term on the free energy balance \(\mathcal{N} \) has been measured. This term should vanish exactly for all times. In practice, the ratio \(\mathcal{N}/\mathcal{D}\) can be used to assess the accuracy of the various algorithms used in GENE to discretize the gyrokinetic equation, both in positions as in the velocity space. Here, \(\mathcal{D}\) is the time-averaged absolute value of the dissipation which is very stable.

Second, the residual:

\[
\Delta = \frac{\left(\frac{\partial E}{\partial t} - G - D\right)}{\mathcal{D}},
\]

(4.62)

can be used to assess the accuracy of the time advancement algorithm used in GENE.

As observed in Fig. 4.1, both tests show that the algorithms used in GENE allow to satisfy the general constraints imposed by the free energy balance very adequately.

4.5.2 Time evolution of the free energy components

The time evolution of the entropy and electrostatic energy are shown in Fig. 4.2 (a). It is observed that \(E_f\) is systematically much greater than \(E_\phi\). It is also noted that both quantities rapidly reach, after a very short transient period, a statistically stationary state corresponding to saturated turbulence. The fact that the entropy term is much greater than the electrostatic term was a priori unexpected. The underlying physics of this mechanism is left for Chapter 5.

The various contributions to the evolution of the free energy are shown in Fig. 4.2 (b). It can be seen that the dissipation term is systematically negative,
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

Figure 4.1: (a) Plot of the residual $\Delta$ versus time. It appears that the time integration scheme satisfies the global free energy balance with a relative error systematically smaller than $5 \times 10^{-4}$. (b) Conservation of the free energy balance by the nonlinear term. The curve shows that the contribution of the nonlinearity to the free energy time derivative is negligible (amounting to machine precision).

Figure 4.2: (a) Time evolution of $\mathcal{E}_f$ and $\mathcal{E}_\phi$. The entropy term is much greater than the electrostatic term for all times. They are given in units of $n_0 e T_0 e \rho_s / R^2$. (b) Free energy balance in units of $n_0 e T_0 e v_T / R (\rho_s / R)^2$. The gradient term ($\mathcal{G}$) is systematically a source of free energy for all times while the dissipation term $\mathcal{D}$ acts as a sink of free energy. Both the parallel and the curvature linear terms ($\mathcal{L}_K, \mathcal{L}_\parallel$) conserve the free energy for all times, see Sec. 4.3.

that is, pumping free energy out the system, while the gradient term is positive, thus injecting energy into the system. The curvature and the parallel contributions, as expected, both conserve the free energy. Finally, the saturated state of the turbulence satisfies ($\partial_t \mathcal{E} \approx 0$). It we take now into account that the linear terms vanish ($\mathcal{L}_K$ and $\mathcal{L}_\parallel$), we end up with the following relation,

$$\frac{\partial \mathcal{E}}{\partial t} = \mathcal{G} + \mathcal{D} \Rightarrow \mathcal{G} \approx - \mathcal{D}, \quad (4.63)$$
which is clearly satisfied for all times in the saturated state (for times larger than
$100 R/v_{Ti}$ units). This relation represents the fact that in a saturated turbulence
state, all free energy injected in the system through the gradient term is dissipated
out of the system by the numerical dissipation term.

4.5.3 Free energy transfers

The nonlinearity has the effect to couple all the modes. Hence, even if the free
energy is conserved globally by the nonlinear term, it may be transferred between
different scales associated to different wave vectors. Following the procedure
used for studying energy transfer in Navier-Stokes and in MHD turbulence \[41, \]
\[42, 43, 44\], we aim to decompose the perpendicular wave vector plane $P_{\perp}$ into
domains and to measure the free energy transfer between these domains. The set
of domains $\{d_\ell\}$ is assumed to be a partition:

$$P_{\perp} = \bigcup_\ell d_\ell,$$

$$d_{\ell_1} \cap d_{\ell_2} = \begin{cases} \emptyset & \text{if } \ell_1 \neq \ell_2, \\ d_{\ell_1} & \text{if } \ell_1 = \ell_2. \end{cases}$$

No intersection between the domains, and all domains together cover the entire
plane. In the following, when needed, we will use $k_{\perp}$ and $k_{\perp} = |k_{\perp}|$ to show
explicitly the perpendicular wave number dependence of the quantities.

The distribution function in a given domain is found to be

$$f_\ell^t = \sum_{k_{\perp} \in d_\ell} f_i(k_{\perp}, z, v_{\parallel}, \mu),$$

and the same for the electrostatic potential:

$$\phi_\ell^t = \sum_{k_{\perp} \in d_\ell} \phi_i(k_{\perp}, z).$$

The distribution function (or electrostatic potential) is thus defined as the parts
of the total distribution function (or electrostatic potential), whose perpendicular
wave numbers belongs to the domain $d_\ell$.

The free energy can also be split into parts which are associated to the domain
$d_\ell$:

$$E = \sum_\ell E_\ell = \sum_\ell E_f^\ell + \sum_\ell E_o^\ell$$

In the problem considered hereafter, both the entropy and the electrostatic con-
tributions to the free energy are conserved separately by the nonlinear term $N$.
It is then legitimate to consider the entropy conservation independently of the
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

conservation of the electrostatic energy. The evolution of $E^f$ due to the nonlinear term can be expressed as,

$$\frac{\partial E^f}{\partial t} = \int d\Theta \frac{T_{0i}}{F_{0i}} f^f_i \frac{\partial f^f_i}{\partial t} = \int d\Theta \frac{T_{0i}}{F_{0i}} \sum_{k \in d_\ell} \frac{\partial f_{ki}}{\partial t}$$  \(4.69\)

and we have used the property

$$\int d\Theta f^f_i f^f_i = \int d\Theta f^f_i \sum_{k \in d_\ell} f_{ki} \text{ with } \int d\Theta = \left( \int d\nu d\mu \pi B_0 n_{0i} \right) \quad (4.70)$$

Introducing the explicit form of the nonlinearity $N[g_{kj}, g_{kj}]$ (hereafter represented by $N_{ki}$) in terms of the domain decomposition we obtain\footnote{We use the form given by Eq. (2.138) but adapted adequately to the domain decomposition performed in this section.}

$$N_{ki} = \sum_{\ell'} \sum_{\ell''} \left( \sum_{k'' \in d_{\ell''}} \sum_{k' \in d_{\ell'}} (k''_y k'_x - k''_x k'_y) J_{0k''} \phi_{1k''} f_{k'i} \delta_{k-k'-k''} \right) \quad (4.71)$$

Taking that into account, we can derive the following expression:

$$\frac{\partial E^f}{\partial t} = \int d\Theta \frac{T_{0i}}{F_{0j}} f^f_i \sum_{k \in d_\ell} N_{ki} = \sum_{\ell'} \sum_{\ell''} T^f_{\ell', \ell''}, \quad (4.72)$$

where the three-domain interaction term is defined as

$$T^f_{\ell', \ell''} = \sum_{k \in d_\ell} \sum_{k'' \in d_{\ell''}} \int d\Theta \frac{T_{0i}}{F_{0k}} f_{ki} (k''_y k'_x - k''_x k'_y) J_{0k''} \phi_{1k''} f_{k'i} \delta_{k-k'-k''} \quad (4.73)$$

Eq. (4.72) shows that the evolution of the entropy associated to the domain $d_\ell$ is the sum of triple interactions between wave vectors associated to the domains $d_\ell$, $d_{\ell'}$, and $d_{\ell''}$. Moreover, considering the structure of these three-domain interaction terms, the following two-domain interaction term is a natural quantity to investigate:

$$T^f_{\ell', \ell} = \sum_{\ell''} T^f_{\ell', \ell''}, \quad (4.74)$$

These two-domain interaction terms, known also as shell-to-shell transfers, will be interpreted as the energy transfers between the domains $d_\ell$ and $d_{\ell'}$, even if the redistribution of the free energy between the different domains by the nonlinear term cannot be fully understood without considering triadic interactions. Moreover, it is easy to show that

$$T^f_{\ell', \ell} = -T^f_{\ell, \ell'}, \quad (4.75)$$
4.5 Simulation results: Cyclone Base Case

which reinforces the interpretation in terms of free energy exchange. Indeed, if the domain \( d \) is considered to receive a certain amount of free energy per unit of time from the domain \( d' \), then the domain \( d' \) is seen as losing exactly the same amount of free energy per unit of time in profit of the domain \( d \).

The same approach can be used to define three-domain and two-domain interaction terms for the electrostatic part of the free energy with the following definitions:

\[
\mathcal{T}_{\phi}^{\ell \ell' \ell''} = \sum_{k \in d_\ell} \sum_{k'' \in d_{\ell''}} \sum_{k' \in d_{\ell'}} \int d\Theta q_i J_{0k' \ell k} \left( k'_x k''_y - k''_x k'_y \right) J_{0k' \ell k'} f_{k''} \delta_{k-k'-k''},
\]

(4.76)

and

\[
\mathcal{T}_{\phi}^{\ell \ell'} = \sum_{\ell''} \mathcal{T}_{\phi}^{\ell \ell'' \ell} \quad \text{with} \quad \mathcal{T}_{\phi}^{\ell \ell'} = -\mathcal{T}_{\phi}^{\ell' \ell}.
\]

(4.77)

Grouping all the terms together, the complete dynamical equation for \( E^{\ell} \) reads:

\[
\frac{\partial E^{\ell}}{\partial t} = \sum_{\ell'} \mathcal{T}_{f}^{\ell \ell'} + \sum_{\ell''} \mathcal{T}_{\phi}^{\ell \ell'' \ell} + \mathcal{G}^{\ell} + \mathcal{L}^{\ell}_{\parallel} + \mathcal{L}^{\ell}_{K} + \mathcal{D}^{\ell},
\]

(4.78)

where the source \( \mathcal{G}^{\ell} \), the linear terms \( \mathcal{L}^{\ell}_{\parallel} \), \( \mathcal{L}^{\ell}_{K} \) and the dissipation \( \mathcal{D}^{\ell} \) terms are given by Eqs. (4.55, 4.56, 4.30, 4.33) but using \( f_{\ell}^{i} \) and \( J^{i}_{0} \phi_{1k}^{i} \) instead of \( f_{ki} \) and \( J_{0ki} \phi_{1k} \). It is worth to mention that in this representation the curvature term conserves the free energy (\( \mathcal{L}^{\ell}_{K} = 0 \)) due to the symmetry of the perpendicular modes. However, the parallel term is not conserved for a given domain (\( \mathcal{L}^{\ell}_{\parallel} \neq 0 \)). The reason was mentioned in the previous section: it is necessary to sum over all \( k_x \) in order to cancel the boundaries, but for a given domain decomposition, only a fraction of the \( k_x \) domain is considered. This term is only conserved globally, i.e., when summing over all the domains (\( \sum_{\ell} \mathcal{L}^{\ell}_{\parallel} = 0 \)).

In this study, for numerical analysis of the Eq. (4.78), the perpendicular wave vector plane \( \mathcal{P}_\perp \) is divided into shells:

\[
d_{\ell} = \{ k_{\perp} \text{ such that } K_{\ell} < |k_{\perp}| \leq K_{\ell+1} \},
\]

(4.79)

where the shell boundaries \( K_{\ell} \) are chosen to grow algebraically \( K_{\ell+1} = \lambda K_{\ell} \), with \( \lambda = 2^{1/5} \) between shell \( \ell = 3 \) and \( \ell = 24 \). The first two shell boundaries have been chosen differently (\( K_1 = 0 \), \( K_2 = 0.2 \rho_s \), \( K_3 = 0.3 \rho_s \)) in order to ensure that enough modes belong to that shells. In addition, in order to limit the number of shells, the last shell (\( \ell = 25 \)) is wider and limited by \( K_{25} = 6.3 \rho_s \) and \( K_{26} = |k_{\perp}|_{\text{max}} = 14.6 \rho_s \).

Fig. 4.3 shows the numerical results for the source and dissipation terms as well as the linear parallel contribution averaged over time during the saturated phase of the simulation.

As expected, the injection of free energy \( \mathcal{G}^{\ell} \) is well localized at low \( k_{\perp} \). However, as it turns out, the dissipative terms \( \mathcal{D}^{\ell} \) are not just active in the high \( k_{\perp} \).
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

Figure 4.3: Shell decompositions in perpendicular wavenumber space of the drive term ($\mathcal{G}^f$), dissipation term ($\mathcal{D}^f$) and the linear terms ($\mathcal{L}^f_K$) and ($\mathcal{L}^f_{L}$) (as well as their sum) from a GENE simulation of ITG turbulence. They are giving in units of $n_0 e v_{Te}/R(\rho_s/R)^2$.

range, but throughout the entire $k_{\perp}$ spectrum, including the drive range. An explanation of this phenomenon may be provided in terms of the nonlinear coupling to damped eigenmodes, as is discussed in Ref. [45] and briefly summarized in the following. In gyrokinetic turbulence each instability generates an unstable mode, which is accompanied by some stable modes. These stable modes are known as damped eigenmodes and due to the nonlinear term, are coupled to the unstable modes. The unstable modes act as source of free energy while the stable mode act as a sink of free energy. Thus, they are responsible for an additional sink of free energy which it is generally localized in similar scales as the unstable modes, i.e. in large scales of the system.

It can also be seen in Fig. 4.3 that the linear parallel term does not affect significantly the overall free energy spectrum. It acts as a dissipative term for low $k_{\perp}$ but a source for higher $k_{\perp}$. Summing all the contributions ($\mathcal{G}^f + \mathcal{D}^f + \mathcal{L}^f_K + \mathcal{L}^f_{L}$), we find that there is a net source of free energy up to shell $\ell = 9$ and a net dissipation beyond that.

The corresponding free energy transfers are shown in Fig. 4.4 and various interesting features can be observed there:

(i) The entropy transfer is larger than the electrostatic energy transfer by 2 orders of magnitude. We will anticipate now (see next chapter and/or Ref. [46]), that this is line with the fact that only $E_f$ is driven directly while $E_{\phi}$ is fed via linear transfer terms. For this reason, we observed in Fig 4.1 that $E_f \gg E_{\phi}$.

(ii) The electrostatic energy exhibits an inverse and non-local cascade behavior. An inverse cascade (in opposite to a direct or forward cascade) corresponds
4.5 Simulation results: Cyclone Base Case

Figure 4.4: Shell-to-shell transfer in perpendicular wavenumber space of entropy (a) and electrostatic energy (b) from a GENE simulation of ITG turbulence.

to a transfer of energy from the smallest to the largest scales of the system. Non-local in this context mean that the transfer of free energy is between domains that are far apart. These properties hardly affect the overall free energy dynamics, given the dominance of $E_f$ over $E_\phi$.

(iii) The entropy transfer (and therefore also the free energy transfer) is from large scales to small ones. It is negative for $\ell' > \ell$ and due to the anti-symmetry property it is positive otherwise. This is commonly known as a forward (or direct) cascade of free energy.

(iv) The free energy transfer is very local in wave number space. Indeed, only values of the total free energy transfer ($\mathcal{T}_{\text{total}}^{\ell,\ell'} \approx \mathcal{T}_f^{\ell,\ell'}$) with $\ell$ close to $\ell'$ are significantly different from zero. In practice, for $|\ell - \ell'| > 5$ the free energy transfer almost vanishes. This corresponds to a ratio of wave numbers between the two shells of the order of 2.

(v) For $\ell > 5$, the total transfer is found to depend mainly on $\ell - \ell'$ and not on the two indices separately. For example, in Fig 4.5 different functions
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

The free energy cascade in gyrokinetic turbulence is illustrated by the functions $\mathcal{T}_{\text{total}}^{\ell} = \mathcal{T}_{\text{total}}^{\ell,\ell'}$ for $\ell' = [13 - 21]$ as shown as a function of $\ell - \ell'$. We observe that these functions tend to collapse in this range. This suggests the existence of an inertial range, despite the finite dissipation that there is in the system for all scales. The explanation of this phenomenon was given in Ref. [45] where it was found that in contrast to the damping rates, the nonlinear frequencies characterizing the free energy transfer increase with $\ell$ and the cascade dynamics is allowed to develop.

![Figure 4.5](image.png)

**Figure 4.5:** It shows $\mathcal{T}_{\text{total}}^{\ell} = \mathcal{T}_{\text{total}}^{\ell,\ell'}$ for $\ell' = [13 - 21]$ as a function of $\ell - \ell'$. The collapse of these functions suggest the existence of an inertial range.

Interestingly, as is shown in Fig. 4.6, the wavenumber spectra of $\mathcal{E}_f$ and $\mathcal{E}_\phi$ exhibit power laws at $k_\perp > 1$ indicative also of an inertial range. Dimensional analysis based on two-dimensional gyrokinetics lead Schekochihin and co-workers [38] to the predictions $\mathcal{E}_f(k_\perp) \propto k_\perp^{-4/3}$ and $\mathcal{E}_\phi(k_\perp) \propto k_\perp^{-10/3}$ which are displayed for comparison. One finds that the measured spectra are relatively close to these expectations, regardless of the fact that terms related to parallel free streaming, magnetic curvature, and inherent drive/damping are all neglected in this theory, and that $\mathcal{E}_f$ and $\mathcal{E}_\phi$ are conserved independently of each other in two dimensions.

4.6 **Summary and conclusions**

In the present chapter we derived the free energy balance for gyrokinetics. We have shown that the free energy is conserved by the nonlinear term and by the parallel and curvature linear terms. As expected, the density and temperature gradients are the only source of free energy while the different dissipation terms (due to numerical hyperdiffusions terms) act as a sink of free energy. We have
then derived the free energy balance equation for the simplified case of adiabatic electrons and the case of adiabatic ions. We computed numerically the free energy transfer for a standard case of ITG turbulence. We found that the electrostatic energy term does not contribute in a significant way and that the transfer is entirely dominated by the entropy part. Interestingly, the entropy (and also the free energy) transfer share most of the properties with kinetic energy transfers measured in fully developed Navier-Stokes turbulence, see Table 4.1 for a comparison. First, it exhibited a forward cascade, i.e., the free energy was systematically transferred from the large scales to the small ones. Second, the cascade is very local, i.e., no significant transfer was observed between scales which are separated more than a factor of two or so. Third, a limited inertial range was observed in the cascade. This last property was rather unexpected. Indeed, the analysis of the source and dissipation terms did not show the existence of a range of scales in which both these terms were negligible. Fourth, the entropy contribution was much greater than the electrostatic one. This fact will be explained in detail in Chapter 5. Finally, the wavenumber spectra of the entropy and electrostatic terms of the free energy exhibit power laws with exponents which are close to the predictions from a simplified two-dimensional analysis.

Figure 4.6: Wavenumber spectra of $E_f$ and $E_\phi$ from a Gene simulation of ITG turbulence. Predictions from a two-dimensional theory are shown for comparison (black solid lines). They are given in units of $n_0eT_{0e}(\rho_s/R)^2$.
4. FREE ENERGY CASCADE IN GYROKINETIC TURBULENCE

\[ \partial_t v + (v \cdot \nabla)v = f_{\text{ext}} - \nabla p + \nu \nabla^2 v \]

\[ \partial_t g = L[g] + N[g,g] + D[g] \]

Kinetic energy is conserved by the advective nonlinearity. Free energy is conserved by the \( \mathbf{E} \times \mathbf{B} \) nonlinearity.

Kinetic energy is injected into the system at the largest scales through mechanical forcing. Free energy is injected into the system via density and temperature gradients.

Kinetic energy is dissipated at the smallest scales by viscous effects. Free energy is dissipated at smallest scales by collision.

The role of the nonlinearity is to transfer kinetic energy from the largest scales to the smallest scales through a cascade process. One role of the nonlinearity is to transfer free energy from the largest perpendicular scales to the smallest ones.

<table>
<thead>
<tr>
<th>Navier-Stokes turbulence</th>
<th>Gyrokinetic turbulence</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \partial_t v + (v \cdot \nabla)v = f_{\text{ext}} - \nabla p + \nu \nabla^2 v ]</td>
<td>[ \partial_t g = L[g] + N[g,g] + D[g] ]</td>
</tr>
<tr>
<td>Kinetic energy is conserved by the advective nonlinearity.</td>
<td>Free energy is conserved by the ( \mathbf{E} \times \mathbf{B} ) nonlinearity.</td>
</tr>
<tr>
<td>Kinetic energy is injected into the system at the largest scales through mechanical forcing.</td>
<td>Free energy is injected into the system via density and temperature gradients.</td>
</tr>
<tr>
<td>Kinetic energy is dissipated at the smallest scales by viscous effects.</td>
<td>Free energy is dissipated at smallest scales by collision.</td>
</tr>
<tr>
<td>The role of the nonlinearity is to transfer kinetic energy from the largest scales to the smallest scales through a cascade process.</td>
<td>One role of the nonlinearity is to transfer free energy from the largest perpendicular scales to the smallest ones.</td>
</tr>
</tbody>
</table>

Table 4.1: Comparison between Navier-Stokes and gyrokinetic turbulence.
Chapter 5

FREE ENERGY STUDIES FOR
GYROKINETICS

The purpose of this chapter is to investigate in detail the free energy balance in gyrokinetic turbulence introduced in Chapter 4. In particular, the interaction between the entropy and electrostatic energy terms that constitute the free energy will be studied numerically. This chapter is structured as follows. In Sec. 5.1 we will derive the entropy and electrostatic balance equations. They will be analyzed numerically with the GENE code in Sec. 5.2. In this section, we will include a spectral representation of the equations that will allow for a better understanding of cascade processes. Finally, a summary and conclusions will be given in Sec. 5.3.

5.1 Entropy and electrostatic energy operators

If we consider only electrostatic fluctuations, the free energy operator $\Xi_h$, can be split into two pieces:

$$\Xi_h = \Xi_f + \Xi_\phi.$$  \hspace{1cm} (5.1)

Here, $\Xi_f$ and $\Xi_\phi$ are known as the entropy and electrostatic energy operators, respectively. They are given by their action on the gyrokinetic (GK) equation:

$$\Xi_f[\text{eq : GK}] + cc := \sum_j \int d\Lambda \frac{T_{0j}}{2F_{0j}} f_{-k_j}[\text{eq : GK}] + cc,$$  \hspace{1cm} (5.2)

$$\Xi_\phi[\text{eq : GK}] + cc := \sum_j \int d\Lambda \frac{q_j}{2} J_{0k_j}\phi_{1-k}[\text{eq : GK}] + cc.$$  \hspace{1cm} (5.3)

For simplicity, we have defined the five-dimensional phase space $\Lambda$ as:

$$\int d\Lambda = \sum_k \int d\Theta \quad \text{with} \quad \int d\Theta = \left\langle \int dv_\parallel d\mu \pi B_0 n_0 \right\rangle_z.$$  \hspace{1cm} (5.4)
Moreover, in the electrostatic case the following relations are fulfilled:

\[ f_{kj} = g_{kj}, \quad \chi_{kj} = J_{0kj} \phi_{1k}, \quad h_{kj} = f_{kj} + \frac{q_j F_{0j}}{T_{0j}} J_{0kj} \phi_{1k}. \]  

(5.5)  

(5.6)  

(5.7)

5.1.1 Derivation of the entropy balance equation

The entropy balance equation is obtained by applying the entropy operator \( \Xi_f \) to the gyrokinetic equation. For the time derivative \( (\partial_t f_{kj}) \), one obtains:

\[ \partial_t S_f := \Xi_f \left[ \partial_t f_{kj} \right] + \text{cc} = \partial_t \left( \sum_j \int d\Lambda \frac{T_{0j}}{2 F_{0j}} \left| f_{kj} \right|^2 \right), \]  

(5.8)

where one can distinguish an associated entropy:

\[ S_f = \sum_j \int d\Lambda T_{0j} \frac{\left| f_{kj} \right|^2}{2 F_{0j}}. \]  

(5.9)

The gradient term \( L_G \) in the right hand side (rhs) of the equation for \( \partial_t f_{kj} \) thus leads to a term \( G_f \) in the equation for \( \partial_t S_f \) that is readily expressed as:

\[ G_f := \Xi_f [L_G f_{kj}] + \text{cc} = \sum_j \int d\Lambda \frac{T_{0j}}{2 F_{0j}} f_{-kj} L_G [f_{kj}] + \text{cc}. \]  

(5.10)

Taking into account the definition of \( L_G [f_{kj}] \), after some operations\(^1\) we end up with the following expression:

\[ G_f = \sum_j \left[ T_{0j} \left( \omega_{nj} - \frac{3}{2} \omega T_j \right) \Gamma_j + \omega T_j Q_j \right] \neq 0. \]  

(5.11)

We mean by different from 0 that the term does not vanish trivially even if it can be 0 in some peculiar cases. The contributions to the equation for \( \partial_t S_f \) from the other linear terms (the curvature term \( L_{K,f} \) and the parallel term \( L_{\parallel,f} \)) are defined similarly:

\[ L_{K,f} := \Xi_f [L_K f_{kj}] + \text{cc} = \sum_j \int d\Lambda \frac{T_{0j}}{2 F_{0j}} f_{-kj} L_K [f_{kj}] + \text{cc} \neq 0 \]  

(5.12)

and

\[ L_{\parallel,f} := \Xi_f [L_{\parallel} f_{kj}] + \text{cc} = \sum_j \int d\Lambda \frac{T_{0j}}{2 F_{0j}} f_{-kj} L_{\parallel} [f_{kj}] + \text{cc} \neq 0. \]  

(5.13)

\(^1\)Most of the operations not shown in this chapter are very similar to the ones performed in Sec. 4.3 Thus, for the clarity of the presentation they will not be repeated again.
5.1 Entropy and electrostatic energy operators

The difference with respect to the free energy balance equation (see Eq. (4.46)) is that these contributions do not conserve the entropy, while they conserve the free energy of the system. Regarding the contribution of the numerical dissipations $D_f$ in the equation for $\partial_t \mathcal{E}_f$, we find similarly:

$$D_f := \Xi_f [D[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{T_{0j}}{2F_{0j}} f_{-kj} D[f_{kj}] + cc \neq 0.$$  \hfill (5.14)

Finally, as we anticipated in Sec. 4.3, the nonlinear term

$$N_f := \Xi_f [N[f_{kj}, f_{kj}]] + cc = \sum_j \int d\Lambda \frac{T_{0j}}{2F_{0j}} f_{-kj} N[f_{kj}, f_{kj}] + cc = 0,$$  \hfill (5.15)

does not contribute to the equation for $\partial_t \mathcal{E}_f$.

5.1.2 Derivation of the electrostatic energy balance equation

The electrostatic energy balance equation can be constructed by applying the electrostatic part of the free energy operator $\Xi_\phi$ to the gyrokinetic equation. For the time derivative one obtains:

$$\partial_t \mathcal{E}_\phi := \Xi_\phi [\partial_t f_{kj}] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_{1-k} \partial_t f_{kj} + cc.$$  \hfill (5.16)

It should be noted that through the Poisson equation $f_{kj}$ is proportional to the $\phi_{1k}$ term. Therefore, Eq. (5.16) is formally quadratic in $\phi_{1k}$ and one can distinguish an associated electrostatic energy term given by:

$$\mathcal{E}_\phi = \sum_k \frac{1}{2} \lambda_k^2 k \left\langle |\phi_{1k}|^2 \right\rangle_z + \sum_{j,k} \frac{r_{0j} q_j^2}{2T_{0j}} \left\langle [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z.$$  \hfill (5.17)

Again, using the explicit decomposition of $\partial_t f_{kj}$ in terms of the linear, dissipation and nonlinear term, it is easy to define the expressions for the contribution of these terms to the electrostatic energy evolution equation ($\mathcal{G}_\phi$, $\mathcal{L}_{K,\phi}$, $\mathcal{L}_{||,\phi}$, $\mathcal{D}_\phi$).

The linear term due to the density and temperature equilibrium gradients $L_G$ leads to a term $\mathcal{G}_\phi$ in the equation for $\partial_t \mathcal{E}_\phi$

$$\mathcal{G}_\phi := \Xi_\phi [L_G[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_{1-k} L_G[f_{kj}] + cc,$$  \hfill (5.18)

that can be shown to vanish.

Moreover, the curvature and the parallel term in the electrostatic energy equation are given by:

$$\mathcal{L}_{K,\phi} := \Xi_\phi [L_K[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_{1-k} L_K[f_{kj}] + cc \neq 0.$$  \hfill (5.19)
and
\[ \mathcal{L}_{\parallel,\phi} := \Xi_\phi[L||[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_1 - k L||[f_{kj}] + cc \neq 0. \] (5.20)

It is worth to remark that these terms have different impact on the balance equations of \( \mathcal{E}_f \) and \( \mathcal{E}_\phi \). For instance, the parallel \( L|| \) linear term was shown to conserve the total free energy \( \mathcal{E} \), but not the entropy and the electrostatic energy individually. Hence, the contributions of these terms to the balance equations satisfy the constraint:
\[ L|| = L||,f + L||,\phi = 0 \rightarrow L||,\phi = -L||,f. \] (5.21)

The curvature \( L_K \) term presents the same property:
\[ L = L_{K,f} + L_{K,\phi} = 0 \rightarrow L_{K,\phi} = -L_{K,f}. \] (5.22)

The numerical dissipations \( D_\phi \) are non-zero in the electrostatic energy equation:
\[ D_\phi := \Xi_\phi[D[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_1 - k D[f_{kj}] + cc \neq 0, \] (5.23)

Finally, the nonlinear term
\[ N_\phi := \Xi_\phi[N[f_{kj}, f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_1 - k N[f_{kj}, f_{kj}] + cc = 0, \] (5.24)

again does not contribute to the equation for \( \partial_t \mathcal{E}_\phi \).

### 5.1.3 Final equations

Taking into account all these properties, the entropy and the electrostatic energy balance equations can be written as:
\[ \frac{\partial \mathcal{E}_f}{\partial t} = G_f + L_{K,f} + L_{||,f} + D_f \quad \text{with} \quad N_f = 0, \] (5.25)
\[ \frac{\partial \mathcal{E}_\phi}{\partial t} = L_{K,\phi} + L_{||,\phi} + D_\phi = -L_{K,f} - L_{||,f} + D_\phi \quad \text{with} \quad G_\phi = 0 \quad \text{and} \quad N_\phi = 0. \] (5.26)

The total free energy balance equation is then given by the sum of these two relations
\[ \frac{\partial \mathcal{E}}{\partial t} = G_f + D_f + D_\phi = G + D, \] (5.27)

which gives the free energy balance equation obtained in Chapter 4.
5.2 Simulation results: Cyclone Base Case

The properties of this system of equations will be analyzed numerically by considering again the Cyclone Base Case [10]. The simulation domain is about 125 ion gyroradii wide in the perpendicular directions, and $128 \times 64 \times 16 \times 32 \times 8$ grid points in $(x, y, z, v_{||}, \mu)$ space. This simulation does not require so much resolution as the one in Chapter 4. In that case, we needed many grid points in order to increase the statistics to analyze the shell-to-shell transfers.

5.2.1 Entropy and electrostatic time evolution

The time evolution of the entropy and electrostatic energy are shown in Fig. 5.1. These components were already shown in Chapter 4 and the fact that the entropy part $E_f$ is much greater than $E_\phi$ motivated this present study.

![Figure 5.1: Time evolution of $E_f$ and $E_\phi$. They are given in units of $n_0eT_0e(\rho_s/R)^2$.](image)

The various contributions to the evolution of $E_f$ and $E_\phi$ are shown in Fig. 5.2. It is observed that the dissipation terms are indeed pumping entropy and electrostatic energy out of the system while entropy is injected through the gradient term. The curvature term appears to transform entropy into electrostatic energy while, on the contrary, the parallel term is transforming electrostatic energy into entropy at approximately the same rate. The same information is presented schematically in Fig. 5.3. The observation that the free energy is largely dominated by its entropy part can be explained by at least two reasons. First, the entropy is the only part that is driven by the gradient term. Second, the almost perfect balance between the curvature and the parallel terms prevents a strong flux of free energy from the entropy to the electrostatic energy. As a consequence, the dissipation of electrostatic energy appears to be almost negligible when compared to the entropy dissipation $D_f/D_\phi \approx 400$. 
5. FREE ENERGY STUDIES FOR GYROKINETICS

Figure 5.2: Different contributions to the time derivatives of $\mathcal{E}_f$ (a) and $\mathcal{E}_\phi$ (b) versus time. They are given in units of $n_0 e T_0 v_T / R (\rho_s / R)^2$.

Figure 5.3: Left: Schematic plot of the different contributions of $\mathcal{E}_f$ and $\mathcal{E}_\phi$ taken from the GENE simulation described in the paper. Right: Diagram of the overall free energy balance. It shows the dominance of the entropy and the passive role of the electrostatic energy term.

5.2.2 The effect of the collision operator

The numerical dissipation terms used in GENE have been implemented to avoid the use of an expensive collision operator. However, it is also possible to run the code with a linearized Landau-Boltzmann collision operator [15]. The evolution of $\mathcal{E}_f$ and $\mathcal{E}_\phi$ are then unchanged except that the dissipation terms $D_f$ and $D_\phi$ have to be replaced, respectively, by collision terms $C_f$ and $C_\phi$ given by

$$ C_f := \Xi_f [C[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{T_{0j}}{2F_{0j}} f_{-kj} C[f_{kj}] + cc, \quad (5.28) $$

$$ C_\phi := \Xi_\phi [C[f_{kj}]] + cc = \sum_j \int d\Lambda \frac{q_j}{2} J_{0-kj} \phi_{1-k} C[f_{kj}] + cc, \quad (5.29) $$

86
where $C[f_{kj}]$ represents the Landau-Boltzmann collision operator. The different terms entering the evolution equations for $\mathcal{E}_f$ and $\mathcal{E}_\phi$ are shown in Fig. 5.4.

![Figure 5.4: Different contributions of $\mathcal{E}_f$ (a) and $\mathcal{E}_\phi$ (b) versus time with a collision operator. They are given in units of $n_0eT_0/v_{ti}/R(\rho_s/R)^2$.](image)

It is observed that the collision operator for the entropy $C_f$ plays the same role as $D_f$. However, $C_\phi$ is now almost negligible. Since a statistically stationary regime is reached, the negligible electrostatic energy collision contribution $C_\phi \approx 0$ implies that the curvature and parallel terms have to be in balance. Except for this minor difference, there is not a significant change in the free energy balance for $\mathcal{E}_f$ or $\mathcal{E}_\phi$ when a realistic collision operator is used instead of numerical dissipation. The fact that $L_{K,f} \approx -L_{\parallel,f}$ when a collisional operator or dissipation term is used supports the idea that numerical dissipation terms are doing a good job in representing the collisional effects.

### 5.2.3 Local free energy balance

The global balance equations analyzed in the preceding section give the overall picture of the fluxes of entropy and electrostatic energy in the system. However, no information is provided on the scales at which these fluxes are the most active. In order to obtain such a scale by scale information, it is necessary to look at the spectral density equations.

The spectral density of entropy will be noted by:

$$\mathcal{E}^k_f = \int d\Theta T_0 |f_{ki}|^2 2F_0.$$

Similarly, a spectral density of electrostatic energy can be defined. Remarkably, the dissipation, injection, curvature and parallel contributions to the balance equations all come from linear terms in the gyrokinetic equation. Their effect on the balance equation can then also be split into spectral density contributions that will be noted $D^k_f, D^k_\phi, G^k_f, L^k_{K,f}$ and $L^k_{\parallel,f}$. This simple mathematical property has a very important physical consequence. None of these terms can be responsible for
5. FREE ENERGY STUDIES FOR GYROKINETICS

a transfer of entropy or of electrostatic energy between different Fourier modes. We already know from Chapter [4] that the only term that can be responsible for such transfers is the nonlinear term. Indeed, even if it does not influence the global free energy balance equations, the nonlinear term has a non-vanishing contribution on each Fourier mode of the entropy and electrostatic energy spectral densities. For instance, its contribution to the evolution of $E_f$ is given by:

$$
\frac{\partial E_f^k}{\partial t} \bigg|_{N'} = \int \frac{d\Theta}{2F_0} \frac{T_{0i}}{2f_{-ki}} N_{ki} + cc = \sum_{k'} T_{f,k'}^{k,k'}.
$$

(5.31)

where $N_{ki}$ is the Fourier mode representation of the nonlinear term \((2.139)\) and where $T_{f,k'}^{k,k'}$ is given by:

$$
T_{f,k'}^{k,k'} = \operatorname{Re} \left[ \int d\Theta \frac{T_{0i}}{F_{0i}} f_{-ki} \left( (k_x - k'_x) J_{0(k-k')} \phi_{1(k-k')} k'_y f_{k'} 
\right. 
- (k_y - k'_y) J_{0(k-k')} \phi_{1(k-k')} k'_x f_{k'} ) \right].
$$

(5.32)

This term will be referred to as the transfer term between the mode $f_k$ and the mode $f_{k'}$. Due to the Poisson equation, the electric potential $\phi_{1(k-k')}$ is a linear function of the distribution $f_{k-k'}$ and the transfer term appears to be a cubic term in $f$ involving modes $f_k, f_{k-k'}$ and $f_{k'}$. Such triadic interactions will be interpreted as an exchange of entropy between two modes ($f_k$ and $f_{k'}$) because of the antisymmetry property:

$$
T_{f,k'}^{k,k'} = -T_{f,k'}^{k,k'}.
$$

(5.33)

A similar approach can be used for the nonlinear term appearing in the equation for the electrostatic energy:

$$
\frac{\partial E_{\phi}^k}{\partial t} \bigg|_{N'} = \int \frac{d\Theta}{2} \frac{q_i}{2} J_{0-k} \phi_{-k} N_k + cc = \sum_{k'} T_{\phi,k'}^{k,k'},
$$

(5.34)

where

$$
T_{\phi,k'}^{k,k'} = \operatorname{Re} \left[ \int d\Theta q_i J_{0-k} \phi_{1-k} \left( k'_x J_{0k'} \phi_{k'} (k_y - k'_y) f_{k-k'} 
\right. 
- k'_y J_{0k'} \phi_{k'} (k_x - k'_x) f_{k-k'} ) \right].
$$

(5.35)

Again, this triadic interaction will be referred to as the electrostatic energy transfer term between the modes $\phi_{1k}$ and $\phi_{1k'}$ because of the property:

$$
T_{\phi,k'}^{k,k'} = -T_{\phi,k'}^{k,k'}.
$$

(5.36)
5.2 Simulation results: Cyclone Base Case

The complete Fourier representation $E^k_f$ and $E^k_\phi$ (including all the linear terms) then reads, respectively, as

$$\frac{\partial E^k_f}{\partial t} = \sum_{k'} T^{k,k'}_f + G^k_f + L^{k}_{K,f} + D^k_f,$$

and

$$\frac{\partial E^k_\phi}{\partial t} = \sum_{k'} T^{k,k'}_\phi + L^k_{K,\phi} + L^{k}_{\parallel,\phi} + D^k_\phi.$$

The different linear contributions of $E^k_f$ and $E^k_\phi$ (averaged over time during the saturated phase) as a function of $k_y$ (summed over $k_x$) are shown in Fig. 5.5. We are not showing the term $\sum_{k'} T^{k,k'}_f$ (or $\sum_{k'} T^{k,k'}_\phi$) in Fig. 5.5 since a saturated turbulence state satisfies $\frac{\partial E^k_f}{\partial t} \approx 0$ and $\frac{\partial E^k_\phi}{\partial t} \approx 0$. Therefore, we have a direct relation between the linear terms and the transfer functions.

![Figure 5.5: Different linear contributions of $E^k_f$ (a) and $E^k_\phi$ (b) as a function of $k_y$ (summed over $k_x$) and average over time. They are given in units of $n_0 v T_i / R (\rho_s / R)^2$.](image)

The injection of entropy $G^k_f$ appears to be well localized at low $k_y$. Hence, the imposed equilibrium gradients directly affects the largest scales of the system without noticeable effect in the smallest scales. However, dissipation is active at all scales. This is in agreement with what we observed for the free energy in the previous section. In fact, it is not surprising since $E_f > E_\phi$ and also $G \approx G_f$ and $D \approx D_f$. An explanation of this phenomenon (due to damped eigenmodes) is provided in Ref. [45] and it was also briefly summarized in Chapter 4.

The linear curvature and parallel terms appear to be important only in the forcing range and are almost always opposite to each other. The net effect of these two terms is thus almost negligible in the entropy equation. However, since
there is no electrostatic energy injection, the small imbalance between these two terms is the only mechanism that acts as a source of $E^k_{\phi}$.

These curves give the net entropy and electrostatic energy injection or dissipation rates due to the various terms appearing in the local balance equations. The impact of these rates depends of course on the value of the entropy and the electrostatic energy. For this reason, it is interesting to compute a frequency associated to each term appearing in the right hand side of Eqs. (5.37-5.38) by dividing these rates by the entropy and electrostatic energy spectral density. For instance, the entropy injection scale frequency is defined by

$$\nu^k_{G_f} = \left| \frac{G^k_f}{E^k_f} \right|.$$  

Clearly, the dominant term in the equation will be characterized by the largest frequency or, equivalently, by the smallest time scale. Fig. 5.6 shows these frequencies as function of $k_y$. According to this criterion, it becomes even clearer that the entropy injection dominates at low $k_y$, while the entropy dissipation dominates at high $k_y$. The linear curvature and parallel terms appear to be characterized by the smallest frequencies at all scales in the entropy equation. In the case of the electrostatic energy equation, there is no energy injection. The linear and parallel terms appear to be dominant in the small scales, while the electrostatic energy dissipation dominates at high $k_y$. Similar figures are easily obtained for these quantities as function of $k_x$ and they show the same trends.

**5.3 Summary and conclusions**

In the present chapter we derived the entropy and electrostatic energy balance equations for gyrokinetics in the simplified case of electrostatic fluctuations. They were evaluated from a numerical simulation using the GENE code for the standard...
5.3 Summary and conclusions

case of ITG turbulence. Several interesting observations can be made from this study.

First, it is observed that the free energy dynamics is largely dominated by the entropy part, while the electrostatic energy plays a passive and subdominant role. The reason is easily found in the global balance equations. Indeed, the average temperature gradient is acting as an external source of entropy, while the electrostatic energy is only driven by internal exchanges with the entropy.

Second, it is observed that the temperature gradients inject entropy mostly at the largest scales of the system, while the dissipation is acting throughout the entire spectrum. An analysis of the typical frequencies as a function of the wave vectors shows that the dominant effect in the entropy balance is clearly the injection in the large scales while it is the dissipation in the small scales. Since the injection and the dissipation are dominant in different ranges of wave vectors, the nonlinear term has to redistribute the entropy in a cascade process as we discussed in Chapter [1].

Third, the role of the artificial dissipation has been explored. Since the results analyzed here refer to the saturated turbulent regime in which all quantities are fluctuating with time but reach statistically stationary values, the dissipation has to compensate the injection on average. When the dissipation is obtained by adding an hyperdiffusion term, its effect on the electrostatic energy is very small (more than two orders of magnitude smaller than its effect on entropy). Such a property for the artificial dissipation used mostly for improving the speed performances of the code is reassuring. Indeed, as shown on Fig. 6, a realistic collision operator barely affects the electrostatic energy and this property is thus quite well reproduced by the hyperdiffusion term.

Finally, it is also observed that the parallel and curvature terms do not play a dominant role in the entropy equation, independently of the wave vector. On the contrary, these two terms are the only contributions to the electrostatic energy balance. Although they are of opposite sign, they both appear to act mostly in the same large scale range. Hence, a strong cascade process of electrostatic energy cannot be triggered by these terms.
5. FREE ENERGY STUDIES FOR GYROKINETICS
In this chapter the large-eddy simulation approach is adapted to the study of plasma micro-turbulence in gyrokinetics. In particular, we study the ion temperature gradient driven turbulence with the \textsc{Gene} code.

This chapter is organized as follows. In Sec. 6.1 we derive the filtered gyrokinetic equation. In this equation the sub-grid term is defined. In order to study the properties of the sub-grid term we derive the filtered free energy balance equation in Sec. 6.2. The properties of the sub-grid term are studied in Sec. 6.3. In Sec. 6.4 we present a simple dissipation model for the sub-grid term. This model contains a coefficient whose value has to be calibrated. The calibration of the model for Cyclone Base Case parameters is also discussed. In addition, in Sec. 6.5 the computational advantages of the LES simulations are commented. In Sec. 6.6 the accuracy of the \textsc{GyroLES} model is discussed. An estimate of the truncated scales is proposed for various quantities in Sec. 6.7. The robustness of the model in terms of parameter changes will be analyzed in Sec. 6.8. Finally, the conclusions are given in Sec. 6.9.

### 6.1 The filtered gyrokinetic equation

As we saw in Chapter 2, the gyrokinetic equation (2.126) can be expressed formally as:

\[
\frac{\partial g_{kj}}{\partial t} = L[g_{kj}] + D[g_{kj}] + N[g_{kj}, g_{kj}],
\]

(6.1)

where \( g_{kj} = g_{1j}(k_x, k_y, z, v_{||}, \mu) \) is the modified distribution function for the species considered. Here, \( L[g_{kj}] \) is a linear operator containing the influence of the density and temperature gradients, the effects due to magnetic curvature and the effects of the parallel dynamics involving magnetic trapping and Landau damping. \( D[g_{kj}] \) is also a linear dissipation term and the nonlinear term that represents the effect of the \( \mathbf{E} \times \mathbf{B} \) drift of the charged particles is denoted by \( N[g_{kj}, g_{kj}] \).

If we now apply a filter operation, denoted by \( \overline{\cdots} \), and represented by a filter operator \( \mathcal{F}_\Delta \) (to be defined later) to the gyrokinetic equation, we obtain the
following equation:
\[ \overline{\partial_t} g_{kj} = L[g_{kj}] + D[g_{kj}] + \mathcal{N}[g_{kj}, g_{kj}]. \] (6.2)

As it was done in N-S and MHD, we will apply the filter operator only to the spatial field aligned coordinates. In addition, we will like to use an homogenous filter that satisfies the following commutation properties:
\[ [\partial_t, \mathcal{F}_\Xi] = 0 \Rightarrow \overline{\partial_t} g_{kj} = \partial_t \overline{g_{kj}}, \] (6.3)
\[ [L[g_{kj}], \mathcal{F}_\Xi] = 0 \Rightarrow \overline{L[g_{kj}]} = L[\overline{g_{kj}}], \] (6.4)
\[ [D[g_{kj}], \mathcal{F}_\Xi] = 0 \Rightarrow \overline{D[g_{kj}]} = D[\overline{g_{kj}}]. \] (6.5)

The first property (6.3) is trivially satisfied for any filter that only depends on the spatial coordinates. It is well-known that an homogenous filter commutes with the spatial derivatives that appears in the operators \( L[g_{kj}] \) and \( D[g_{kj}] \). However, the filter will not commute with these operators if they depend explicitly on the spatial coordinates. Fortunately, in the flux-tube approximation there is no explicit spatial dependence in the perpendicular directions.

On the other hand, \( L[g_{kj}] \) and \( D[g_{kj}] \) depend on the parallel \((z)\) coordinate. Therefore, the simplest filter that satisfies (6.4) and (6.5) for the flux-tube approximation must act only in the perpendicular spatial coordinates.

This choice fits our problem because in gyrokinetics the perpendicular plane usually requires much higher resolution than the other coordinates. As an example, DNS can use grids that go up to \( N_x \times N_y \times N_z \times N_{\parallel} \times N_{\perp} = 768 \times 384 \times 16 \times 32 \times 8 \) [47]. Physically, this choice is also convenient because the cascade processes take place in the perpendicular plane. For all these reasons, the LES technique will be limited here to a filtering in the \((k_x, k_y)\) grid.

The filter is implemented numerically by reducing the number of grid points in \((k_x, k_y)\) space. The reduction of number of grid points can be viewed as a low-pass filter operation, with a characteristic length \( \overline{\Delta} \), represented by the Heaviside step function \( H \) and defined in the perpendicular Fourier space \( k \) (with \( k = |k_x| \) or \( |k_y| \)) as:
\[ \mathcal{F}_\Xi[g_{kj}] := H(K_{\text{LES}} - k)[g_{kj}] = \begin{cases} g_{kj} & \text{for } 0 < k < K_{\text{LES}} \text{ with } K_{\text{LES}} = 1/\overline{\Delta}, \\ 0 & \text{for } K_{\text{LES}} < k < K_{\text{DNS}} \text{ with } K_{\text{DNS}} = 1/\Delta_{\text{DNS}}. \end{cases} \]

The filter sets to zero the smallest scales of \( g_{kj} \), characterized by all modes larger than \( K_{\text{LES}} = 1/\overline{\Delta} \) up to the maximum wave number represented by \( K_{\text{DNS}} = 1/\Delta_{\text{DNS}} \), as shown in Fig. 6.1. Consequently, this technique reduces the computational cost of a gyrokinetic simulation. Taking into account all the previous considerations, we can write Eq. (6.2) as:
\[ \partial_t \overline{g_{kj}} = L[\overline{g_{kj}}] + D[\overline{g_{kj}}] + \mathcal{N}[g_{kj}, g_{kj}]. \] (6.6)

\(^1\)A direct consequence of that fact is that we are able to use a Fourier decomposition in the perpendicular directions.
6.1 The filtered gyrokinetic equation

The filtered nonlinear term $\mathcal{N}[g_{kj}, g_{kj}]$ still depends on the complete distribution function $g_{kj}$. It is convenient to split this term into a term which depends only on the filtered distribution function $\tilde{g}_{kj}$ and a term which contains the information of complete distribution function $g_{kj}$:

$$
\mathcal{N}[g_{kj}, g_{kj}] = \mathcal{N}[\tilde{g}_{kj}, \tilde{g}_{kj}] + \mathcal{N}[g_{kj}, g_{kj}] - \mathcal{N}[\tilde{g}_{kj}, \tilde{g}_{kj}].
$$

(6.7)

The last two terms in the above equation defined the sub-grid term, which for clarity of the presentation, will be represented by a notation that remarks the fact that this term contains the influence of both the resolved scales ($\Delta$) and the under-resolved scales ($\Delta_{DNS}$):

$$
T_{\Delta, \Delta_{DNS}} = \mathcal{N}[g_{kj}, g_{kj}] - \mathcal{N}[\tilde{g}_{kj}, \tilde{g}_{kj}].
$$

(6.8)

With this definition, the filtered gyrokinetic equation reads:

$$
\partial_t \tilde{g}_{kj} = L[\tilde{g}_{kj}] + D[\tilde{g}_{kj}] + \mathcal{N}[\tilde{g}_{kj}, \tilde{g}_{kj}] + T_{\Delta, \Delta_{DNS}}.
$$

(6.9)

The LES technique for gyrokinetics (GyroLES in the following) consists in replacing the sub-grid term by a model $M$ which depends only on the resolved unknowns ($\tilde{g}_{kj}$):

$$
T_{\Delta, \Delta_{DNS}} \approx M[\tilde{g}_{kj}].
$$

(6.10)
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

6.2 The filtered free energy balance equation

In order to correctly model the sub-grid term, we need to understand its role in the filtered gyrokinetic equation. For this purpose, it is convenient to look at the filtered free energy balance equation. The filtered free energy balance equation can be obtained by applying the filtered kinetic operator \( \Xi_h \) to filtered gyrokinetic equation (6.9) (GK) and adding its complex conjugate part (cc):

\[
\Xi_h[\text{eq : GK}] + \text{cc} := \sum_j \int d\Lambda_k \frac{T_{0j}}{2 F_{0j}} h_{-kj} [\text{eq : GK}] + \text{cc},
\]  

(6.11)

where the above quantity is defined using a phase-space volume integration over \( d\Lambda_k \) in which the sums have to be understood to be up to \( K_{x}^{\text{LES}} \) and \( K_{y}^{\text{LES}} \):

\[
\int d\Lambda_k = \sum_{|k_x| \leq K_{x}^{\text{LES}}} \sum_{|k_y| \leq K_{y}^{\text{LES}}} \int d\Theta \quad \text{with} \quad \int d\Theta = \left\langle \int d\nu \| d\mu \right\rangle_{z} \pi B_0 n_{0j}.
\]

(6.12)

As we have already mentioned in the previous chapters, the nonlinear term has the fundamental role of transferring the free energy across perpendicular scales. Indeed, in a DNS, these transfers have globally a vanishing contribution of the free energy balance:

\[
N := \Xi_h [N[g_{kj}, g_{kj}]] + \text{cc} = \sum_j \int d\Lambda_k \frac{T_{0j}}{2 F_{0j}} h_{-kj} N_k[g_{kj}, g_{kj}] + \text{cc} = 0,
\]  

(6.13)

where in this case the sum goes up to maximum wave number, that is, \( K_{x}^{\text{DNS}} \) and \( K_{y}^{\text{DNS}} \). If a filter is introduced, the same property also holds for the nonlinear term in the filtered gyrokinetic equation:

\[
\overline{N} := \Xi_h [\overline{N}[\overline{g}_{kj}, \overline{g}_{kj}]] + \text{cc} = \sum_j \int d\Lambda_k \frac{T_{0j}}{2 F_{0j}} h_{-kj} \overline{N}_k[\overline{g}_{kj}, \overline{g}_{kj}] + \text{cc} = 0.
\]

(6.14)

On the contrary, the filtered free energy operator has a non vanishing contribution when it is applied to the sub-grid term:

\[
\mathcal{T}_{\Xi_DNS} := \Xi_h [\mathcal{T}_{\Xi_DNS}[j]] + \text{cc} = \sum_j \int d\Lambda_k \frac{T_{0j}}{2 F_{0j}} h_{-kj} \mathcal{T}_{\Xi_DNS}[j] + \text{cc} \neq 0.
\]

(6.15)

Therefore, the filtered free energy balance can then be expressed as

\[
\partial_t \mathcal{E} = \mathcal{G} + \mathcal{D} + \mathcal{T}_{\Xi_DNS},
\]

(6.16)

where filtered quantities are obtained from the action of the filtered free energy operator \( \Xi_h \) on the filtered gyrokinetic equation (6.9). Thus, the quantities \( \mathcal{E}, \mathcal{G}, \mathcal{D} \) are the same as \( \mathcal{E}, \mathcal{G}, \mathcal{D} \) (see Eqs. (4.47, 4.55, 4.56)), except that they are defined using \( \overline{g}_{kj} \) instead of \( g_{kj} \).
6.3 The physics of the sub-grid term

In this section, we will study numerically the physics of the sub-grid term for the standard case of CBC [40] for ITG driven turbulence ($\omega_{ni} = 2.22, \omega_{Ti} = 6.92, q = 1.4, \delta = 0.796$). Furthermore, the DNS and LES grid correspond, respectively, to $N_x \times N_y = 128 \times 64$ and $N_x \times N_y = 48 \times 24$, while $N_z = 16, N_{v_x} = 32$, and $N_{v_y} = 8$ are held constant. In the following, we will try to answer the following questions: can we neglect the sub-grid term contribution? and, what is the role of the sub-grid term?

6.3.1 The sub-grid term contribution

First, we compare the free energy spectrum of two numerical simulations: a DNS, whose free energy equation is given by:

$$\partial_t \mathcal{E} = \mathcal{G} + \mathcal{D}$$

and a LES

$$\partial_t \overline{\mathcal{E}} = \overline{\mathcal{G}} + \overline{\mathcal{D}} + \overline{T_{DNS}}_{\Delta \text{neglect}}$$

but where we have neglected the sub-grid term contribution. This is the simplest LES model, i.e., no model for the sub-grid term.

Fig. 6.2 shows the free energy spectra versus $k_x$ (summed over $k_y$). The black dotted line represents the DNS spectrum (which for clarity, is shown only until the maximum wavenumber of the LES simulation, $K_{\text{LES}}^x = 1.15 \rho_s$) and the blue dashed line represents the LES spectrum. They are defined, respectively, from the two-dimensional spectrum as:

$$\mathcal{E}^{kx}_{k_y} = \sum_{|k_y| \leq K_{\text{DNS}}^y} \mathcal{E}^{kx,k_y} \quad \text{and} \quad \overline{\mathcal{E}}^{kx}_{k_y} = \sum_{|k_y| \leq K_{\text{LES}}^y} \overline{\mathcal{E}}^{kx,k_y}.$$

Clearly, the free energy is piling up in the high $k_x$ range in the LES case due to the reduced high wavenumber dissipation in the absence of small scales. Therefore, we cannot neglect the sub-grid term.

6.3.2 Role of the sub-grid term

Second, we now consider again a DNS but where a test filter $\overline{\Delta}$ is applied to it. This test filter operation allows us to calculate explicitly the filtered distribution function $\overline{\mathcal{E}}$, and therefore the sub-grid term for all times. We want to remark

\[\text{\footnotesize\footnote{For clarity of the presentation, the two-dimensional spectrum which was defined previously by } \mathcal{E}^{k} \text{ is now represented by } \mathcal{E}^{kx,k_y}.}\]
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

Figure 6.2: Free energy: comparison between highly resolved DNS (black), and LES without model (blue) for the Cyclone Base test Case (CBC). The resolution for the DNS is $N_x = 128$ and $N_y = 64$ and for the LES $N_x = 48$ and $N_y = 24$. The free energy is given in units of $n_0eT_0eK_s/L^2$.

that this is not a LES, since we are not reducing the simulation domain. Our simulation still contains the complete distribution $g_{kj}$. Therefore, the free energy equation with the test filter $\Delta$ reads:

$$\partial_t \overline{\mathcal{E}} = \overline{\mathcal{G}} + \overline{\mathcal{D}} + \tau_{\Delta\text{DNS}}.$$  \hspace{1cm} (6.20)

The numerical results are shown in Fig. 6.3. Here, the sub-grid term contribution (red dash-dotted) represents a loss of free energy. Its amplitude is compared to the free energy injection $\overline{\mathcal{G}}$ and dissipation $\overline{\mathcal{D}}$. On average, once a statistically stationary turbulent state is reached, these three terms should be in balance, that is:

$$\overline{\mathcal{G}} \approx -\overline{\mathcal{D}} - \tau_{\Delta\text{DNS}}.$$  \hspace{1cm} (6.21)

In the run corresponding to Fig. 6.3, the ratio

$$\frac{\tau_{\Delta\text{DNS}}}{\overline{\mathcal{D}}} \approx 1,$$  \hspace{1cm} (6.22)

appears to be close to unity. Hence, we conclude that the transfer of free energy between the largest (resolved) scales and the smallest (under-resolved) scales, represented by the sub-grid term, cannot be neglected.

6.3.3 Final remarks

We could have anticipated these results from what we obtained in the previous chapters. The free energy injected into the system in the largest scales is transferred through the smallest ones in a cascade process where it is dissipated. If
6.4 Developing a gyrokinetic LES model

The development of models for representing the effect of small on the large scales has been the subject of countless efforts in LES for fluid turbulence \[23, 48\] and conductive fluids \[31, 32\]. Nevertheless, the most commonly used models simply attempt to reproduce the transfer of kinetic energy towards small scales by a dissipative mechanism represented by an eddy viscosity. The simplest example of a viscosity model is the Smagorinsky model \[48\] introduced previously in Chapter \[2\]. Taking into account the analogy between fluid and plasma turbulence, in the area of gyrofluid turbulence, LES techniques have been explored by Smith and
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

Hammett [49], considering hyper-viscosity models for two-dimensional drift-wave turbulence. The aim of the present section is to extend the LES methodology to gyrokinetics in three spatial dimensions. For this reason, it is proposed to also use an effective dissipation which is modeled by a hyperdiffusion term

\[ M[c, \gk] = -c_\perp k_\perp^4 \hbar_{kj}. \quad \text{(6.25)} \]

It is easy to verify that this model always gives a negative contribution to the filtered free energy balance equation:

\[ \mathcal{M} := \sum_j \int d\Lambda_k \frac{T_{0j}}{F_{0j}} \hbar_{kj} M[c, \gk] + cc = -c_\perp \sum_j \int d\Lambda_k \frac{T_{0j}}{F_{0j}} \left| k_\perp^4 \hbar_{kj} \right|^2 < 0, \]

(6.26)

if the hyperdiffusion coefficient \(c_\perp\) is defined positive. The \(k_\perp^4\) dependency is due to the evidence that the turbulence appears to be very close to isotropy in the plane perpendicular to the magnetic field at scales smaller than the driving range [47]. However, the power four dependence is not trivial at all. It must be acknowledged at this point that no strong theoretical support can be given to this choice. At least one other choice (\( \approx k_\perp^2 \)) has been tested but led to slightly less satisfactory results and is not discussed here.

6.4.1 Calibration of the model

The model we have defined in Eq (6.25) is shown to dissipate free energy. However, before we can apply it to a LES, the model must be calibrated in order to ensure that it dissipates the correct amount of free energy. This can be done by adjusting the hyperdiffusion coefficient \(c_\perp\) in such a way that the free energy spectra given by a DNS (\(N_x \times N_y = 128 \times 64\)) and a LES (\(\overline{N_x} \times \overline{N_y} = 48 \times 24\)) match.

In Fig. 6.4 the free energy spectra are displayed for various values of the parameter \(c_\perp\). The black curve corresponds to the DNS run. It is compared to four LES with runs corresponding to \(c_\perp = \{0, 0.025, 0.375, 1.0\}\). Other values of \(c_\perp\) have also been tested but are not shown here for clarity. All the spectra are time-averaged during the saturated state of the turbulence. From this figure, we can make the following observations:

i) A too small coefficient \(c_\perp = 0.025\) (red dash-dotted) does not significantly improve the results when compared to the no model case (black dotted). Here, there is a lot of artificial accumulation of free energy in the small scales. In addition, the large scales are also not well represented in this case.

ii) If we now increase the value of the coefficient, we start to have less free energy accumulation in the small scales together with a better representation of the large scales. There is a “plateau of values” \(c_\perp \in [0.25, 0.625]\) for
which we have a good agreement, its optimal value being close to $c_\perp = 0.375$ (blue dashed line). Here, the corresponding LES reproduces fairly well the spectra of the free energy in $k_x$ and in $k_y$.

iii) A too large value of the $c_\perp$ (red × dotted) tends to over-damp the small scales which leads to an artificial accumulation of the free energy in the large scales.

![Figure 6.4: Resolved free energy spectra versus $k_x$ (left) and versus $k_y$ (right) obtained by varying the model coefficient compared with DNS. The free energy spectra are given in units of $n_0eT_0e(\rho_s/R)^2$.](image)

In conclusion, the value of the coefficient that is able to dissipate the correct amount of free energy is around $c_\perp = 0.375$.

### 6.5 Computational gain

It is interesting to discuss the computational gain obtained in the LES presented in the previous section. Although for the present case, the DNS does not use a very large grid, the LES grid and hence the required memory can be reduced by 86%. In terms of CPU time, the gain is even higher. Indeed, the LES can be performed with a larger time step since the smallest scales are larger than in the DNS. In practice, with the grid resolution chosen in this study, the time step is increased by a factor of about two in the LES when compared to the DNS. As a consequence, the overall computational effort required for the LES runs is more than 30 times smaller than in the DNS runs.

### 6.6 Accuracy of the GyroLES model

In the previous section, the use of a properly calibrated model was shown to give a good agreement between DNS and LES. In addition, in terms of free energy,
it is also possible to compare the contribution of the sub-grid term with the dissipation introduced with the GyroLES model. The sub-grid contribution to the resolved free energy balance can be expressed:

\[
T_{k_x,k_y}\Delta_{DNS} = \sum_{k'_x,k'_y} T_{k_x,k_y,k'_x,k'_y} \Delta_{DNS},
\]

where the four-dimensional quantity \( T_{k_x,k_y} \Delta_{DNS} \) arises from the nonlinearities in Eq. (6.8) and can be interpreted as a nonlinear transfer function from modes \((k'_x,k'_y)\) to modes \((k_x,k_y)\) \[46,50\].

A comparison between the one-dimensional spectra defined as:

\[
T_{k_x} = \sum_{k_y \leq K_{y,LES}} T_{k_x,k_y} \Delta_{DNS} \text{ and } T_{k_y} = \sum_{k_x \leq K_{x,LES}} T_{k_x,k_y} \Delta_{DNS},
\]

\[
M_{k_x} = \sum_{k_y \leq K_{y,LES}} M_{k_x,k_y} \text{ and } M_{k_y} = \sum_{k_x \leq K_{x,LES}} M_{k_x,k_y},
\]

are shown in Fig. 6.5.

Figure 6.5: Resolved sub-grid spectra \( T_{k_x} \Delta_{DNS} \) (left), \( T_{k_y} \Delta_{DNS} \) (right) compared with dissipations due to model \( M_{k_x} \) and \( M_{k_y} \). They are given in units of \( n_0 e T_0 v_T / R (\rho_s/R)^2 \).

The model presents an overall agreement with the sub-grid spectra obtained from the DNS, while the detailed structure is smoothed down by the model. By overall agreement we mean that both curves are of the same order of magnitude and both \( T_{k_x} \Delta_{DNS} \) and \( M \) dissipate the same amount of free energy.

### 6.7 Estimate for the global quantities

Since small scales are truncated in the LES runs, it is not possible in LES to predict directly global quantities such as the total free energy and the total free
6.7 Estimate for the global quantities

energy injection (or equivalently, the total heat flux in the case of electrostatic fluctuations). An estimate of the contribution from the truncated scales to these global quantities is certainly desirable if a comparison has to be made with experimental results.

In this section, a simple estimate for the truncated scale contribution to these quantities is proposed. It is noted that all these quantities (\(E\) or \(G\)), generically denoted in the following by \(Q\), can be represented either by their two-dimensional spectrum \(Q_{k_x,k_y}\) or by their one-dimensional \(k_x\) spectrum \((Q^{k_x})\) and \(k_y\) spectrum \((Q^{k_y})\). In a LES, only the resolved part of \(Q\), denoted hereafter by \(\overline{Q}\), is directly accessible. It is given by:

\[
\overline{Q} = \sum_{|k_x| \leq K_{LES}^x} Q^{k_x} = \sum_{|k_y| \leq K_{LES}^y} Q^{k_y}. \tag{6.30}
\]

The under-resolved part of \(Q\), denoted by \(\delta Q\), contains three contributions:

\[
\delta Q = \delta_x Q + \delta_y Q + \delta_{xy} Q, \tag{6.31}
\]

with

\[
\delta_x Q = \sum_{|k_x| > K_{LES}^x} \sum_{|k_y| \leq K_{LES}^y} Q^{k_x,k_y}, \tag{6.32}
\]

\[
\delta_y Q = \sum_{|k_x| \leq K_{LES}^x} \sum_{|k_y| > K_{LES}^y} Q^{k_x,k_y}, \tag{6.33}
\]

\[
\delta_{xy} Q = \sum_{|k_x| > K_{LES}^x} \sum_{|k_y| > K_{LES}^y} Q^{k_x,k_y}. \tag{6.34}
\]

The different contributions of \(Q\) are illustrated in Fig. 6.6.

In a DNS, \(\delta Q\) can be computed, but in LES it has to be estimated. In this thesis, we estimate \(\delta Q\) by noting that in the large \(k_x\) and \(k_y\) ranges of LES runs, the quantity \(Q\) can often be approximated by decaying power laws:

\[
Q^{k_x} \approx A_x k_x^{-\alpha_x} \quad \text{with} \quad |k_x| \leq K_{LES}^x, \tag{6.35}
\]

\[
Q^{k_y} \approx A_y k_y^{-\alpha_y} \quad \text{with} \quad |k_y| \leq K_{LES}^y. \tag{6.36}
\]

The amplitudes \(A_x\) and \(A_y\) as well as the exponents \(\alpha_x\) and \(\alpha_y\) can be estimated by linear regression from the LES spectra. In that case, the following estimates can be obtained:

\[
\delta_x Q \approx \sum_{|k_x| > K_{LES}^x} K_{DNS}^{k_x} A_x k_x^{-\alpha_x}, \tag{6.37}
\]

\[
\delta_y Q \approx \sum_{|k_y| > K_{LES}^y} K_{DNS}^{k_y} A_y k_y^{-\alpha_y}. \tag{6.38}
\]
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

**Figure 6.6:** Different contributions to any quantity $Q = \mathcal{E}$ or $\mathcal{G}$. Bottom left, the resolved $\overline{Q}$, containing modes that are resolved both in $|k_x| \leq K_{x}\text{LES}$ and $|k_y| \leq K_{y}\text{LES}$. Top left, the under-resolved spectrum in $k_y$ represented by $\delta_y Q$. It contains modes which are resolved in $|k_x| \leq K_{x}\text{LES}$ but under-resolved in $|k_y| > K_{y}\text{LES}$. Bottom right, the under-resolved spectrum in $k_x$ represented by $\delta_x Q$. It contains modes which are resolved in $|k_y| \leq K_{y}\text{LES}$ but under-resolved in $|k_x| > K_{x}\text{LES}$. Top right, the under-resolved spectrum in both dimensions, represented by $\delta_{xy} Q$. It contains modes which are under-resolved in both $|k_x| > K_{x}\text{LES}$ and $|k_y| > K_{y}\text{LES}$.

Since these sums are finite, there is a priori no restriction on the values of the exponents. However, if the wave vector range is extended to infinity, these sums converge if and only if $\alpha_x > 1$ and $\alpha_y > 1$.

Estimating $\delta_{xy} Q$ is more difficult. However, assuming a separable spectrum

$$Q^{k_x,k_y} = q_1^{k_x} q_2^{k_y}, \quad (6.39)$$

it can be shown that

$$\delta_{xy} Q = \delta_x Q \frac{\delta_y Q/\overline{Q}}{\delta_y Q}. \quad (6.40)$$

In general, it is thus expected that the correction due to $\delta_{xy} Q$ is very small and can be neglected compared to $\delta_x Q$ or $\delta_y Q$:

$$\delta_{xy} Q \ll \delta_x Q, \delta_y Q. \quad (6.41)$$

Therefore, the global value of $Q$ can be approximated by:

$$Q \approx \overline{Q} + \delta_x Q + \delta_y Q \approx \overline{Q} + \sum_{|k_x| > K_{x}\text{LES}} A_x k_x^{-\alpha_x} + \sum_{|k_y| > K_{y}\text{LES}} A_y k_y^{-\alpha_y}. \quad (6.42)$$
6.7 Estimate for the global quantities

This procedure has been used to estimate the total value of both the free energy and the free energy injection from the LES with the optimal value of $c_\perp = 0.375$ and for the LES without model.

As far as the free energy is concerned, the best fit of the one-dimensional spectra yields $\alpha_x = 2.21$, $\alpha_y = 1.74$ for $c_\perp = 0.375$. These values are then used to compute the corrections $\delta_\alpha \mathcal{E}$ and $\delta_\beta \mathcal{E}$. The LES estimate $(\mathcal{E}^{\text{LES}})$ for the total free energy can then be compared to the value measured from the DNS value $(\mathcal{E}^{\text{DNS}})$. It is found that the LES estimate is in good agreement with the DNS value $\mathcal{E}^{\text{LES}} = 1.10 \mathcal{E}^{\text{DNS}}$. On the contrary, without a model ($c_\perp = 0$), the best fit of the free energy one-dimensional spectra yields $\alpha_x = 0.79$, $\alpha_y = 0.85$. In that case, the estimates given by equations (6.37) and (6.38) would be divergent if the sums had to be extended to infinity. However, if the sums are limited to $K_x^{\text{DNS}}$ and $K_y^{\text{DNS}}$, it is possible to reconstruct the total free energy from the LES without model but the estimate is more than twice the value of the DNS: $\mathcal{E}^{\text{No Model}} = 2.1 \mathcal{E}^{\text{DNS}}$.

The same procedure has been used for the free energy injection $\mathcal{G}$, see Fig 6.7. For $c_\perp = 0.375$, the regression method yields $\alpha_x = 3.60$ and $\alpha_y = 2.20$, which gives the following estimate $\mathcal{G}^{\text{LES}} = 1.11 \mathcal{G}^{\text{DNS}}$. Again, the value computed from the LES slightly overestimate the DNS value of the free energy injection. However, this prediction is still in reasonable agreement with the DNS and provides a much better estimate than the no model simulation for which the regression method gives $\alpha_x = 2.95$ and $\alpha_y = 1.72$, resulting in $\mathcal{G}^{\text{No Model}} = 1.38 \mathcal{G}^{\text{DNS}}$. The comparisons described above are summarized in table 6.1.
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

<table>
<thead>
<tr>
<th>No Model</th>
<th>$\mathcal{E} = 2.10\mathcal{E}^{DNS}$</th>
<th>$\alpha_x = 0.79$</th>
<th>$\alpha_y = 0.85$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES</td>
<td>$\mathcal{E} = 1.10\mathcal{E}^{DNS}$</td>
<td>$\alpha_x = 2.21$</td>
<td>$\alpha_y = 1.74$</td>
</tr>
<tr>
<td>No Model</td>
<td>$\mathcal{G} = 1.38\mathcal{G}^{DNS}$</td>
<td>$\alpha_x = 2.95$</td>
<td>$\alpha_y = 1.72$</td>
</tr>
<tr>
<td>LES</td>
<td>$\mathcal{G} = 1.11\mathcal{G}^{DNS}$</td>
<td>$\alpha_x = 3.60$</td>
<td>$\alpha_y = 2.20$</td>
</tr>
</tbody>
</table>

Table 6.1: Comparisons of a LES $(c_\perp = 0.375)$ and a no model LES $(c_\perp = 0)$ respect to the DNS simulation, for the free energy and the free energy injection terms.

6.8 Limitations of the GyroLES model

In the previous section, we have shown that the choice $c_\perp = 0.375$ gave a reasonable agreement between the LES and the DNS runs for the standard CBC parameters. However, the LES methodology is only useful if the model coefficient does not have to be calibrated for each set of parameters. In this section, it is proposed to explore the robustness of the LES approach by varying the logarithmic temperature gradient $\omega_{Ti}$. This choice is motivated by the fact that an ITG simulation is driven by the equilibrium ion temperature gradient. Therefore, its variation allows us to change the turbulent level of the system. For this reason, in the following, all the parameters characterizing the CBC have been kept constant, except the logarithmic temperature gradient which is varied from the standard CBC value of $\omega_{Ti} = 6.96$ to a lower turbulent case with $\omega_{Ti} = 6.0$ and a higher turbulent case with $\omega_{Ti} = 8.0$.

6.8.1 Lower turbulent case

For the lower turbulent case ($\omega_{Ti} = 6.0$), Fig. 6.8 shows the comparisons between LES with $c_\perp = 0.375$ (red dash-dotted), LES with $c_\perp = 0$ (blue dashed) and DNS (black pointed) of the free energy spectrum. Here, although the LES prediction is still acceptable and there is a clear improvement when compared with the no model run, the predictions tend to deviate significantly from the DNS results in the large scale range. This is not surprising, since in this case, the turbulence strength is decreased with respect to CBC. As a consequence, the amplitude of the model is slightly bigger than it should be: we are over-damping the small scales. The same effect was observed in Sec. 6.4 when the amplitude of the model was too big.

6.8.2 Higher turbulent case

On the other hand, when the turbulent strength is increased ($\omega_{Ti} = 8.0$), we observe in Fig. 6.9 that in the LES run with $c_\perp = 0.375$ (red dash-dotted), there
6.8 Limitations of the GyroLES model

Figure 6.8: Resolved free energy spectra $\mathcal{E}^{k_x}$ (left) and $\mathcal{E}^{k_y}$ (right) obtained with the model of Eq (6.25) with $c_\perp = 0.375$ for $\omega_{Ti} = 6.0$. Comparison with a highly resolved DNS with $\omega_{Ti} = 6.0$ and with LES without model. The free energy spectra are given in units of $n_0eT_{0e}(\rho_s/R)^2$.

is now an artificial accumulation of the free energy at small scales in comparison with the DNS run (black pointed). However, there is still a clear improvement when comparing the LES run with no model (blue dashed). Again, this can be understood in terms of the turbulent level of the simulation. Since this is a higher turbulent state, the amplitude of the model should be increase accordingly in order to dissipate the correct amount of free energy and avoiding its accumulation at the small scales.

Figure 6.9: Resolved free energy spectra $\mathcal{E}^{k_x}$ (left) and $\mathcal{E}^{k_y}$ (right) obtained with the model (6.25) $c_\perp = 0.375$ for $\omega_{Ti} = 8.0$. Comparison with a highly resolved DNS with $\omega_{Ti} = 8.0$ and with LES without model. The free energy spectra is given in units of $n_0eT_{0e}(\rho_s/R)^2$. 

107
6. EXTENSION OF THE LES APPROACH TO GYROKINETICS

6.9 Conclusions

In this chapter we presented the extension of the LES approaches to gyrokinetic simulations. First, we derived the filtered gyrokinetic equation where the sub-grid term was defined. Second, we derived the filtered free energy balance equation in order to study the properties of the sub-grid term. It was observed, as expected from our analyses in the previous chapters, that the role of the sub-grid term is to dissipate free energy. For this reason, and based on previous studies by Smith and Hammett [49], we used an hyperdiffusion model that dissipates free energy. This model has a coefficient whose value has to be calibrated in each simulation. This was done for the CBC parameters, and we found that a value for the parameter of $c_\perp = 0.375$ gives good agreement when comparing the free energy spectra of the DNS and the LES runs. As a consequence, we found that the overall computational effort required for the LES runs is approximately 30 times smaller than in the DNS runs. These findings indicated that the LES approach is quite promising in the context of gyrokinetics. Furthermore, we developed a method to estimate the global quantities, such as the free energy and the heat flux. In this case, we found a quite good agreement between DNS and LES runs, which encouraged our findings.

Finally, we tested the robustness of our model by changing the turbulence drive, i.e., the temperature gradient. We observed that the model coefficient must change accordingly. When the turbulence level is lowered the agreement between the under-resolved and the fully resolved simulations becomes less and less satisfactory—although such behavior can be understood and even anticipated. In order to make LES useful, we need to apply a method that is able to calibrate automatically the amplitude of the model. In this work, we will use the method developed for fluid dynamics by Germano (see Chapter 2), known as the dynamic procedure. The implementation of the dynamic procedure for gyrokinetics is discussed in the next chapter.
Chapter 7

Dynamic procedure for GyroLES

In the previous chapter we extended LES techniques to gyrokinetics using a hyperdiffusion model. However, the robustness of the model was not proved in the most general sense. For instance, the coefficient must change when varying the logarithmic temperature gradient. The main objective of the present chapter is to overcome this problem by adapting the dynamic procedure \[23, 26\] to GyroLES. The dynamic procedure is an optimization approach that allows to calibrate the model amplitude in the course of the simulation.

The chapter is organized as follows. After a brief review of the model used so far, the effect of the filter width will be discussed. The aim of this study is to develop a more general model before introducing the dynamic procedure. Then, the dynamic procedure for gyrokinetics will be discussed. Numerical results obtained for various logarithmic temperature gradient and magnetic shear values will be presented. Finally, conclusions will be given.

7.1 An improved model for the sub-grid term

In the previous chapter, the proposed model for the sub-grid term

\[
T_{j,\Delta}\approx M[c, y_{kj}] = -c_{\perp} k_{\perp} h_{kj}
\]

(7.1)
did not take into account the filter width dependency $\Delta$. However, Fig. 7.1 shows the time evolution of the sub-grid contribution to the filtered free energy balance equation

\[
T_{\Delta,\text{DNS}} := \Xi_{h} [T_{j,\Delta}\text{DNS}] + cc = \sum_{j} \int d\Lambda_{k} \frac{T_{0j}}{2F_{0j}} \bar{h}_{kj} T_{\Delta,\text{DNS}} + cc
\]

(7.2)

for different values of the filter width $\Delta$ for the CBC parameters. Here, one observes that the amplitude of the sub-grid dissipation increases with the filter width.

For this reason, a more general model for the sub-grid term should behave like

\[
T_{j,\Delta,\text{DNS}} \approx M[c, \Delta, y_{kj}] = -c_{\perp} \Delta^{\alpha} k_{\perp}^{n} h_{kj}
\]

(7.3)
where in the last expression, we have proposed a hyperdiffusion model of order \( n \) which ensures analytically that the model acts as a sink of free energy. The model amplitude is proportional to a coefficient \( c_\perp \) and to the filter width \( \Delta \) to the power \( \alpha \). The latter being positive in order to take into account that the dissipation of free energy increases with the filter width.

The disadvantage of this model is that we have introduced another free parameter in the problem, since the exact value of \( \alpha \) is unknown. However, it is still possible to estimate its value. For instance, in fluid turbulence it is common to assume that the kinetic energy flux from scale to scale is a constant in the inertial range. Based on the finding that gyrokinetic ITG turbulence also exhibits a local and direct cascade of free energy [46, 50], and in analogy to the fluid case, we also assume that the free energy flux \( \varepsilon_\mathcal{E} \) is constant from scale to scale in the plane perpendicular to the magnetic field line. Hereafter, this scale range is called the gyrokinetic inertial range.

Therefore, based on the previous arguments, it is reasonable to assume that the model depends only on the free energy flux \( \varepsilon_\mathcal{E} \) and the filter width \( \Delta \),

\[
M[c, \Delta, g_{kj}] = -\varepsilon_\mathcal{E}^{\alpha} \Delta^n k_\perp h_{kj}.
\]  

(7.4)

Here, the free energy flux is dimensionally related to the model coefficient by 
\[ [c] = [\varepsilon_\mathcal{E}]^\beta. \]

We can now proceed to a dimensional analysis of the model in order to obtain the exponent \( \alpha \). The free energy has the dimension of an energy density \( 1/LT^2 \),
so that the free energy flux $\varepsilon$ is an energy density per unit of time,
\[ [\varepsilon_E] = \frac{1}{L^2 T^2} = \frac{1}{L^2 T^3}, \]  
(7.5)
where $T$ and $L$ represent characteristic time and length scales. In addition, from the filtered gyrokinetic equation (6.9) and taking into account that $[g_{kj}]$ and $[h_{kj}]$ have the same dimensions, we find:
\[ [\partial_t g_{kj}] = [M[c, \overline{\Delta}, \overline{g_{kj}}]] \Rightarrow [\partial_t] [\overline{g_{kj}}] = [\varepsilon_E^\beta] [\overline{\Delta}^\alpha] [k_n^\perp] [\overline{h_{kj}}] \]  
(7.6)
thus
\[ T^{-1} = \left( \frac{1}{L^3 T^3} \right)^\beta L^n \left( \frac{1}{L^3} \right)^n, \]  
(7.7)
giving
\[ T^{-1} = T^{-3\beta} \Rightarrow \beta = 1/3, \]  
(7.8)
\[ 1 = L^{-\beta} L^{-n} \Rightarrow \alpha = n + 1/3. \]  
(7.9)
The last relation allows to fix the unknown filter width exponent $\alpha$ accordingly to the model parameter $n$. Thus, the model can be expressed as:
\[ M[c, \overline{\Delta}, \overline{g_{kj}}] = -\varepsilon_E^{1/3} \overline{\Delta}^{n+1/3} k_n^\perp \overline{h_{kj}} = -c_{\perp} \overline{\Delta}^{n+1/3} k_n^\perp \overline{h_{kj}}, \]  
(7.10)
in terms of the free energy flux or the model coefficient, respectively. It is worth to notice that, since the derivative order $n$ is positive, the filter width exponent $n + 1/3$ is also positive. This is in line with the observations from the numerical results of Fig 7.1.

This model has again only one free parameter, the model coefficient $c_{\perp}$. In the next section we will introduce the dynamic procedure for gyrokinetics: a method used to calculate this free parameter in the course of a GyroLES run.

### 7.2 Dynamic procedure for gyrokinetics

The following steps describe how the dynamic procedure can be derived for gyrokinetic LES:

1) We consider a LES equation with a filter width satisfying $\overline{\Delta} > \Delta_{DNS}$:
\[ \partial_t \overline{g_{kj}} = L[\overline{g_{kj}}] + D[\overline{g_{kj}}] + N[\overline{g_{kj}}, \overline{g_{kj}}] + T_{\overline{\Delta}_{DNS}}^j, \]  
(7.11)
where in the last expression, the sub-grid term $T_{\overline{\Delta}_{DNS}}^j$ has been modeled by a term that depends on the coefficient $c$ and on the filter width $\overline{\Delta}$. 

111
2) We now consider another LES equation but with a broader filter width, thus satisfying \( \Delta > \overline{\Delta} > \Delta_{\text{DNS}} \):

\[
\partial_t \tilde{g}_{kj} = L[\tilde{g}_{kj}] + D[\tilde{g}_{kj}] + N[\tilde{g}_{kj}, \tilde{g}_{kj}] + T^j_{\Delta_{\text{DNS}}}
\approx L[\tilde{g}_{kj}] + D[\tilde{g}_{kj}] + N[\tilde{g}_{kj}, \tilde{g}_{kj}] + M[c, \Delta, \tilde{g}_{kj}].
\] (7.12)

Here, the sub-grid term has been modeled with a term that depends on the filter width \( \Delta \) and the same coefficient \( c \) as in the previous case. This implies that \( c \) does not depend on the filter widths \( \Delta, \Delta_{\text{DNS}} \). This assumption is valid provided that the range of scales between the filters belongs to the gyrokinetic inertial range.

3) If we now apply a test filter operator with width \( \Delta \) to Eq. (7.11), we obtain:

\[
\partial_t \hat{g}_{kj} = L[\hat{g}_{kj}] + D[\hat{g}_{kj}] + \hat{N}[\hat{g}_{kj}, \hat{g}_{kj}] + M[c, \overline{\Delta}, \hat{g}_{kj}].
\] (7.13)

Note that in the last term the model coefficient and the filter width are constant. Therefore, they are not affected by the test filter operation. Furthermore, we can re-express the nonlinearity in terms of the sub-grid contribution between the \( \overline{\Delta} \) and \( \Delta \) filters:

\[
\hat{N}[\hat{g}_{kj}, \hat{g}_{kj}] = N[\hat{g}_{kj}, \hat{g}_{kj}] + \hat{N}[\hat{g}_{kj}, \hat{g}_{kj}] - N[\tilde{g}_{kj}, \tilde{g}_{kj}]
\approx N[\tilde{g}_{kj}, \tilde{g}_{kj}] + T^j_{\overline{\Delta}, \Delta}.
\] (7.14)

(7.15)

Using the previous relation and the use of the very important property \( \cdots \approx \cdots \) of Fourier low-pass filters, we can re-write Eq. (7.13) as

\[
\partial_t \hat{g}_{kj} = L[\hat{g}_{kj}] + D[\hat{g}_{kj}] + \hat{N}[\hat{g}_{kj}, \hat{g}_{kj}] + M[c, \overline{\Delta}, \hat{g}_{kj}] + T^j_{\overline{\Delta}, \Delta}.
\] (7.16)

4) Taking into account that Eq. (7.11) and Eq. (7.16) are acting on the same quantity \( \partial_t \hat{g}_{kj} \), we can equal both equations, giving the Germano identity \([23, 26]\):

\[
M[c, \Delta, \hat{g}_{kj}] = M[c, \overline{\Delta}, \hat{g}_{kj}] + T^j_{\overline{\Delta}, \Delta}.
\] (7.17)

In the Germano identity everything is known except the model coefficient. During a LES the sub-grid term \( T^j_{\overline{\Delta}, \Delta} \) can be computed exactly since it involves test filtering \( \Delta \) of the LES quantities \( \overline{\Delta} \).

5) In order to obtain the model coefficient, one can define the squared distance

\[
d^2 = \sum_j \int d\Delta \left( T_{\Delta, \Delta} + M[c, \overline{\Delta}, \hat{g}_{kj}] - M[c, \Delta, \hat{g}_{kj}] \right)^2
\approx \left( T_{\Delta, \Delta} + M[c, \overline{\Delta}, \hat{g}_{kj}] - M[c, \Delta, \hat{g}_{kj}] \right)^2.
\] (7.18)
where here, $\langle \cdots \rangle_{\Lambda,j}$ stands for integration over the entire phase space and sum over species. This definition assumes that besides the coefficient being constant in the perpendicular plane, it is also constant in the other coordinates ($z, v_{||}, \mu$ and species $j$) and it only depends on time.\footnote{This condition can be relax if we limit our integration to the perpendicular plane. In this case, the resulting coefficients will depend on the rest of coordinates and time.}

6) An optimization of this difference with respect to the unknown parameter

$$\frac{\partial d^2}{\partial c} = \frac{\partial}{\partial c} \left( T_{\Delta, \bar{\Delta}} + M[c, \bar{\Delta}, \bar{g}_k] - M[c, \Delta, \bar{g}_k] \right)_{\Lambda,j} = 0. \quad (7.19)$$

give us an expression to calculate $c$ at each time during a LES. A schematic view of the dynamic procedure is given in Fig. 7.2.

The optimization can be done even if the model depends on many coefficients. For instance, so far we have only considered one coefficient ($c_\perp$) in our model:

$$M[c, \bar{\Delta}, \bar{g}_k] = -c_\perp \bar{\Delta}^{n+1/3} \frac{1}{k_\perp} h_{kj}. \quad (7.20)$$

However, the use of $k_\perp$ implies that the relative dissipation in $k_x$ and $k_y$ is fixed, since $k_\perp$ is related to $k_x$ and $k_y$ by the following relation: $k_\perp^2 = g^{x\perp} k_x^2 + 2g^{\perp x} k_x k_y + g^{y\perp} k_y^2$. Now, since we can use the dynamic procedure to calculate several free parameters we can construct a more flexible model which takes into account the anisotropy in the perpendicular plane. The new model depends on four parameters ($c_x, c_y, \bar{\Delta}_x, \bar{\Delta}_y$):

$$M[c, \bar{\Delta}, \bar{g}_k] = -\left( c_x \bar{\Delta}_x^{n+1/3} k_x^n + c_y \bar{\Delta}_y^{n+1/3} k_y^n \right) h_{kj}. \quad (7.21)$$

Within this model:

$$M[c, \bar{\Delta}, \bar{g}_k] = -\left( c_x \bar{\Delta}_x^{n+1/3} k_x^n + c_y \bar{\Delta}_y^{n+1/3} k_y^n \right) h_{kj}, \quad (7.22)$$

$$M[c, \bar{\Delta}, \bar{g}_k] = -\left( c_x \bar{\Delta}_x^{n+1/3} k_x^n + c_y \bar{\Delta}_y^{n+1/3} k_y^n \right) h_{kj}. \quad (7.23)$$

Therefore, the Germano identity (7.17) can be expressed as:

$$T_{\Delta, \bar{\Delta}}^j = -c_x m_x^j - c_y m_y^j. \quad (7.24)$$

Here, the notation

$$m_{x,y}^j = \left( \bar{\Delta}_x^{n+1/3} - \bar{\Delta}_x^{n+1/3} \right) k_{x,y}^n h_{kj} \quad (7.25)$$

has been introduced.
7. DYNAMIC PROCEDURE FOR GYROLES

Figure 7.2: Schematic view of the dynamic for LES. Top) A LES with a filter width satisfying $\Delta > \Delta^{DNS}$. Middle) Another LES with a broader filter width satisfying: $\hat{\Delta} > \Delta > \Delta^{DNS}$. Bottom) A test filter with width $\hat{\Delta}$ is apply to the LES in the domain $\Delta$. 

114
Using Eq. (7.24), the squared distance can be expressed in terms of the model amplitudes $c_x$ and $c_y$ according to

$$d^2 = \left\langle \left( T^j_{\Delta,\Delta} + c_x m^i_x + c_y m^i_y \right)^2 \right\rangle_{\Lambda,j}.$$  \hspace{1cm} (7.26)

The optimization is performed by taking the derivatives with respect to each parameter:

$$\frac{\partial d^2}{\partial c_x} = \frac{\partial}{\partial c_x} \left\langle \left( T^j_{\Delta,\Delta} + c_x m^i_x + c_y m^i_y \right)^2 \right\rangle_{\Lambda,j} = 0, \hspace{1cm} (7.27)$$

$$\frac{\partial d^2}{\partial c_y} = \frac{\partial}{\partial c_y} \left\langle \left( T^j_{\Delta,\Delta} + c_x m^i_x + c_y m^i_y \right)^2 \right\rangle_{\Lambda,j} = 0, \hspace{1cm} (7.28)$$

from which we get the following system of equations:

$$-c_x \left\langle (m^i_x)^2 \right\rangle_{\Lambda} = \left\langle m^i_x \left( T^j_{\Delta,\Delta} + c_y m^i_y \right) \right\rangle_{\Lambda,j}, \hspace{1cm} (7.29)$$

$$-c_y \left\langle (m^i_y)^2 \right\rangle_{\Lambda} = \left\langle m^i_y \left( T^j_{\Delta,\Delta} + c_x m^i_x \right) \right\rangle_{\Lambda,j} \hspace{1cm} (7.30)$$

One finally obtains the rules for computing the model parameters:

$$c_x = \frac{\left\langle m_x T_{\Delta,\Delta} \right\rangle_{\Lambda} \left\langle m_y^2 \right\rangle_{\Lambda} - \left\langle m_y T_{\Delta,\Delta} \right\rangle_{\Lambda} \left\langle m_y m_x \right\rangle_{\Lambda}}{\left\langle m_x m_y \right\rangle_{\Lambda}^2 - \left\langle m_x^2 \right\rangle_{\Lambda} \left\langle m_y^2 \right\rangle_{\Lambda}}, \hspace{1cm} (7.31)$$

$$c_y = \frac{\left\langle m_y T_{\Delta,\Delta} \right\rangle_{\Lambda} \left\langle m_x^2 \right\rangle_{\Lambda} - \left\langle m_x T_{\Delta,\Delta} \right\rangle_{\Lambda} \left\langle m_x m_y \right\rangle_{\Lambda}}{\left\langle m_x m_y \right\rangle_{\Lambda}^2 - \left\langle m_x^2 \right\rangle_{\Lambda} \left\langle m_y^2 \right\rangle_{\Lambda}} \hspace{1cm} (7.32)$$

Thus, these two coefficients can be computed dynamically during a numerical simulation from Eqs. (7.31) and (7.32).

Finally, the dissipative effect of the model on free energy is guaranteed by setting to zero any negative coefficient value:

$$\text{If} \quad c_x < 0 \Rightarrow c_x = 0, \hspace{1cm} (7.33)$$

$$\text{If} \quad c_y < 0 \Rightarrow c_y = 0. \hspace{1cm} (7.34)$$

7.3 Numerical results: Cyclone Base Case

In this section we present numerical results obtained by means of the dynamic procedure with the GENE code. The set of parameters corresponds to the Cyclone Base Case (CBC) \[40\] used for studying Ion Temperature Gradient (ITG)

\[1\]For the sake of clarity, the species dependence $j$ is omitted in their respective terms.
7. DYNAMIC PROCEDURE FOR GYROLES

driven turbulence. Moreover, a perpendicular grid of $N_x \times N_y = 128 \times 64$ is used for the DNS. This grid has been used both with and without a LES model, and the results obtained have not been affected, indicating that the simulation is well resolved. On the other hand, a minimal perpendicular grid for GyroLES should be $N_x \times N_y = 48 \times 32$, allowing the dynamic procedure to work. Indeed, the use of the latter involves the introduction (in the LES domain $\bar{\Delta}$) of a test filter corresponding to a more filtered grid, $\Delta > \bar{\Delta}$. However, it is necessary for the dynamic procedure that the range of scales between the filters belongs to the gyrokinetic inertial range, so that the model coefficients have the same values in the two domains. This sets the minimum resolution for the LES.

Here we employ a test filter width which corresponds to the half of the LES domain: $\Delta_x = 2\bar{\Delta}_x$, $\Delta_y = 2\bar{\Delta}_x$. This means that the optimization in the dynamic procedure is related to a sub-grid term $T_{3,\Delta}$ defined by 24 $k_x$ modes and 16 $k_y$ modes: $\hat{N}_x \times \hat{N}_y = 24 \times 16$. The parameters given in Eqs. (7.31) and (7.32) are computed at each time step of the simulation. The parallel and velocity grids are kept fixed at $N_z = 32$, $N_{v||} = 64$, and $N_\mu = 8$. It is understood that the quantities showing in the following are averaged during the quasi stationary turbulent state over sufficiently long time windows. The model order is chosen to be $n = 4$, leading to

$$M_4 := - \left( c_x \bar{\Delta}^{13/3} k_x^4 + c_y \bar{\Delta}^{13/3} k_y^4 \right) \bar{h}_{k_3}. \quad (7.35)$$

For comparison, we also show simulations without any model (LES M0), with a perpendicular grid identical to the LES M4 one.

The free energy injection spectra from DNS, GyroLES, and a simulation without a model are shown in Fig. 7.3. The $k_x$ spectra for all three cases are found to exhibit a surprisingly good level of agreement, but the $k_y$ spectra illustrate

![Figure 7.3: Free energy injection spectra $G^{k_x}$ (left), $G^{k_y}$ (right) for the fourth-order model (M4) at reduced resolution, compared with a DNS and the case without a model (M0). The free energy injection is given in units of $n_0eT_0v_0T_i/R(\rho_s/R)^2$.](image-url)
that the use of a LES model diminishes the accumulation at the smallest scales, improving the agreement at the largest scales with the DNS.

The free energy spectra is shown in Fig. 7.4. The GyroLES clearly prevents the accumulation of free energy at the smallest scales. However, there still exists an overestimation of the free energy at the largest scales when compared with the DNS.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7.4}
\caption{Free energy spectra $E^{k_x}$ (left), $E^{k_y}$ (right) for the fourth order model (M4) at reduced resolution, compared with a DNS and the case without a model (M0). The free energy is given in units of $n_0 e T_0 \rho_s / R^2$.}
\end{figure}

Since the LES spectra are truncated with respect to the DNS ones, estimates for the neglected parts of the spectra are required for computing global values of the free energy and the free energy injection. Such estimates are provided via a power law regression of the spectra method introduced in the previous chapter and in Ref. [51]. The estimate from the GyroLES run yields $E^{M4} = 1.49 E^{DNS}$, while for the case without a model (M0), one obtains $E^{M0} = 2.36 E^{DNS}$. The free energy injection term from DNS and LES are in very good agreement, $G^{M4} = 1.06 G^{DNS}$. In the case without a model, one finds $G^{M0} = 1.20 G^{DNS}$ due to an overestimate at the smallest scales. The mean values of the coefficients $c_x$ and $c_y$ computed dynamically are $c_x = 0.0140$, $c_y = 0.0212$.

### 7.4 Computational gain

In order to optimize the free parameter of the model during the course of a GyroLES, we need to evaluate Eqs. (7.31) and (7.32) at every time step. Obviously, this requires additional CPU time when one compares with the case of LES without the dynamic procedure. However, in terms of computational cost, the dynamic approach still saves a factor of 20, requiring only about 250 CPU-hours per single run. This allows for the possibility to perform nonlinear gyrokinetic simulations on any modest cluster with relatively little effort.
7. DYNAMIC PROCEDURE FOR GYROLES

7.5 Robustness while varying the logarithmic temperature gradient

As we commented in the previous chapter, the logarithmic temperature gradient \( \omega_{T1} \) is a key parameter for ITG turbulence, given that the equilibrium temperature gradient acts as a source of free energy for the system. In the following, the robustness of the LES approach is tested for two values of the temperature gradient which differ from the CBC standard value. They correspond to a weakly driven turbulence case \( (\omega_{T1} = 6.0) \) and to a strongly driven turbulence case \( (\omega_{T1} = 8.0) \) as in Chapter 6. Furthermore, for the sake of clarity, all further comparisons will focus on the spectra \( \mathcal{E}^{ky} \) and \( \mathcal{G}^{ky} \) which have been found to be the most sensitive.

The case of weakly driven ITG turbulence is shown in Fig. 7.5. The M4 model yields a very reasonable agreement with the DNS regarding both the free energy spectrum \( \mathcal{E}^{ky} \) and the free energy injection spectrum \( \mathcal{G}^{ky} \). The total values \( \mathcal{E}^{M4} = 0.99 \mathcal{E}^{DNS} \) and \( \mathcal{G}^{M4} = 0.75 \mathcal{G}^{DNS} \) are also in good agreement. Without a model, one obtains \( \mathcal{E}^{M0} = 1.79 \mathcal{E}^{DNS} \) and \( \mathcal{G}^{M0} = 1.04 \mathcal{G}^{DNS} \). However, the latter result is accidental. It results from a compensation between an underestimation at large scales and an overestimation at small ones.

![Figure 7.5: Wavenumber spectra \( \mathcal{E}^{ky} \) (left) and \( \mathcal{G}^{ky} \) (right): Comparison between DNS and LES for the case of weakly driven ITG turbulence at \( \omega_{T1} = 6.0 \). The free energy is given in units of \( n_0 e T_0 e T_{ij}/R \) and the free energy injection is given in units of \( n_0 e T_{ij}/\rho_s R \).](image)

Fig. 7.6 displays the results for the case of strongly driven ITG turbulence. The LES is found to systematically overestimate the DNS free energy spectrum \( \mathcal{E}^{ky} \), while the prediction of the free energy injection spectrum \( \mathcal{G}^{ky} \) is in reasonable agreement. One finds \( \mathcal{E}^{M4} = 1.67 \mathcal{E}^{DNS} \) and \( \mathcal{G}^{M4} = 1.14 \mathcal{G}^{DNS} \), whereas the values exhibit a substantial disagreement without a model, leading to \( \mathcal{E}^{M0} = 3.00 \mathcal{E}^{DNS} \) and \( \mathcal{G}^{M0} = 1.42 \mathcal{G}^{DNS} \). The model amplitudes \( c_x \) and \( c_y \) computed dynamically are found to be quite robust when varying the temperature gradient. The mean...
7.5 Robustness while varying the logarithmic temperature gradient

Figure 7.6: Wavenumber spectra $\mathcal{E}^{k_y}$ (left) and $\mathcal{G}^{k_y}$ (right): Comparison between DNS and LES for the case of strongly driven ITG turbulence at $\omega_T = 8.0$. The free energy is given in units of $n_0eT_0(\rho_s/R)^2$ and the free energy injection is given in units of $n_0eTv_T_i(R(\rho_s/R)^2$.

values are $c_x = 0.0155$, $c_y = 0.0179$ in the weakly driven case and $c_x = 0.0140$, $c_y = 0.0219$ for the strongly driven case.

In summary, the LES model leads to a far better agreement with the DNS than the runs without a model. As far as the free energy injection term levels are concerned, the relative error with respect to the DNS is acceptable, amounting to less than 30% in all the three cases considered. See Table 7.1 for a result summary.

<table>
<thead>
<tr>
<th>$\omega_T$</th>
<th>$\mathcal{E}^{M0}$</th>
<th>$\mathcal{E}^{DNS}$</th>
<th>$\mathcal{G}^{M0}$</th>
<th>$\mathcal{G}^{DNS}$</th>
<th>$c_x$</th>
<th>$c_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>1.79 $\mathcal{E}^{DNS}$</td>
<td>0.99 $\mathcal{E}^{DNS}$</td>
<td>1.04 $\mathcal{G}^{DNS}$</td>
<td>0.75 $\mathcal{G}^{DNS}$</td>
<td>0.0155</td>
<td>0.0179</td>
</tr>
<tr>
<td>6.96 (CBC)</td>
<td>2.36 $\mathcal{E}^{DNS}$</td>
<td>1.49 $\mathcal{E}^{DNS}$</td>
<td>1.20 $\mathcal{G}^{DNS}$</td>
<td>1.06 $\mathcal{G}^{DNS}$</td>
<td>0.0140</td>
<td>0.0212</td>
</tr>
<tr>
<td>8</td>
<td>3.00 $\mathcal{E}^{DNS}$</td>
<td>1.67 $\mathcal{E}^{DNS}$</td>
<td>1.42 $\mathcal{G}^{DNS}$</td>
<td>1.14 $\mathcal{G}^{DNS}$</td>
<td>0.0140</td>
<td>0.0219</td>
</tr>
</tbody>
</table>

Table 7.1: Comparisons of a LES and a no model LES respect to the DNS, for the free energy $\mathcal{E}$ and the free energy injection $\mathcal{G}$ terms for $\omega_T = 6, 6.96, 8$.  

119
Next, we would like to investigate the robustness of the LES approach with respect to variations of the magnetic shear $\hat{s}$. The effects of the latter on plasma turbulence have been the subject of numerous experimental [32, 53, 54, 55, 56], theoretical [57], as well as numerical [58, 59, 60, 61] studies. In this context, it was also found that negative magnetic shear can help to improve the plasma confinement in a tokamak by decreasing the level of turbulence. Apart from the CBC case, three highly resolved DNS runs have been performed, corresponding to reversed ($\hat{s} = -0.4$), low ($\hat{s} = 0.2$), and high ($\hat{s} = 1.4$) magnetic shear cases, compared to the CBC standard value ($\hat{s} = 0.796$). In the case of reversed shear, the free energy and free energy injection spectra peak at a slightly higher $k_y$ value ($k_y\rho_i \approx 0.3$ compared to $k_y\rho_i \approx 0.2$ for CBC), as shown in Fig. 7.7. The total free energy is very small compared to the CBC, indicating a low level of turbulence. This effect has already been observed in a previous numerical study based on the spectral heat flux [59]. The LES offers a satisfying agreement with the DNS spectra, except for an underestimation of the free energy injection peak. The total free energy agrees reasonably well with the value, $E_{M4} = 1.35 E_{DNS}$, while $E_{M0} = 2.12 E_{DNS}$. Considering the free energy injection term, one finds the same trend: $G_{M4} = 1.04 G_{DNS}$ and $G_{M0} = 1.31 G_{DNS}$.

Figure 7.7: Wavenumber spectra $\mathcal{E}_y$ (left) and $\mathcal{G}_y$ (right): Comparison between DNS and LES for the case of reversed shear ($\hat{s} = -0.4$). The free energy is given in units of $n_0eT_0(\rho_s/R)^2$ and the free energy injection is given in units of $n_0eT_0\nu T_i/R(\rho_s/R)^2$.

In Fig. 7.8 the results for the case of low shear ($\hat{s} = 0.2$) are presented. Here, the turbulence level lies between those of the reversed shear and CBC cases. The free energy and free energy injection spectra, $\mathcal{E}_y$ and $\mathcal{G}_y$, are fairly extended, up to $k_y\rho_i \approx 0.4$. The use of a LES model prevents the accumulation of free energy.
7.6 Robustness while varying the magnetic shear

energy at small scales. The LES model also moderates the appearance of large-scale structures although it cannot suppress them completely (at small non-zero $k_y$). The total free energy obtained by the LES model deviates from the DNS value, $E_{M4} = 1.78 E_{DNS}$, but it is much better than the estimate obtained without a model, $E_{M0} = 2.89 E_{DNS}$. The disagreement regarding the free energy injection terms is again found to be more acceptable, according to $G_{M4} = 1.17 G_{DNS}$ and $G_{M0} = 1.56 G_{DNS}$.

Figure 7.8: Wavenumber spectra $\mathcal{E}^{k_y}$ (left) and $\mathcal{G}^{k_y}$ (right): Comparison between DNS and LES for the case of low shear ($\hat{s} = 0.2$). The free energy is given in units of $n_0 e T_0 (\rho_s/R)^2$ and the free energy injection is given in units of $n_0 e T_0 v_T (\rho_s/R)^2$.

Finally, the results for the case of high shear ($\hat{s} = 1.4$) are displayed in Fig. 7.9. The turbulence level is slightly lower than for CBC parameters and the free energy and free energy injection spectra are very similar to the CBC ones. A very satisfying agreement between LES and DNS is found regarding both the total free energy ($E_{M4} = 1.23 E_{DNS}$) and the total free energy injection term ($G_{M4} = 0.96 G_{DNS}$). Again, without using a model the accumulation of free energy at small scales leads to larger differences: $E_{M0} = 1.98 E_{DNS}$ and $G_{M0} = 1.15 G_{DNS}$.

In all three cases, an important consequence of the use of a LES model is that it prevents the accumulation of free energy at small scales. In addition, for low magnetic shear, unphysical features at small $k_y$ are strongly reduced. Although not shown explicitly in the figures, the $k_x$ spectra of free energy $\mathcal{E}^{k_x}$ and free energy injection $\mathcal{G}^{k_x}$ are always in good agreement. One notes that the total free energy appears to be a very sensitive diagnostic. The presence of a model considerably enhances the agreement between DNS and GyroLES runs. The total free energy injection term is estimated with an encouraging relative error of less than 20% for all cases.

In contrast to the findings of the temperature gradient scan, the LES model amplitudes exhibit substantial variations for changes in the magnetic shear. In particular, the value of $c_x$ is found to be close to zero in the reversed shear case ($c_x \approx 5 \times 10^{-5}$) as well as in the low shear case ($c_x \approx 2 \times 10^{-3}$). Meanwhile, it departs from the CBC value ($c_x = 0.0140$) only moderately in the high shear case.
7. DYNAMIC PROCEDURE FOR GYROLES

Figure 7.9: Wavenumber spectra $\mathcal{E}^{k_y}$ (left) and $G^{k_y}$ (right): Comparison between DNS and LES for the case of high shear ($\hat{s} = 1.4$). The free energy is given in units of $n_0eT_0(\rho_s/R)^2$ and the free energy injection is given in units of $n_0eT_i(\rho_s/R)^2$.

Figure 7.10: Model amplitude $c_x$ as a function of time for different values of the magnetic shear $\hat{s}$.

($c_x = 0.0102$). The time traces of $c_x$ are shown in Fig. 7.10. On the other hand, the $c_y$ values do not vary much; one obtains $c_y = 0.0192$, $c_y = 0.0223$, $c_y = 0.0212$, and $c_y = 0.0185$ for the four values of magnetic shear (in increasing order). These results are a reflection of the effect of the magnetic shear on the turbulence which includes the twisting of the perpendicular eddies along the magnetic field. Eddy twisting leads the turbulence to distribute up to higher $k_x$ as increasing the positive magnetic shear [62]. Therefore, $c_x$ has to increase with the magnetic shear in order to dissipate an increasing amount of free energy. A summary of the results is given in Table 7.2.
7.7 Conclusions

In the present chapter the dynamic procedure has been applied to gyrokinetic turbulence as described by the GENE code. This approach provides an automatic calibration of the free parameters associated with dissipative GyroLES models. The dynamic procedure has been found to be robust in a wide parameter range of the logarithmic temperature gradient and the magnetic shear.

Comparisons between DNS and GyroLES have been based on free energy and free energy injection spectra, $E_k$ and $G_k$. Generally, the use of a LES model prevents the accumulation of free energy at small scales. While the differences regarding the total free energy can exceed 50%, simulations without a LES model are even much more inaccurate, exhibiting relative errors up to 200%. Moreover, when considering the total free energy injection term, the GyroLES results are really encouraging, with relative errors below about 20%. In terms of computational cost, the GyroLES approach has been found to be around 20 times faster than the DNS. These results show that GyroLES is a good candidate to reduce the computational cost of gyrokinetic simulations.

<table>
<thead>
<tr>
<th>$\hat{s}$</th>
<th>$E^M_0$</th>
<th>$G^M_0$</th>
<th>$x$ approximate value</th>
<th>$E^M_4$</th>
<th>$G^M_4$</th>
<th>$y$ approximate value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-0.4$</td>
<td>$2.12E_{DNS}$</td>
<td>$1.31G_{DNS}$</td>
<td>$5 \times 10^{-5}$</td>
<td>$1.35E_{DNS}$</td>
<td>$1.04G_{DNS}$</td>
<td>$0.0192$</td>
</tr>
<tr>
<td>$0.2$</td>
<td>$2.89E_{DNS}$</td>
<td>$1.56G_{DNS}$</td>
<td>$2 \times 10^{-3}$</td>
<td>$1.78E_{DNS}$</td>
<td>$1.17G_{DNS}$</td>
<td>$0.0223$</td>
</tr>
<tr>
<td>$0.796$</td>
<td>$2.36E_{DNS}$</td>
<td>$1.20G_{DNS}$</td>
<td>$0.0140$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1.4$</td>
<td>$1.98E_{DNS}$</td>
<td>$1.15G_{DNS}$</td>
<td>$0.0102$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(CBC)</td>
<td>$1.49E_{DNS}$</td>
<td>$1.06G_{DNS}$</td>
<td>$0.0212$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1.4$</td>
<td>$1.23E_{DNS}$</td>
<td>$0.96G_{DNS}$</td>
<td>$0.0185$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 7.2: Comparisons of a LES and a no model LES respect to the DNS, for the free energy $E$ and the free energy injection $G$ terms for $\hat{s} = -0.4, 0.2, 0.796, 1.4$. 

7.7 Conclusions

In the present chapter the dynamic procedure has been applied to gyrokinetic turbulence as described by the GENE code. This approach provides an automatic calibration of the free parameters associated with dissipative GyroLES models. The dynamic procedure has been found to be robust in a wide parameter range of the logarithmic temperature gradient and the magnetic shear.

Comparisons between DNS and GyroLES have been based on free energy and free energy injection spectra, $E_k$ and $G_k$. Generally, the use of a LES model prevents the accumulation of free energy at small scales. While the differences regarding the total free energy can exceed 50%, simulations without a LES model are even much more inaccurate, exhibiting relative errors up to 200%. Moreover, when considering the total free energy injection term, the GyroLES results are really encouraging, with relative errors below about 20%. In terms of computational cost, the GyroLES approach has been found to be around 20 times faster than the DNS. These results show that GyroLES is a good candidate to reduce the computational cost of gyrokinetic simulations.
7. DYNAMIC PROCEDURE FOR GYROLES
Chapter 8

Conclusions

In this work we have developed the concept of Gyrokinetic Large Eddy Simulations (GyroLES) in computational plasma physics. GyroLES is an extension of the LES technique used in fluid turbulence to gyrokinetic simulations of tokamak plasmas. We have implemented this technique in the Gyrokinetic Electromagnetic Numerical Experiment (Gene) code. Below, a short overview of the main results of this thesis is given. More detailed summaries can be found at the end of the respective chapters. Furthermore, an outlook on possible future research topics is also given.

Brief description of the GyroLES approach

The GyroLES methodology consists of filtering out the small turbulent scales from the gyrokinetic equation. The benefit of this approach is that the filtered equation can be solved on a smaller computational grid and, consequently, the simulation cost is significantly reduced. In practice, the filtering of the gyrokinetic equation has been limited to the spatial directions perpendicular to the magnetic field lines. These directions normally require large numbers of grid points. Hence, reducing the resolution in the directions perpendicular to the magnetic lines is extremely effective in reducing numerical costs. Since Gene uses a Fourier representation in these perpendicular directions, filtering the small scales of turbulence is equivalent to setting to zero the Fourier modes corresponding to the highest perpendicular wave vectors.

Although the transport properties are essentially captured by the large scales, the small scales are considered important to get well-converged transport levels. Therefore, the filtered scales play an important role in the dynamics of the system and their impact on the large scale has to be taken into account through a model. These small scales are usually considered to have a universal behavior by opposition to the largest ones that are mostly problem dependent. This property suggests that sub-grid models for the small turbulent scales should not be too much problem dependent, i.e. that the model should be independent on the mechanisms that drive turbulence. As in fluid mechanics, sub-grid models for the small scales are based on the physics of the cascade process for the nonlinear invariant quantities. In gyrokinetics, the nonlinear invariant is the free energy (mixing of entropy and electromagnetic energy).
8. CONCLUSIONS

Free energy cascade in gyrokinetic turbulence

In Chapter 4, the free energy transfers has been analyzed for the case of ion temperature gradient (ITG) driven turbulence. It was found that the free energy dynamics shares most of the properties with the kinetic energy transfers measured in Navier-Stokes turbulence. First, it exhibits a cascade of free energy from the largest scales dominated by the background temperature gradient to the smallest scales at which most of the dissipation takes places. Moreover, this cascade process appears to be essentially local in wavenumber space. The nonlinear exchanges of free energy are dominated by mode-to-mode transfer between wave vectors with similar amplitudes. Finally, a limited self-similarity range has been identified in which the free energy exchanges only depends on the ratios of the wave vector amplitudes and not on the absolute value of these wave vectors.

Free energy studies for gyrokinetics

In Chapter 5, we have studied further the free energy dynamics by investigating in detail components of the free energy for ITG driven turbulence. We found that the entropy part was systematically bigger than the electrostatic term for all times. The reason was found in their balance equations. Only the entropy contribution was driven directly, the electrostatic energy could only grow by internal changes with the entropy. Here, the entropy-electrostatic term transfers channels were represented by the linear parallel and curvature terms. However, these exchanges were found to be very small as a consequence of the almost perfect balance between the curvature and parallel terms.

Extension of the LES approach for gyrokinetics

The first GyroLES have been performed in Chapter 6. By means of the previous work done by Smith and Hammett [49], free energy based diagnostics and the results obtained in the previous chapters, a perpendicular hyperdiffusion model was proposed. The free parameter of the model was calibrated by a trial and error process for the Cyclone Base Case parameters. An optimal value for the parameter was found and as a consequence, we found that GyroLES allow to gain a factor of 30 in terms of computational time. Finally, this model was tested for different turbulent drives by varying the temperature gradient. We found that the model parameter must change accordingly: it must increase when the turbulence drive increases and vice-versa. Therefore, we concluded that in order to make GyroLES useful, it would be convenient to apply a method that calibrates automatically the amplitude of the model.
Dynamic procedure for GyroLES

For this reason, in Chapter 7, a dynamic procedure have been implemented in the GENE code. This method allows for a dynamic optimization of the GyroLES model by setting its amplitude. In this case, we used a more flexible model that took into account the turbulence anisotropy in the perpendicular directions. Here, different amplitudes values where considered along \( k_x \) and \( k_y \). With this model, comparisons between GyroLES and Direct Numerical Simulations (DNS) were performed. They were based on the free energy and the free energy injection spectra for different values of the ion temperature gradient and magnetic shear. We found the relative error below 20% for the energy injection term and below 50% for the free energy spectra. On contrast, relative errors up to 200% were found when no model was used. In addition, the dynamic approach saves a factor of 20 in terms of computational cost. These results were really encouraging and showed that GyroLES is a good candidate to reduce the computational cost of gyrokinetic simulations.

Outlook

Finally, current and future research lines include:

- Free energy studies of collisionless trapped electron mode (TEM) turbulence:
  
  So far, GyroLES approach has been tested for ion temperature gradient (ITG) driven turbulence where adiabatic electrons were considered. Obviously, future GyroLES will have to take kinetic and electrons and their contribution to the overall free energy into account. The same methodology used in Chapter 4 to study ITG driven turbulence can be extended to the study of trapped electron modes. Here, the free energy exchanges between the different particle channels (electrons and ions) could be analyzed.

- The study of the locality and universality of gyrokinetic turbulence:
  
  In Chapter 4 we showed that the exchange of free energy takes place between similar scales. However, although the energy exchanges are local, the fundamental question regarding the locality of the interactions has never been addressed so far in GK turbulence. Preliminary results of this topic can be found in 63.

- Dynamic procedure with scale dependent coefficient:
  
  The dynamic procedure introduced in Chapter 7 is based on the scale invariant assumption that the model coefficient is the same at the LES grid and test filter levels. However, this condition is not entirely satisfied in our case due to the fact that the dissipation term was active at all cases. For many applications in fluid dynamics, the scale invariant assumption was also not met. Meneveau and Lund proposed different dynamic models.
8. CONCLUSIONS

which consider a scale dependent coefficient, see Ref. [64]. The extension of these dynamic models for gyrokinetics is currently under study.

- A model amplitude not constant in phase space:
  One could also consider a model whose amplitude depends on the \( z, v_z, \mu \), species coordinates and time. For instance, for more than two kinetic species (like the TEM case), one could expect that the model dissipation should be different for both species.

**Future applications of GyroLES**

These studies would help to test and develop new models for GyroLES. It is expected that GyroLES will also be of great benefit in this wider context. Therefore, GyroLES could be used:

- to perform large parameter scans of gyrokinetic turbulence. These scans could be used to efficiently couple turbulence to transport codes, see Ref. [65].

- as a predictive tool to explore runs that are not accessible to DNS. For instance, one could reproduce the results by T. Görler [47] using GyroLES with a realistic ion/electron mass ratio, which is an extremely expensive run if one wants to perform it without the used of GyroLES.
Appendix A

**Generic derivation of a Poisson bracket integration**

Let us perform in a very general manner an integration of a Poisson bracket, similarly to the application of the free energy operator,

\[
\int_a^b f[f, g]_{ab} \, da \, db = \int_a^b \left[ f \frac{\partial f}{\partial a} \frac{\partial g}{\partial b} - f \frac{\partial f}{\partial b} \frac{\partial g}{\partial a} \right] \, da \, db. \tag{A.1}
\]

We consider now the first term

\[
\int_a^b \int_b^a f \frac{\partial f}{\partial a} \frac{\partial g}{\partial b} \, da \, db = \frac{1}{2} \int_a^b \int_b^a \frac{\partial f^2}{\partial a} \frac{\partial g}{\partial b} \, da \, db, \tag{A.2}
\]

on which we perform an integration by parts with respect to \( a \),

\[
\frac{1}{2} \int_b^a \left( f^2 \frac{\partial g}{\partial b} \right)_{\text{a boundaries}} - \int_a^b f^2 \frac{\partial^2 g}{\partial a \partial b} \, da \, db. \tag{A.3}
\]

The second term,

\[
- \int_a^b \int_b^a f \frac{\partial f}{\partial b} \frac{\partial g}{\partial a} \, da \, db = -\frac{1}{2} \int_a^b \int_b^a \frac{\partial f^2}{\partial b} \frac{\partial g}{\partial a} \, da \, db, \tag{A.4}
\]

easily shows the following shape if performing a similar integration by parts with respect to \( b \),

\[
-\frac{1}{2} \int_a^b \left( f^2 \frac{\partial g}{\partial a} \right)_{\text{b boundaries}} - \int_b^a f^2 \frac{\partial^2 g}{\partial a \partial b} \, da \, db. \tag{A.5}
\]

We have indeed cancellation,

\[
-\frac{1}{2} \int_a^b \int_b^a f^2 \frac{\partial^2 g}{\partial a \partial b} \, da \, db + \frac{1}{2} \int_a^b \int_b^a f^2 \frac{\partial^2 g}{\partial a \partial b} \, da \, db = 0, \tag{A.6}
\]

upon fulfillment of the following condition,

\[
\frac{1}{2} \int_b^a \left( f^2 \frac{\partial g}{\partial b} \right)_{\text{a boundaries}} \, db - \frac{1}{2} \int_a^b \left( f^2 \frac{\partial g}{\partial a} \right)_{\text{b boundaries}} \, da = 0. \tag{A.7}
\]
A. GENERIC DERIVATION OF A POISSON BRACKET INTEGRATION
In this section, we will show that the definition of the free energy given for kinetic systems in (4.7):

\[ E = -T_0 S + \mathcal{E}_E + \mathcal{E}_M = \sum_j T_{0j} \int d^3x d^3v \frac{\tilde{f}_{ij}^2}{2 F_{0j}} + \int d^3x \frac{E^2}{8\pi} + \int d^3x \frac{B^2}{8\pi}. \]  

(B.1)

is equivalent the one given by the sum of Eqs. (4.47), (4.48) and (4.49).

This can be done by expressing the particle distribution function \( \tilde{f}_{ij} \) in terms of the gyro-center distribution function \( f_{1j} \), by expressing the electromagnetic fields in terms of their potentials \( \phi_1 \) and \( A_{1\parallel} \) and by normalizing the resulting equations in the units of the GENE code.

Regarding the part of the gyro-center distribution function, we need to perform similar operations as those done in Sec 2.5 to obtain the gyrokinetic field equations. We need to express the gyro-center distribution function \( f_{1j} \) in terms of the guiding center distribution function \( F_{1j} \) by the use of the pull-back operator \( T \). In a second step we go from guiding-center space to particle space. For instance, the application of the pull-back operator to the gyrokinetic distribution function \( f_{1j} \) and its square gives:

\[ F_{1j} = T f_{1j} = f_{1j} - q_j \frac{F_{0j}}{T_{0j}} \tilde{\phi}_1 \Rightarrow F_{1j}^2 = \frac{1}{T_{0j}} \frac{T_{0j}^2}{8\pi} \tilde{\phi}_1 \tilde{\phi}_1 - \frac{1}{T_{0j}} \frac{T_{0j}^2}{8\pi} \tilde{\phi}_1 \tilde{\phi}_1. \]
Therefore, the first term in Eq. (B.1) is expressed as:

\[-T_0 S = \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{F_{1j}^2}{2F_{0j}}\]

\[= \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{(T_{1j})^2}{2F_{0j}}\]

\[= \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{f_{1j}^2}{2F_{0j}}\]

\[+ \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{q_j^2}{2T_{0j}^2} \theta_1^2\]

\[ - \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{q_j}{T_{0j}} f_{1j} \theta_1. \quad (B.2)\]

The first term in Eq. (B.2) gives:

\[\sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || d^3X \delta^3(X + \rho_j a(\theta) - x) \frac{f_{1j}^2}{2F_{0j}}\]

\[= \sum_j \int d^3x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || \frac{1}{2F_{0j}} f_{1j}^2(x - \rho_j a(\theta)). \quad (B.3)\]

In the local flux-tube approximation, we can use the Fourier representation in the direction perpendicular to the magnetic field \((k = k_x, k_y)\). In this case, a spatial average for the free energy is also considered. As a result, we have:

\[= \sum_j \int \frac{1}{J(z)dx dy dz} \int J(z) d^2x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || \frac{1}{2F_{0j}} \sum_{k,k'} f_{1kj} f_{1k'j} e^{i(k+k') \times} e^{-i(k+k') \rho_j a(\theta)}\]

\[= \sum_j \int \frac{1}{L_x L_y} \int d^2x T_{0j} \frac{B_0}{m_j} \int d\theta d\mu dv || \frac{1}{2F_{0j}} \sum_{k,k'} f_{1kj} f_{1k'j} e^{i(k+k') \times} e^{-i(k+k') \rho_j a(\theta)}\]

\[= \sum_j \int \frac{2\pi B_0}{m_j} \int d\mu dv || \frac{1}{2F_{0j}} \sum_{k,k'} f_{1kj} f_{1k'j} e^{-i(k+k') \rho_j a(\theta)}\]

\[= \sum_j \sum_k \int \frac{2\pi B_0}{m_j} \int d\mu dv || \frac{|f_{1kj}|^2}{2F_{0j}}. \quad (B.4)\]

Here, the definition of the \(\delta\)-Dirac for the perpendicular plane \(d^2x = dx dy\) has been used: \(\delta_{k+k'} = \int d^2x e^{i(k+k') \times} / L_x L_y\).

In the normalized units of the GENE code, the above equation reads:

\[\sum_j \sum_k \int \frac{\pi B_0 n_{0j} T_{0j}}{2F_{0j}} \int d\mu dv || \frac{|f_{1kj}|^2}{2F_{0j}}. \quad (B.5)\]
It is given in $n_{\text{ref}} T_{\text{ref}} \rho_{\text{ref}}^2 / L_{\text{ref}}^2$ units.

The second term in Eq. (B.2) has the following contributions:

$$\sum_j \int d^3x \frac{B_0}{m_j} \int d\theta d\mu dv_l \int d^3x \frac{B_0}{m_j} q_j^2 \frac{F_{0j}}{2 T_{0j}} \phi_1^2$$

$$= \sum_j \int d^3x \frac{B_0}{m_j} \int d\theta d\mu dv_l \int d^3x \frac{B_0}{m_j} q_j^2 \frac{F_{0j}}{2 T_{0j}} (\phi_1 - \langle \phi_1 \rangle)^2$$

$$= \sum_j \int d^3x \frac{q_j^2}{2 T_{0j} m_j} \int d\theta d\mu dv_l \int d^3x \frac{q_j^2}{2 T_{0j} m_j} (\phi_1 - \langle \phi_1 \rangle)^2 F_{0j} (\phi_1^2 + \langle \phi_1 \rangle^2 - 2 \phi_1 \langle \phi_1 \rangle). \quad (B.6)$$

In the first contribution of Eq. (B.6), the term $\phi_1$ neither depends on the velocity variables nor on the guiding center coordinates. Therefore, it can be taken out from the guiding center integral:

$$\sum_j \int d^3x \frac{q_j^2}{2 T_{0j}} \frac{B_0}{m_j} \phi_1^2 \int d\theta d\mu dv_l \frac{d^3x}{m_j} \frac{B_0}{m_j} \phi_1^2 F_{0j}$$

$$= \sum_j \int d^3x \frac{q_j^2}{2 T_{0j} m_j} \phi_1^2 F_{0j}$$

$$= \sum_j \int d^3x \frac{q_j^2}{2 T_{0j}} \phi_1^2 n_{0j} = \sum_j \sum_k \left\langle \frac{q_j^2}{2 T_{0j}} n_{0j} \phi_{1k}^2 \right\rangle_z. \quad (B.7)$$

In addition, the following integral has been evaluated:

$$\int d\theta d\mu dv_l F_{0j} = \frac{m_j}{B_0} n_{0j}. \quad (B.8)$$

The second contribution of Eq. (B.6) gives:

$$\sum_j \int d^3x \frac{q_j^2}{2 T_{0j} m_j} \frac{B_0}{m_j} \int d\theta d\mu dv_l F_{0j} \langle \phi_1 (x - \rho_j a(\theta))^2 \rangle$$

$$= \sum_j \int \frac{1}{L_x L_y} d^2x \frac{q_j^2}{2 T_{0j} m_j} \frac{B_0}{m_j} \int d\theta d\mu dv_l F_{0j} \frac{1}{2\pi} \int d\theta' \sum_{k, k'} \phi_{1k} \phi_{1k'} e^{i(k + k')(x - \rho_j a(\theta) + \rho_j a(\theta'))} \right\rangle_z$$

$$= \sum_j \left\langle q_j^2 \frac{B_0}{2 T_{0j} m_j} \int d\theta d\mu dv_l F_{0j} \frac{1}{2\pi} \int d\theta' \sum_k |\phi_{1k}|^2 \right\rangle_z$$

$$= \sum_j \sum_k \left\langle q_j^2 \frac{B_0}{2 T_{0j} m_j} n_{0j} |\phi_{1k}|^2 \right\rangle_z. \quad (B.9)$$
The third contribution of Eq. (B.6) gives:

\[- \sum \int d^3x \frac{q_j^2}{T_{0j}} \frac{B_0}{m_j} \phi_1(\mathbf{x}) \int d\theta d\mu dv || F_{0j} \langle \phi_1(\mathbf{x} - \rho_j a(\theta)) \rangle\]

\[= - \sum \left\langle \frac{1}{L_x L_y} \int d^2x \frac{q_j^2}{T_{0j}} \frac{B_0}{m_j} \phi_{1k} e^{ik \cdot x} \int d\theta d\mu dv || F_{0j} \frac{1}{2\pi} \int d\theta' \sum_{k'} \phi_{1k'} e^{ik' \cdot (x - \rho_j a(\theta) + \rho_j a(\theta'))} \right\rangle_z \]

\[= - \sum \left\langle \frac{q_j^2 B_0}{T_{0j} m_j} \sum_{k} |\phi_{1k}|^2 \int d\theta d\mu dv || F_{0j} \frac{1}{2\pi} \int d\theta' e^{-ik \cdot (\rho_j a(\theta) + \rho_j a(\theta'))} \right\rangle_z \]

\[= - \sum \left\langle \frac{q_j^2}{T_{0j}} 2\pi B_0 \sum_{k} |\phi_{1k}|^2 \int d\mu dv || F_{0j} |J_{0kj}|^2 \right\rangle \]

\[= - \sum \sum_{k} \left\langle \frac{q_j^2}{T_{0j}} n_{0j}(b_j) |\phi_{1k}|^2 \right\rangle_z. \quad \text{(B.10)} \]

In addition to the definition of the Bessel function in Fourier space:

\[J_{0kj} = \frac{1}{2\pi} \int d\theta e^{ik \cdot \rho_j a(\theta)}, \quad \text{(B.11)} \]

the following integral has been also performed:

\[\int d\mu dv || F_{0j} |J_{0kj}|^2 = n_{0j} \frac{m_j}{2\pi B_0} \Gamma_0(b_j). \quad \text{(B.12)} \]

Grouping all the terms of Eq. (B.6) we obtain:

\[\sum \sum_{k} \left\langle \frac{q_j^2}{T_{0j}} n_{0j} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z. \quad \text{(B.13)} \]

Taking into account the normalized units of GENE. This yields:

\[\sum \sum_{k} \left\langle \frac{n_{0j} q_j^2}{2 T_{0j}} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z. \quad \text{(B.14)} \]

in \(n_{\text{ref}} T_{\text{ref}} \rho_{\text{ref}}^2 / L_{\text{ref}}^2\) units.

The third term in Eq. (B.2) has the following contributions:

\[- \sum \int d^3x \frac{B_0}{m_j} \int d\theta d\mu dv || d^3x \delta^3(\mathbf{x} + \rho_j a(\theta) - \mathbf{X}) \frac{q_j}{T_{0j}} f_{1j} \tilde{\phi}_1 \]

\[= - \sum \int d^3x \frac{B_0}{m_j} \int d\theta d\mu dv || d^3x \delta^3(\mathbf{x} + \rho_j a(\theta) - \mathbf{X}) f_{1j} (\phi_1 - \langle \phi_1 \rangle). \quad \text{(B.15)} \]
The first contribution of Eq. (B.15) gives:

$$- \sum_j \int d^3x \frac{B_0}{m_j} q_j \phi_1 \int d\theta \, d\mu \, dv f_{ij}(x - \rho_j a(\theta))$$

$$= - \sum_j \left\langle \int d^2x \, \frac{q_j}{L_x L_y} \frac{B_0}{m_j} \sum_k \phi_{1k} e^{ikx} \sum_{k'} \int d\theta \, d\mu \, dv f_{1k'j} e^{ik'(x - \rho_j a(\theta))} \right\rangle_z$$

$$= - \sum_j \left\langle \frac{B_0}{m_j} \sum_k \phi_{1k} \sum_{k'} \int d\theta \, d\mu \, dv f_{1k'j} \delta_{k+k'} e^{-ik\rho_j a(\theta)} \right\rangle_z$$

$$= - \sum_j \sum_k \left\langle \frac{2\pi B_0}{m_j} \phi_{1k} \int d\mu \, dv J_{0kj} f_{1-kj} \right\rangle_z. \quad (B.16)$$

The second contribution of Eq. (B.15) gives:

$$\sum_j \int d^3x \frac{B_0}{m_j} q_j \phi_1(x - \rho_j a(\theta)) f_{ij}(x - \rho_j a(\theta))$$

$$= \sum_j \left\langle \int d^2x \, \frac{q_j}{L_x L_y} \frac{B_0}{m_j} \int d\theta \, d\mu \, dv f_{ij} \frac{1}{2\pi} \int d\theta' \sum_{k,k'} \phi_{1k} e^{ik(x - \rho_j a(\theta) + \rho_j a(\theta'))} f_{1k'j} e^{ik'(x - \rho_j a(\theta))} \right\rangle_z$$

$$= \sum_j \left\langle \frac{B_0}{m_j} \sum_k \phi_{1k} \int d\theta \, d\mu \, dv f_{ij} \frac{1}{2\pi} \int d\theta' \sum_{k,k'} e^{ik(-\rho_j a(\theta) + \rho_j a(\theta'))} f_{1k'j} e^{-ik\rho_j a(\theta)} \delta_{k+k'} \right\rangle_z$$

$$= \sum_j \sum_k \left\langle \frac{2\pi B_0}{m_j} \phi_{1k} \int d\mu \, dv J_{0kj} f_{1-kj} \right\rangle_z. \quad (B.17)$$

Thus, both contribution in Eq. (B.15) cancel. Therefore, the first term in Eq. (B.1) gives:

$$- T S_0 = \sum_j \sum_k \left\langle \pi B_0 n_{0j} T_{0j} \int d\mu \, dv \left| \frac{f_{1kj}}{2F_{0j}} \right|^2 \right\rangle_z$$

$$+ \sum_j \sum_k \left\langle \frac{n_{0j} q_j^2}{2T_{0j}} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z. \quad (B.18)$$

The electromagnetic terms of Eq. (B.1)

$$\mathcal{E}_E = \int d^3x \frac{\mathbf{E}^2}{8\pi} \quad \text{and} \quad \mathcal{E}_M = \int d^3x \frac{\mathbf{B}^2}{8\pi}, \quad (B.19)$$
B. ON THE FREE ENERGY

can be expressed in terms of the potentials $\phi_1$ and $A_{1\parallel}$:

\[
E_E = \int \frac{d^3x}{8\pi} \mathbf{E}^2 = \int \frac{d^3x}{8\pi} \left(-\nabla \phi_1 \right)^2 = \sum_k \left\langle \frac{k_\perp^2 \phi_k^2}{8\pi} \right\rangle_z, \tag{B.20}
\]

\[
E_M = \int \frac{d^3x}{8\pi} \mathbf{B}^2 = \int \frac{d^3x}{8\pi} \left(\nabla \times \mathbf{A}\right)^2 = \sum_k \left\langle \frac{k_\perp^2 A_{1\parallel k}^2}{8\pi} \right\rangle_z. \tag{B.21}
\]

We can normalize them in terms of the GENE units $(n_{\text{ref}} T_{\text{ref}} \rho_{\text{ref}}^2 / L_{\text{ref}}^2)$:

\[
E_E = \sum_k \frac{1}{2} \lambda_D^2 k_\perp^2 \left\langle |\phi_{1k}|^2 \right\rangle_z \quad \text{and} \quad E_M = \sum_k \left\langle \frac{k_\perp^2}{\beta} A_{1\parallel k}^2 \right\rangle_z. \tag{B.22}
\]

In conclusion, the free energy expressed in GENE units reads:

\[
\mathcal{E} = \sum_j \sum_k \left\langle \pi B_0 n_{0j} T_{0j} \int d\mu \, d\nu \frac{|f_{1kj}|^2}{2F_{0j}} \right\rangle_z
+ \sum_j \sum_k \left\langle \frac{n_{0j} q_j^2}{2T_{0j}} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z
+ \sum_k \frac{1}{2} \lambda_D^2 k_\perp^2 \left\langle |\phi_{1k}|^2 \right\rangle_z
+ \sum_k \left\langle \frac{k_\perp^2}{\beta} A_{1\parallel k}^2 \right\rangle_z. \tag{B.23}
\]

Grouping the term that depends on $f$ in $\mathcal{E}_f$, the terms that depend on $\phi_1$ in $\mathcal{E}_\phi$ and the term that depends on $A_{1\parallel}$ in $\mathcal{E}_A$, we have:

\[
\mathcal{E} = \mathcal{E}_f + \mathcal{E}_\phi + \mathcal{E}_A, \tag{B.24}
\]

where the entropic term is defined as:

\[
\mathcal{E}_f = \sum_j \sum_k \left\langle \pi B_0 n_{0j} T_{0j} \int d\mu \, d\nu \frac{|f_{1kj}|^2}{2F_{0j}} \right\rangle_z, \tag{B.25}
\]

the electrostatic term is defined as

\[
\mathcal{E}_\phi = \sum_j \sum_k \left\langle \frac{n_{0j} q_j^2}{2T_{0j}} [1 - \Gamma_0(b_j)] |\phi_{1k}|^2 \right\rangle_z
+ \sum_k \frac{1}{2} \lambda_D^2 k_\perp^2 \left\langle |\phi_{1k}|^2 \right\rangle_z. \tag{B.26}
\]

and the magnetic energy term is defined as:

\[
\mathcal{E}_A = \left\langle \frac{k_\perp^2}{\beta} A_{1\parallel k}^2 \right\rangle_z. \tag{B.27}
\]

This is the expression of the free energy given by Eqs. (4.47), (4.48) and (4.49).
Appendix C

ON HYPERDIFFUSION AND ASSOCIATED FREE ENERGY

Two different functional dependencies of numerical dissipations are involved in Gene, both for the parallel (||) directions \( z \) or \( v_\parallel \),

\[
D_{\parallel}[f_{kj}] \propto \frac{\partial^4 f_{kj}}{\partial^4 ||}, \quad D_{\parallel}[h_{kj}] \propto \frac{\partial^4 h_{kj}}{\partial^4 ||}, \quad (C.1)
\]

and likewise for perpendicular (\( \perp \)) directions \( k_x, k_y \) or \( k_{\perp} \) which generally use a fourth order scheme:

\[
D_{\perp}[f_{kj}] \propto \frac{\partial^4 f_{kj}}{\partial^4 \perp}, \quad D_{\perp}[h_{kj}] \propto \frac{\partial^4 h_{kj}}{\partial^4 \perp}. \quad (C.2)
\]

It is of the greatest importance to ensure that in Gene, the numerical diffusion terms have a definite sign \cite{39}. Thus, with a negative constant prefactor, these terms will dissipate free energy. In order to analyze their sign, for simplicity, will be express the different hyperdiffusions shapes using the following notation:

\[
D_{\parallel/\perp}[f_{kj}/h_{kj}]. \quad (C.3)
\]

Taking that into account, we can define the associated free energy as

\[
D_{\parallel/\perp} := \Xi [D_{\parallel/\perp}[f_{kj}/h_{kj}]] + cc 
\]

\[
\begin{align*}
&= \sum_{j,k} \left< \int d\mu \, dv_\parallel \frac{\pi}{2} B_0 n_{0j} \left( T_{0j} \frac{g_{-kj}}{F_{0j}} + q_j \chi_{-kj} \right) D_{\parallel/\perp}[f_{kj}/h_{kj}] \right>_{z} + cc \\
&= \sum_{j,k} \left< \int d\mu \, dv_\parallel \frac{\pi}{2} B_0 n_{0j} T_{0j} h_{-kj} D_{\parallel/\perp}[f_{kj}/h_{kj}] \right>_{z} + cc. \quad (C.4)
\end{align*}
\]

After two steps of integration by parts, we are left with the very general term:

\[
D_{\parallel/\perp} = \sum_{j,k} \left< \int d\mu \, dv_\parallel \pi B_0 n_{0j} T_{0j} \frac{\partial^2}{\partial^2 ||/\perp} \left( \frac{h_{-kj}}{F_{0j}} \right) \frac{\partial^2 (f/h)_{kj}}{\partial^2 ||/\perp} \right>_{z}. \quad (C.5)
\]

where the boundary terms arising from the integration by parts vanish properly because they essentially depend on distribution and electrostatic potential physical boundary conditions. In the following, we will study the signs of the different hyperdiffusion terms defined above.
C. ON HYPERDIFFUSION AND ASSOCIATED FREE ENERGY

Parallel hyperdiffusion

For the parallel hyperdiffusion terms (both \( z \) and \( v \)) we have:

\[
D_{||} = \sum_{j,k} \left\langle \int d\mu d\nu \pi B_0 n_0 T_{0j} \frac{\partial^2 (h_{-kj})}{\partial \parallel^2} \left( \frac{\partial^2 (f/h)_{kj}}{\partial \parallel^2} \right) \right\rangle_z , \tag{C.6}
\]

and there is apparently no way to ensure a definite sign of such terms.

Parallel hyperdiffusion with \( \frac{h_{kj}}{\pi B_0 n_0 T_{0j}} \) shape

However, if one, inspired by the shape of the free energy operator, now constructs the dissipation as

\[
D_{||} \left[ \frac{h_{kj}}{\pi B_0 n_0 T_{0j}} \right] \propto \frac{\partial^4}{\partial \parallel^4} \left( \frac{h_{kj}}{\pi B_0 n_0 T_{0j}} \right) , \tag{C.7}
\]

the associated free energy, after the two same steps of integration by parts as above, becomes:

\[
D_{||} = \sum_{j,k} \left\langle \int d\mu d\nu \pi B_0 n_0 T_{0j} \frac{\partial^2 h_{kj}}{\partial \parallel^2} \left( \frac{\partial^2 (f/h)_{kj}}{\partial \parallel^2} \right)^2 \right\rangle_z . \tag{C.8}
\]

This term has definite (positive) sign. Thus, multiplying it by a negative constant, we make sure that Eq. (C.8) is \(< 0\) and acts as a dissipation term.

Perpendicular hyperdiffusions

Since perpendicular directions are treated numerically in Fourier space directly, the fourth-order derivatives reduces the following way,

\[
\frac{\partial^4}{\partial x, y, z^4} \rightarrow k_{x, y, \perp}^4 . \tag{C.9}
\]

Therefore, one can also re-write the free energy associated to the perpendicular hyperdiffusion as

\[
D_{\perp} = \sum_{j,k} \left\langle \int d\mu d\nu \pi B_0 n_0 T_{0j} \frac{h_{-kj}}{\pi B_0 n_0 T_{0j}} k_{x, y, \perp}^4 \left( f, h \right)_{kj} \right\rangle_z . \tag{C.10}
\]

It is quite clear that if the hyperdiffusion acts on \( h \), for any of the perpendicular directions \((k_x, k_y \text{ or } k_{\perp})\), we obtain straight the following result,

\[
D_{\perp} = \sum_{j,k} \left\langle \int d\mu d\nu \pi B_0 n_0 T_{0j} \frac{|h_{kj}|^2}{\pi B_0 n_0 T_{0j}} \right\rangle_z . \tag{C.11}
\]

In this way, the definite sign for these perpendicular terms is also ensured.
Glossary

Roman Symbols

\( \delta E, E_1 \) Perturbed electric field.

\( \delta B, B_1 \) Perturbed magnetic field.

\( \delta A_{\parallel}, A_{1\parallel} \) Parallel vector potential.

\( \Gamma_0 \) Gamma function. It is proportional to the modified Bessel function.

\( \hat{s} \) Dimensionless magnetic shear.

\( \langle A_{\parallel\parallel} \rangle \) Gyro-phase independent part of the parallel vector potential.

\( C \) Free energy contribution to the collisional dissipation term.

\( C_\phi \) Electrostatic energy contribution to the collisional dissipation term.

\( C_f \) Entropy contribution to the collisional dissipation term.

\( D \) Free energy contribution to the numerical dissipation term.

\( D_\phi \) Electrostatic energy contribution to the dissipation term.

\( D_f \) Entropy contribution to the numerical dissipation term.

\( E \) Free energy.

\( E_\phi \) Electrostatic energy.

\( E_A \) Magnetic energy.

\( E_f \) Entropy.

\( F_{\Delta}, F_{\Delta} \) Filter operators.

\( G \) Free energy contribution to the drive term.

\( G_\phi \) Electrostatic energy contribution to the drive term.

\( G_f \) Entropy contribution to the drive term.

\( K_v \) Kinetic energy operator.

\( L_{\parallel,\phi} \) Electrostatic energy contribution to the linear parallel term.

\( L_{\parallel,f} \) Entropy contribution to the linear parallel term.

\( L_\parallel \) Free energy contribution to the linear parallel term.

\( L_{K,\phi} \) Electrostatic energy contribution to the linear curvature term.

\( L_{K,f} \) Entropy contribution to the linear curvature term.

\( L_K \) Free energy contribution to the linear curvature term.

\( M \) Free energy contribution to the gyrokinetic model.

\( T^j_{\Delta,\Delta_{DNS}} \) Free energy contribution to the sub-grid term.

\( T^f_{\parallel,\parallel} \) Entropy shell-to-shell transfer.

\( T^f_{\phi,\phi} \) Electrostatic energy shell-to-shell transfer.

\( \mathbf{J}_{ij} \) Parallel current density of the gyro-centers of the species \( j \).

\( \pi_j \) Density of the gyro-centers of the species \( j \).

\( c \) Speed of light. In Gyrokinetic Large Eddy Simulations corresponds also to the model coefficient.
GLOSSARY

\( \tilde{\mathbf{A}}_{1\parallel} \)  \hspace{1cm} \text{Gyro-phase dependent part of the parallel vector potential.}

\( c_x, c_y, c_\perp \)  \hspace{1cm} \text{Model coefficients in the } k_x, k_y \text{ and } k_\perp \text{ directions, respectively.}

\( E(k) \)  \hspace{1cm} \text{In fluid dynamics, spectral energy density.}

\( E_v \)  \hspace{1cm} \text{In fluid dynamics, kinetic energy of the flow.}

\( F_{0j} \)  \hspace{1cm} \text{Maxwellian distribution function of the species } j.

\( f_{1j}, f_{kj} \)  \hspace{1cm} \text{Perturbed gyrokinetic distribution function of the species } j \text{ and its Fourier representation.}

\( g^{ij} \)  \hspace{1cm} \text{Metric coefficients.}

\( g_{1j}, g_{kj} \)  \hspace{1cm} \text{Modified gyrokinetic distribution function of the species } j \text{ and its Fourier representation.}

\( h_{1j}, h_{kj} \)  \hspace{1cm} \text{Non-adiabatic part of the gyrokinetic distribution function of the species } j \text{ and its Fourier representation.}

\( I_0 \)  \hspace{1cm} \text{Modified Bessel function.}

\( J \)  \hspace{1cm} \text{Jacobian of the transformation from a cartesian coordinate system to a flux-tube coordinate system.}

\( J_{0kj} \)  \hspace{1cm} \text{Bessel function.}

\( k_{\parallel} \)  \hspace{1cm} \text{Wave number parallel to the magnetic field.}

\( k_{\perp} \)  \hspace{1cm} \text{Wave number perpendicular to the magnetic field.}

\( L \)  \hspace{1cm} \text{Characteristic scale length of the system.}

\( L_x, L_y \)  \hspace{1cm} \text{In gyrokinetics, length of the simulation domain in the perpendicular directions.}

\( L_z \)  \hspace{1cm} \text{In gyrokinetics, length of simulation domain in the parallel directions.}

\( l_\nu \)  \hspace{1cm} \text{In fluid dynamics, Kolmogorov scale.}

\( M \)  \hspace{1cm} \text{Gyrokinetic model.}

\( m_j \)  \hspace{1cm} \text{Mass of the } j \text{ species.}

\( n_j \)  \hspace{1cm} \text{Particle density of the } j \text{ species.}

\( n_{0j} \)  \hspace{1cm} \text{Equilibrium particle density of the species } j.

\( n_{1j} \)  \hspace{1cm} \text{Perturbed particle density of the species } j.

\( p \)  \hspace{1cm} \text{Pressure.}

\( q \)  \hspace{1cm} \text{Safety factor.}

\( q_j \)  \hspace{1cm} \text{Charge of the species } j.

\( Q_j \)  \hspace{1cm} \text{Heat flux of the species } j.

\( R_0 \)  \hspace{1cm} \text{Tokamak major radius.}

\( Re \)  \hspace{1cm} \text{Reynolds number.}

\( Rm \)  \hspace{1cm} \text{Magnetic Reynolds number.}

\( S_{ij} \)  \hspace{1cm} \text{Strain-stress tensor.}

\( T \)  \hspace{1cm} \text{Characteristic scale time of the system.}

\( T^j_{\Delta DNS} \)  \hspace{1cm} \text{In gyrokinetics, the sub-grid term.}

\( t_\nu \)  \hspace{1cm} \text{In fluid dynamics, time associated with the smallest scale of the system.}

\( V \)  \hspace{1cm} \text{In fluid dynamics, characteristic velocity of the flow.}

\( v_i \)  \hspace{1cm} \text{In fluid dynamics, velocity field with } i = x, y, z.

\( v_{\parallel} \)  \hspace{1cm} \text{In gyrokinetics, velocity parallel to the equilibrium magnetic field.}

\( v_{\perp} \)  \hspace{1cm} \text{In gyrokinetics, velocity perpendicular to the equilibrium magnetic field.}
Glossary

\( v_{Tj} \) Thermal speed of the species \( j \).

\( x, k_x \) Radial field aligned coordinates and its Fourier representation.

\( y, k_y \) Toroidal field aligned coordinate and its Fourier representation.

\( z \) Parallel field aligned coordinates.

\( B_0, b_0 \) Equilibrium magnetic field and its unit vector.

\( E \) Electric field.

\( j_j \) Current density of the species \( j \).

\( \dot{j}_{ij} \) Parallel current density of the species \( j \).

**Greek Symbols**

\( \chi_1, \chi_{kj} \) Modified electromagnetic potential and its Fourier representation.

\( \beta \) Beta plasma. It represents the ratio of the plasma pressure to the magnetic field pressure.

\( \epsilon \) In fluid dynamics, energy flux. In gyrokinetics, small parameter in the gyrokinetic ordering.

\( \epsilon_e \) In gyrokinetics, free energy flux.

\( \epsilon_d \) In fluid dynamics, dissipation rate.

\( \epsilon_i \) In fluid dynamics, injection rate.

\( \epsilon_t \) Inverse aspect ratio.

\( \Gamma_j \) Particle flux of the species \( j \).

\( \Lambda \) Phase space.

\( \lambda_D \) Debye length.

\( \langle \phi_1 \rangle \) Gyro-phase independent of the perturbed electrostatic potential.

\( \mu \) Magnetic moment.

\( \nu \) In fluid dynamics, kinematic viscosity.

\( \nu_e \) In fluid dynamics, eddy viscosity.

\( \omega \) Frequency.

\( \Omega_j \) Gyro-frequency of the \( j \) species.

\( \omega_n \) Normalized density gradient.

\( \omega_T \) Normalized temperature gradient.

\( \partial_i \) Partial derivative respect to the spatial coordinate with \( i = x, y, z \).

\( \partial_t \) Partial derivative respect time.

\( \phi_{1,\phi_{1k}} \) Perturbed electrostatic potential and its Fourier representation.

\( \rho \) In fluid dynamics, the density of a fluid.

\( \rho_j \) Larmor radius of the \( j \) species.

\( \tau_{ij} \) In fluid dynamics, the sub-grid term.

\( \theta \) Gyro-angle coordinate.

\( \tilde{\phi}_1 \) Gyro-phase dependent of the perturbed electrostatic potential.

\( \Xi_\phi \) Electrostatic energy operator.

\( \Xi_f \) Entropy operator.

\( \Xi_h \) Free energy operator.

\( Q_j \) Heat flux of the species \( j \).

**Miscellaneous**

\( \langle \cdot \rangle \) Gyro-average operation.

\( \langle \cdot \rangle_V \) Volume integral.

\( \langle \cdot \rangle_{FS} \) Flux surface average.

\( \langle \cdot \rangle_z \) \( z \) - average.

\( \cdots, \ddots \) Filter operations.

**Acronyms**

CBC Cyclone Base Case.

cc complex conjugate.
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETG</td>
<td>Electron temperature gradient.</td>
<td>lhs</td>
<td>left hand side.</td>
</tr>
<tr>
<td>GK</td>
<td>Gyrokinetic equation.</td>
<td>MHD</td>
<td>Magnetohydrodynamics.</td>
</tr>
<tr>
<td>GyroLES</td>
<td>Gyrokinetic Large Eddy Simulations.</td>
<td>N-S</td>
<td>Navier-Stokes equation.</td>
</tr>
<tr>
<td>ITG</td>
<td>Ion temperature gradient.</td>
<td>rhs</td>
<td>right hand side.</td>
</tr>
<tr>
<td>LES</td>
<td>Large-Eddy Simulations.</td>
<td>TEM</td>
<td>Trapped electron mode.</td>
</tr>
</tbody>
</table>
Bibliography


ACKNOWLEDGEMENTS

I would like to express my acknowledgments to those who have helped me during the three years of my Ph.D studies. Since my studies could be divided into two stages (a two year period in Belgium and then another year in Germany) my acknowledgments will be also divided into these two stages.

In Belgium, at the Université Libre de Bruxelles (ULB), I would like to thank my supervisor, Prof. Daniele Carati. He gave me the opportunity to work with him, and has always been available for advice and consultation. I would also like to thank my colleagues Pierre and Michel. I have learned a lot from them and I had a very good time with them. Besides, I would like to thank Gabriel and Bogdan, from whom I learned a lot about turbulence theory. It cannot be missed the great support from the Statistical and Plasma Physics group for their financial assistance; the support from Prof. Bernard Knaepen; my ex-office mate Chichi; and the secretaries, Fabienne and Mari-France. I would also like to thank my friends in Brussels, Tania, Marta and Fani.

In Germany, at the Max-Planck Institute for Plasma Physics (IPP) in Garching, I am deeply indebted to Prof. Frank Jenko for giving me the possibility to join his group and providing the primary support during the last year of my work. Many thanks to my office mates, Tobias, David and Daniel for their warm welcome in their office. Special thanks go to all careful proofreaders of my thesis, Andrés, Daniel and also Angelo and Josefine who have read part of the thesis and have contributed with their suggestions and corrections. Moreover, I would like to thank Angelo, Vasil and my neighbors Francis and David, from whom I have profited from useful discussions, advice and a great time during my stay in Garching. In addition, I would also like to thank other colleagues from IPP–Mirjam, Hauke and Michael.

Last but not least, I would like to thank my family Phuong Anh, Papi, Mami, Marta, Noa and Chiki and my friends Joaquín and Mario for their support during the Ph.D. studies.
DECLARATION

I declare that the work presented in this thesis is my own except where stated otherwise, and was carried out at the Université Libre de Bruxelles during the period of September 2009 to August 2012, under the supervision of Prof. Daniele Carati.

Some parts of the work reported in this thesis have been published in peer reviewed journals, as listed below:


Publication 1 in the above list is the basis of Chapter [4] of this thesis. Publication 2 is the basis of Chapter [5] of this thesis. Publications 3 and 4 in the above list are the basis of Chapters [6] and [7]. While I am not the first author of this material, I was intimately involved in the production of all results and scientific conclusions.
LIST OF PUBLICATIONS

Papers in Peer-Reviewed Journals


Published Conference Proceedings


Invited Talks and Oral Conference Contributions


