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DEPARTMENT OF MECHANICAL AND AEROSPACE ENGINEERING

Master's Degree in Aerospace Engineering

MASTER'S DEGREE THESIS

**On modified Navier-Stokes equations for viscous  
non-Newtonian incompressible fluid motion and their  
numerical solution**

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*To Grandma Nunzia and Uncle Gerardo*  
*A Nonna Nunzia e Zio Gerardo*





## Abstract

The aim of this study is to investigate numerically some modified Navier-Stokes equations, namely O. A. Ladyzhenskaya's set of equations, which describe viscous non-Newtonian incompressible fluid motion. Employing pseudo-spectral methods (Fourier-Galerkin method) Navier-Stokes equations and Ladyzhenskaya equations are solved in a cubic domain assuming periodic boundary conditions and the Taylor-Green Vortex as initial condition, in order to compare solutions and explore alternative fluid dynamics models whose hypotheses are less restrictive.

The study consists of two Parts named Theoretical Formulation and Numerical Investigation. In Part I governing equations of Fluid Dynamics are derived using the continuum hypothesis and the conservation laws; then equations are specialized for incompressible flows, defining also the conditions under which flows can be considered incompressible and the role of the pressure. Viscous behavior is analyzed in Chapter 2 where expressions for the viscous stress tensor are derived for the cases of Newtonian fluids and general Reiner-Rivlin fluids. These expressions are then used in Chapter 3 to obtain incompressible Navier-Stokes equations and Ladyzhenskaya's models which contain non-linear additional viscous terms. In the same Chapter global regularity problem for Navier-Stokes equations and mathematical results for Ladyzhenskaya equations are presented pointing out turbulence's possible role in the *Millennium Problem*. Chapter 4 then covers Turbulence, its characteristics, its statistical description and statistical symmetries. Part I ends with some considerations on Navier-Stokes equations and the reasons why one should investigate also alternative models.

In Part II the mathematical problems to solve are presented defining equations, domain and initial conditions. In Chapter 6 spectral methods are then introduced and some applications of the Fourier-Galerkin method to linear and non-linear partial differential equations are shown. Assuming the arising turbulence to be homogeneous and isotropic, Navier-Stokes and Ladyzhenskaya equations are discretized in space through the Fourier-Galerkin method, whereas advancement in time is realized through the fourth-order Runge-Kutta scheme. The MPI program which implements the numerical scheme described is presented. Simulations' results are shown and analyzed in Chapter 7.

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# Part I

## Theoretical Formulation

# Chapter 1

## Governing Equations of Fluid Dynamics

The physical model which leads to formulate the governing equations of fluid motion is based on the assumption of fluid as a continuum and on some fundamental principals of physics.

### 1.1 The Continuum Hypothesis

The matter is not continuous: at microscopic scale homogeneous materials, such as solids, liquids and gases are composed of molecules separated by space. Every molecule has its own mass, momentum and energy so that at this scale material properties (density and velocity) present discontinuities. In everyday experience, however, there are many physical phenomena - such as fluid motion in pipes and bodies deformation under loads - that can be described and predicted accurately using theories which neglect the molecular structure of matter. Fluid mechanics is indeed normally concerned with the behavior of matter on scales which are much larger than the distance between molecules so that molecular structure of fluid does not need to be taken into account explicitly.

As an example, taking air under atmospheric condition the average spacing between molecules is  $3 \cdot 10^{-9}$  m, the mean distance between two successive collisions of a molecule (the *mean free path*) is  $\lambda = 6 \cdot 10^{-8}$  m, whereas the mean time necessary to cover this distance is  $\tau = 10^{-10}$  s. In a flow, instead, the smallest geometric length scale is about  $L = 0.1$  mm =  $10^{-4}$  m and for flow velocities up to  $u = 100$  m/s the flow time scale results larger than  $t = 10^{-6}$  s. It seems clear that even for flows with small length and time scales, the macroscopic scales are some order of magnitude greater than molecular scales. The separation between molecular length scale and flow length scale is quantified by the *Knudsen number*:

$$\text{Kn} := \frac{\lambda}{L} \quad (1.1)$$

and in general if  $\text{Kn} \ll 1$  the approach that neglects the molecular structure of matter is justified.

The theory that regards matter as indefinitely divisible and describes its behavior from a macroscopic point of view is known as *Continuum Theory*. Within this theory materials are considered to be composed of infinitesimal volumes, referred as *particles*, which contain a huge number of molecules such that a statistical description of particle properties is possible and holds. In a *continuum* the matter is assumed to be continuously distributed and to fill the entire region of space it occupies; physical quantities such as mass, momentum and energy associated with the matter in the particle are regarded as

being spread uniformly over its volume. The continuum hypothesis implies that it is possible the notion of value *at a point* of the various fluid properties such as density, velocity and temperature and that in general these quantities are continuous functions of position and time. For very small Knudsen number, indeed, there exist intermediate length scales  $l$  such that  $l$  is large compared with molecular scales, but small compared with flow scales and the continuum properties can be thought of as the molecular properties averaged over a volume  $\mathcal{V}$  of size  $l^3$ . If in the  $\mathbb{R}^3$  space at the time  $t$  this small volume  $\mathcal{V}$  located in  $\mathbf{x}$  contains a number of  $N(t)$  molecules each of which has its own mass  $m_n$  and velocity  $\mathbf{u}_n$ , then the density of the material is

$$\rho(\mathbf{x}, t) = \frac{1}{l^3} \sum_{n=1}^{N(t)} m_n \quad (1.2)$$

and can be considered as uniformly spread within the volume. The velocity of the center of mass of this volume is

$$\mathbf{u}(\mathbf{x}, t) = \frac{\sum_{n=1}^{N(t)} m_n \mathbf{u}_n}{\sum_{n=1}^{N(t)} m_n} \quad (1.3)$$

and it can be regarded as the velocity of the entire small volume (the fluid particle) as well. The continuum hypothesis allows to introduce the notion of the *fluid particle*: a point that moves with the local fluid velocity.

From a mathematical point of view, giving meaning to the notion of value at a point and leading to continuous functions of space and time, the continuum assumption makes differentiation possible. Fundamental physical laws such as the conservation of mass, the conservation of momentum, and the conservation of energy may then be applied to such model to derive differential equations that describe the phenomenon (motion, equilibrium, deformation, etc).

## 1.2 Eulerian and Lagrangian descriptions of fluid motions

In order to obtain some differential equations for the fluid motion, it is necessary a frame and a set of mathematical tools to represent physical quantities and their variations with time and space. There are two main ways to describe the physical fields variations in a fluid motion: the *Eulerian* approach and the *Lagrangian* approach. In a fluid motion physical quantities of interest can be expressed as function of time and fixed points position in an inertial frame that is equivalent to assign to every fixed point a quantity which varies with time (*Eulerian* description) or they can be regarded as quantities associated to each fluid particle which can varies with time and as the particle moves along its trajectory (*Lagrangian* description).

### 1.2.1 Eulerian description

Considering an inertial reference frame with the coordinate system  $\mathbf{x}$  in the  $\mathbb{R}^3$  space, the Eulerian representation of a (scalar or vectorial) physical variable  $f$  consists of the continuum field  $f(x_1, x_2, x_3, t)$ . The continuum density and velocity fields,  $\rho(\mathbf{x}, t)$  and  $\mathbf{u}(\mathbf{x}, t)$ , are Eulerian fields. Fluid properties are specified at a fixed point and a chosen time.



### 1.2.2 Lagrangian description

The *Lagrangian* approach follows all fluid particles and describes the variations around each fluid particle along its trajectory. Considering an inertial reference frame with the coordinate system  $\mathbf{x}$  in the  $\mathbb{R}^3$  space, a particle can be identified by its initial position that is the position at time  $t^{(0)}$  assumed as reference time,

$$\mathbf{y} = \{x_1^{(0)}, x_2^{(0)}, x_3^{(0)}\} \quad (1.4)$$

Let

$$\mathbf{x}^* = \mathbf{x}^*(t, \mathbf{y}) \quad (1.5)$$

denote the position at time  $t$  of the particle initially located in  $\mathbf{y}$ . Mathematically, the fluid particle position  $\mathbf{x}^*(t, \mathbf{y})$  is completely defined by two equations:

- the definition of the position at the reference time  $t^{(0)}$

$$\mathbf{x}^*(t^{(0)}, \mathbf{y}) = \mathbf{y} \quad (1.6)$$

- the equation that expresses the fact that the fluid particle moves with the local fluid velocity  $\mathbf{u}(\mathbf{x}^*, t)$ :

$$\frac{\partial}{\partial t} \mathbf{x}^*(t, \mathbf{y}) = \mathbf{u}(\mathbf{x}^*(t, \mathbf{y}), t) \quad (1.7)$$

Given the Eulerian velocity field  $\mathbf{u}(\mathbf{x}, t)$ , for any particle, i.e. for any initial position  $\mathbf{y}$ , equation (1.7) can be integrated backward and forward in time to obtain particles positions  $\mathbf{x}^*(t, \mathbf{y})$  for all the time  $t$ . Lagrangian fields of density and velocity can be then expressed in term of their Eulerian fields:

$$\rho^*(t, \mathbf{y}) = \rho(\mathbf{x}^*(t, \mathbf{y}), t)$$

$$\mathbf{u}^*(t, \mathbf{y}) = \mathbf{u}(\mathbf{x}^*(t, \mathbf{y}), t)$$

The Eulerian fields are indexed by the position  $\mathbf{x}$  in the inertial frame, whereas the Lagrangian fields are indexed by the position  $\mathbf{y} = \{x_1^{(0)}, x_2^{(0)}, x_3^{(0)}\}$  the particle has at the reference time  $t^{(0)}$ . The coordinate  $\mathbf{y}$  is called *Lagrangian* or *material* coordinate.

For a given initial position  $\mathbf{y}$ ,  $\mathbf{x}^*(t, \mathbf{y})$  defines the path and  $\rho^*(t, \mathbf{y})$  the density of the fluid particle initially positioned in  $\mathbf{y}$ . The rate of change of density associated with this particle is

$$\begin{aligned} \frac{\partial}{\partial t} \rho^*(t, \mathbf{y}) &= \frac{\partial}{\partial t} \rho(\mathbf{x}^*(t, \mathbf{y}), t) = \left( \frac{\partial}{\partial t} \rho(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*} + \frac{\partial}{\partial t} x_i^*(t, \mathbf{y}) \left( \frac{\partial}{\partial x_i} \rho(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*} = \\ &= \left( \frac{\partial}{\partial t} \rho(\mathbf{x}, t) + u_i(\mathbf{x}, t) \frac{\partial}{\partial x_i} \rho(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*} = \left( \frac{D}{Dt} \rho(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*} \end{aligned} \quad (1.8)$$

where the operator  $D(\cdot)/Dt$  is the *material derivative* defined by

$$\frac{D}{Dt}(\cdot) := \frac{\partial}{\partial t}(\cdot) + v_i \frac{\partial}{\partial x_i}(\cdot) = \frac{\partial}{\partial t}(\cdot) + (\mathbf{u} \cdot \nabla)(\cdot) \quad (1.9)$$

Thus the variation of density following the fluid particle is due to the local time rate of change of Eulerian field and the term  $\mathbf{u} \cdot \nabla \rho$ , referred to as *convective* variation, which arises because the fluid particle moves with local velocity to a new position. Similarly, the rate of change of fluid particle velocity, i.e. the particle acceleration, is given by

$$\frac{\partial}{\partial t} \mathbf{u}^*(t, \mathbf{y}) = \left( \frac{D}{Dt} \mathbf{u}(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*} = \left( \frac{\partial}{\partial t} \mathbf{u}(\mathbf{x}, t) + (\mathbf{u}(\mathbf{x}, t) \cdot \nabla) \mathbf{u}(\mathbf{x}, t) \right)_{\mathbf{x}=\mathbf{x}^*}. \quad (1.10)$$

### 1.3 Conservation laws of fluid dynamics

Many of laws of continuum mechanics state that the total amount of some particular quantities associated with a material body either is invariant or changes in a certain way under the action of known external influences. The total mass of an arbitrary given volume of fluid, for example, is the most obvious conserved quantity; in general given an arbitrary extensive property of the fluid, the amount of which per unit of mass of fluid is an intensive quantity denoted by  $\theta(\mathbf{x}, t)$ , it is possible to write a *conservation* law for this extensive quantity associated with the a material volume  $\Omega$  which has the following form:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \theta(\mathbf{x}, t) d\Omega = \int_{\Omega} Q(\mathbf{x}, t) d\Omega \quad (1.11)$$

where  $Q(\mathbf{x}, t)$  represents the density of the source of the extensive quantity and may depend on the instantaneous fluid motion in some way. The exact form of the function  $Q(\mathbf{x}, t)$  depends on the nature of the extensive quantity corresponding to  $\theta$ .

Since for a material element of fluid the integral relation

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \theta d\Omega = \int_{\Omega} \frac{D}{Dt} (\rho \theta) d\Omega + \int_{\Omega} \rho \theta \nabla \cdot \mathbf{u} d\Omega \quad (1.12)$$

holds, then

$$\int_{\Omega} \frac{D}{Dt} (\rho \theta) d\Omega + \int_{\Omega} \rho \theta \nabla \cdot \mathbf{u} d\Omega = \int_{\Omega} Q d\Omega \quad (1.13)$$

Since  $\Omega$  is an arbitrary volume, the quantity  $\rho \theta$  must satisfy the following differential equation

$$\frac{D}{Dt} (\rho \theta) + \rho \theta \nabla \cdot \mathbf{u} = Q(\mathbf{x}, t) \quad (1.14)$$

which represents the differential form of a conservation law for the generic extensive property  $\rho \theta$ .

#### 1.3.1 Mass Conservation

Considering the mass itself as a extensive property then  $\theta = 1$  and the equation (1.14) becomes

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = Q$$

and by the definition of the material derivative

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} &= Q \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= Q \end{aligned} \quad (1.15)$$

If there is not any source of mass,  $Q(\mathbf{x}, t) = 0$  everywhere and (1.15) becomes

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.16)$$

which is the mass conservation law in differential form. Integrating this equation over a finite material volume  $\Omega$  of fluid the mass conservation becomes

$$\int_{\Omega} \frac{\partial \rho}{\partial t} d\Omega + \int_{\Omega} \nabla \cdot (\rho \mathbf{u}) d\Omega = 0$$

and by applying the divergence theorem

$$\int_{\Omega} \frac{\partial \rho}{\partial t} d\Omega + \int_S \rho \mathbf{u} \cdot \mathbf{n} dS = 0 \quad (1.17)$$

where  $S$  is the boundary of the fluid volume ( $S = \partial\Omega$ ) that has unit outward normal  $\mathbf{n}$ . The integral equation (1.17) states that the rate of increasing of the mass of fluid enclosed by the surface  $S$

$$\int_{\Omega} \frac{\partial \rho}{\partial t} d\Omega$$

is equal to the net rate at which mass is flowing inward across the surface  $S$ , i.e. the net flux of mass entering the control volume through the boundary:

$$- \int_S \rho \mathbf{u} \cdot \mathbf{n} dS$$

If mass is conserved then

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u} \quad (1.18)$$

and the integral conservation law for extensive properties (1.13)

$$\int_{\Omega} \theta \frac{D\rho}{Dt} d\Omega + \int_{\Omega} \rho \frac{D\theta}{Dt} d\Omega + \int_{\Omega} \rho \theta \nabla \cdot \mathbf{u} d\Omega = \int_{\Omega} Q d\Omega$$

is reduced to

$$\int_{\Omega} \rho \frac{D\theta}{Dt} d\Omega = \int_{\Omega} Q d\Omega \quad (1.19)$$

which has the differential form

$$\rho \frac{D\theta}{Dt} := \rho \frac{\partial \theta}{\partial t} + \rho \mathbf{u} \cdot \nabla \theta = Q \quad (1.20)$$

### 1.3.2 Momentum Conservation

Considering the momentum as extensive property,  $\theta = \mathbf{u}$  and the integral form of the conservation law will be

$$\int_{\Omega} \rho \frac{D\mathbf{u}}{Dt} d\Omega = \int_{\Omega} \mathbf{Q} d\Omega$$

In this equation the term on the left-hand side represents the sum of the product of mass and acceleration for all the elements of the material volume  $\Omega$  or alternatively the time rate of change of momentum of the entire fluid volume. For Newton's second law this time rate of change of momentum equals the resultant of the external forces  $\mathbf{F}$  (both surface and body forces) acting on the fluid:

$$\int_{\Omega} \rho \frac{D\mathbf{u}}{Dt} d\Omega = \mathbf{F}(\mathbf{x}, t) \quad (1.21)$$

In general surface forces, which are of molecular origin and act on the volume boundary  $S = \partial\Omega$ , are described by a second order symmetric tensor  $\boldsymbol{\sigma} = \sigma_{ij}(\mathbf{x}, t)$  called *stress tensor* which expresses the mutual reactions of the adjacent parts of fluid, while body forces per

unit mass are described by their vector resultant  $\mathbf{f} = f_i(\mathbf{x}, t)$ . The total body force on the selected volume of fluid is then the vector

$$\int_{\Omega} \rho \mathbf{f} \, d\Omega$$

The  $i$ -component of the surface force exerted on a surface element of area  $dS$  and normal unit vector  $\mathbf{n}$  is represented as  $\sigma_{ij}n_j \, dS$ . The total surface force exerted on the selected portion of fluid by the surrounding matter is then the vector

$$\int_S \sigma_{ij}n_j \, dS = \int_S \boldsymbol{\sigma} \cdot \mathbf{n} \, dS = \int_{\Omega} \nabla \cdot \boldsymbol{\sigma} \, d\Omega = \int_{\Omega} \frac{\partial \sigma_{ij}}{\partial x_j} \, d\Omega$$

Therefore the integral conservation law (1.21), which is a vector equation, will be

$$\int_{\Omega} \rho \frac{D\mathbf{u}}{Dt} \, d\Omega = \int_{\Omega} \rho \mathbf{f} \, d\Omega + \int_{\Omega} \nabla \cdot \boldsymbol{\sigma} \, d\Omega \quad (1.22)$$

or by component ( $i = 1, 2, 3$ )

$$\int_{\Omega} \rho \frac{Du_i}{Dt} \, d\Omega = \int_{\Omega} \rho f_i \, d\Omega + \int_{\Omega} \frac{\partial \sigma_{ij}}{\partial x_j} \, d\Omega \quad (1.23)$$

Since  $\Omega$  is arbitrary then the following differential equation holds

$$\rho \frac{D\mathbf{u}}{Dt} := \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \rho \mathbf{f} + \nabla \cdot \boldsymbol{\sigma} \quad (1.24)$$

The equation (1.24) represents the differential form of the *conservation* law for momentum. Angular momentum is conserved as consequence of the symmetry of the stress tensor.

Body forces acting on fluid are generally due to earth gravitational fields, so that  $\mathbf{f}$  is simply equal to the gravitational acceleration  $\mathbf{g}$ ; in other particular cases such as treating fluids with electromagnetic properties, for example, an appropriate expression for  $\mathbf{f}$  has to be specified.

As symmetric tensor, the stress tensor  $\sigma_{ij}$  can be decomposed in a isotropic part and an anisotropic (or deviatoric) part:

$$\sigma_{ij} = \frac{1}{3} \sigma_{ii} \delta_{ij} + \tau_{ij} \quad (1.25)$$

The isotropic part is

$$\sigma_{ij}^0 = \frac{1}{3} \sigma_{ii} \delta_{ij} \quad (1.26)$$

where  $\sigma_{ii}$  is the trace of the tensor. This part is characterized by invariance under any frame rotation and represents the mean normal stress. If the fluid is at rest only these stresses are present and are equal to the static pressure  $p$ :

$$\sigma_{ij} = \frac{1}{3} \sigma_{ii} \delta_{ij} = -p \delta_{ij} \quad (1.27)$$

This pressure is also the thermodynamic pressure: a state variable that can be determined by the temperature and the density and may be function of position in the fluid. There is no reason to expect that the notion of pressure, intended as normal stress acting equally in all the directions, is valid for a fluid in motion as well since in general the normal

component of the stress acting on a surface element depends on the direction of the normal to the element. It is useful however to define a scalar quantity for a moving fluid which is analogous to the static pressure which measures the amount of the compression exerted on the fluid element by the surrounding matter. In this sense the quantity  $-\frac{1}{3}\sigma_{ii}$  can generalise the notion of pressure to moving fluids since it is invariant under rotation and represents the mean stress acting normally on the fluid element. Thus the pressure at a point in a moving fluid can be defined as

$$p = -\frac{1}{3}\sigma_{ii} \quad (1.28)$$

This is a purely mechanical definition of *pressure* and nothing is implied about the connection with the thermodynamic pressure. In conclusion when the fluid is moving the pressure is defined as the average normal force on a fluid element and is not necessarily the thermodynamic pressure.

Subtracting the mean normal stress from the stress tensor produces the deviatoric stresses

$$\tau_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{ii}\delta_{ij} \quad (1.29)$$

The deviatoric stress tensor is due entirely to the existence of the motion of the fluid; it will be discussed later in the Chapter 2.

Using the stress tensor decomposition in isotropic and deviatoric part the integral conservation law of momentum becomes

$$\int_{\Omega} \rho \frac{Du_i}{Dt} d\Omega = \int_{\Omega} \rho f_i d\Omega - \int_{\Omega} \frac{\partial p}{\partial x_i} d\Omega + \int_{\Omega} \frac{\partial \tau_{ij}}{\partial x_j} d\Omega \quad (1.30)$$

which has differential form

$$\rho \frac{D\mathbf{u}}{Dt} := \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \rho \mathbf{f} - \nabla p + \nabla \cdot \boldsymbol{\tau} \quad (1.31)$$

or by components (for  $i = 1, 2, 3$ )

$$\rho \frac{Du_i}{Dt} := \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (1.32)$$

### 1.3.3 Energy Conservation

Classical thermodynamics is concerned with equilibrium states of uniform matter: states in which all local mechanical, physical and thermal quantities are virtually independent of both position and time. Therefore, in order to obtain a conservation law for the energy in a fluid motion it is necessary to extend classical thermodynamics concepts and results to systems which are in non-uniform and non-equilibrium states; observations show that classical thermodynamics results are approximately valid for the fluid motion in practical fluid dynamics when the non-uniformities are considered to generate a succession of states in each of which the departure from equilibrium at any instant is small and can be neglected. If a given mass of fluid is in thermodynamic equilibrium, its state is completely defined by two parameters, for example the density  $\rho$  and the pressure  $p$ ; thus all the other quantities (such as the temperature, the internal energy and the entropy) which describe the state of the fluid are function of these two *parameters of state* through equations of state. When the fluid presents non-uniformities, instead, it is necessary to define

thermodynamics quantities which are not dependent on the existence of exact equilibrium; the simplest independent quantity that can be defined is the density: the instantaneous ratio of the mass to volume of the fluid element. Another important quantity is the internal energy per unit of mass  $E$ . Assuming that  $E$  refers to an equilibrium state that is achieved instantaneously by isolating the fluid element and letting it to come to equilibrium, the internal energy can be defined at every instant using the first law of thermodynamics

$$\Delta E = Q + W \quad (1.33)$$

in which the heat gained by the fluid per unit of mass ( $Q$ ) and the work per unit of mass performed on the fluid ( $W$ ) between two instants are quantities whose definitions are independent on the existence of equilibrium. Once  $\rho$  and  $E$  are defined, it is possible to use them to define other quantities such as the temperature  $T$  and the entropy per unit of mass  $S$  which describe the state of the moving fluid. It is possible at this point to determine the internal energy balance for a mass of homogeneous fluid using the first principle of thermodynamics which, derived in time, states that the rate of change of internal energy is due to the rate at which work is performed on fluid and the rate at which heat is gained by the fluid:

$$\frac{DE}{Dt} = \dot{Q} + \dot{W} \quad (1.34)$$

The rate at which the work is done on the fluid in the volume  $\Omega$  by the body forces is

$$\int_{\Omega} \rho u_i f_i d\Omega \quad (1.35)$$

whereas that done by surface forces is

$$\int_S u_i \sigma_{ij} n_j dS = \int_{\Omega} \frac{\partial (u_i \sigma_{ij})}{\partial x_j} d\Omega = \int_{\Omega} \left[ \frac{\partial (u_i \tau_{ij})}{\partial x_j} - \frac{\partial (u_i p \delta_{ij})}{\partial x_j} \right] d\Omega \quad (1.36)$$

Thus the total rate of working on a material element per unit of mass of fluid is

$$u_i f_i + \frac{1}{\rho} \frac{\partial (u_i \tau_{ij})}{\partial x_j} - \frac{1}{\rho} \frac{\partial (u_i p \delta_{ij})}{\partial x_j} \quad (1.37)$$

It can be written also as follows

$$\begin{aligned} & u_i f_i + \frac{u_i}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{u_i}{\rho} \frac{\partial (p \delta_{ij})}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} = \\ & = \frac{u_i}{\rho} \left[ \rho f_i + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} \right] + \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} \end{aligned} \quad (1.38)$$

and using the momentum equation (1.32):

$$u_i \frac{Du_i}{Dt} + \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} \quad (1.39)$$

It can be seen that the term in (1.38)

$$\frac{u_i}{\rho} \left[ \rho f_i + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} \right] = \frac{D}{Dt} \left( \frac{\mathbf{u}^2}{2} \right) \quad (1.40)$$

is due to the difference between the stresses on opposite sides of the element and to the volume force and contributes only to the gain in kinetic energy  $\mathbf{u}^2/2$  (per unit of mass) of the material element, whereas the term

$$\frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i}$$

is due to the difference between the velocities on opposite side of the element and represents the work done in deforming the element without changing its velocity. This term contributes only to the gain of internal energy. Thus the rate of working done by surface and body forces which determines a change of internal energy will be simply:

$$\dot{W} = \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} \quad (1.41)$$

Assuming that there is no heat source and that the heat is transferred in the fluid by molecular conduction, the net heat's flux entering the control volume through the boundary  $S$  can be written using Fourier's law of heat conduction

$$\int_S k \frac{\partial T}{\partial x_i} n_i dS = \int_\Omega \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) d\Omega \quad (1.42)$$

where  $T$  is the local temperature and  $k$  the thermal conductivity of the fluid. Thus the rate of gain of heat by a material element per unit of mass is

$$\dot{Q} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) \quad (1.43)$$

Therefore using the first principle of thermodynamics (1.34), the rate of change of internal energy per unit of mass is

$$\frac{DE}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} - \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} \quad (1.44)$$

This equation represents the balance of internal energy in differential form; the balance of kinetic energy  $K$  for unit of mass associated with the material element is given by equation (1.40):

$$\frac{DK}{Dt} = \frac{D}{Dt} \left( \frac{\mathbf{u}^2}{2} \right) = u_i f_i + \frac{u_i}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} - \frac{u_i}{\rho} \frac{\partial p}{\partial x_i} \quad (1.45)$$

Summing equations (1.44) and (1.45) the total energy balance equation can be obtained

$$\rho \frac{D}{Dt} \left( E + \frac{\mathbf{u}^2}{2} \right) = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j} - p \frac{\partial u_i}{\partial x_i} + \rho u_i f_i + u_i \frac{\partial \tau_{ij}}{\partial x_j} - u_i \frac{\partial p}{\partial x_i} \quad (1.46)$$

In these equations the pressure  $p$  has a mechanical definition, as previously explained it is defined as minus the mean normal stress. Given the values of density  $\rho$  and internal energy  $E$  it is possible to obtain the value of pressure  $p_e$  corresponding to the instantaneous thermodynamic equilibrium using an equilibrium equation of state for the fluid. In absence of relative motion of the fluid the pressure  $p$  equals the thermodynamic equilibrium pressure  $p_e$ , but when relative motion occurs they may be different. For sufficiently small magnitude of the velocity gradient, the difference  $p - p_e$  can be assumed to be a

linear function of the non-uniformities in velocity field, that are the various components of the tensor  $\partial u_i / \partial x_j$ :

$$p - p_e = B_{ij} \frac{\partial u_i}{\partial x_j} \quad (1.47)$$

where the tensor coefficient  $B_{ij}$  depends on the local state of the fluid but not directly on the velocity field. The response of the pressure to an imposed velocity gradient can be assumed also to be independent on the direction so that  $B_{ij}$  is an isotropic tensor

$$B_{ij} = -\kappa \delta_{ij} \quad (1.48)$$

where  $\kappa$  is a scalar coefficient dependent on the local state of fluid. Thus the relation (1.47) reduces to

$$p = p_e - \kappa \delta_{ij} \frac{\partial u_i}{\partial x_j} = p_e - \kappa \frac{\partial u_i}{\partial x_i} \quad (1.49)$$

The rate at which the isotropic part of the stress tensor, i.e. the pressure, contributes to change the internal energy in equation (1.44) is then

$$-\frac{p}{\rho} \frac{\partial u_i}{\partial x_i} = -\frac{p_e}{\rho} \frac{\partial u_i}{\partial x_i} + \frac{\kappa}{\rho} \left( \frac{\partial u_i}{\partial x_i} \right)^2 \quad (1.50)$$

in which the term

$$\frac{\kappa}{\rho} \left( \frac{\partial u_i}{\partial x_i} \right)^2$$

provided that  $\kappa$  is positive, represents a dissipation of mechanical energy due to the expansion caused by  $\partial u_i / \partial x_i$  in the departure from the equilibrium state;  $\kappa$  represents indeed a expansion damping coefficient usually called *bulk viscosity*. This term is in general small compared to the first term on right-hand side of the relation (1.50) since the velocity gradient is assumed to be small, however it can determine a considerable amount of dissipation of mechanical energy when the rate of expansion  $\partial u_i / \partial x_i$  is periodic and goes through many cycles, like in propagation of acoustic waves on long distances.

The set of equations which describes the fluid motion under the assumptions made is formed by

- Mass conservation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (1.51)$$

- Momentum conservation (for  $i = 1, 2, 3$ )

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (1.52)$$

- Energy conservation

$$\rho \frac{D}{Dt} \left( E + \frac{\mathbf{u}^2}{2} \right) = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j} - p \frac{\partial u_i}{\partial x_i} + \rho u_i f_i + u_i \frac{\partial \tau_{ij}}{\partial x_j} - u_i \frac{\partial p}{\partial x_i} \quad (1.53)$$

If we assume for the moment that the deviatoric part of stresses is a known function of the velocity gradient and the local thermodynamic state (it will be explained later), then the unknown functions in these five differential equations are eight: the three components



of the velocity field  $\mathbf{u}$ , the density field  $\rho$ , the pressure field  $p$ , the temperature field  $T$ , the thermal conductivity of the fluid  $k$  and the internal energy field  $E$ . We thus miss three equations in order to close the system of equations. These missing equations are given by thermodynamic relations between  $\rho$ ,  $T$ ,  $E$ ,  $p$  and  $k$ . We have assumed that non-uniformities generate a succession of states in each of which the departure from equilibrium is small and an intermediate equilibrium state is achieved instantaneously by the fluid element; thus this intermediate thermodynamic state of the fluid is completely defined by two parameter of state, for example the density  $\rho$  and the temperature  $T$ . Therefore, given  $\rho$  and  $T$ , the other thermodynamic variables can be determined through known relations called *constitutive equations* which are proper of the fluid:

$$p = p(\rho, T) \quad (1.54)$$

$$E = E(\rho, T) \quad (1.55)$$

$$k = k(\rho, T) \quad (1.56)$$

Using these three relations and the expression of  $\tau_{ij}$  which, for the moment, is supposed known, the five equations can be expressed in function of the following five variables:  $u_1$ ,  $u_2$ ,  $u_3$ ,  $\rho$ ,  $T$ .

## 1.4 Incompressible flows

In certain flow conditions that will be soon discussed, the density of the fluid element does not change during its motion and the flow is said to be *incompressible*. Therefore when the flow is incompressible, the rate change of density of the material fluid element is zero:

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + u_i \frac{\partial\rho}{\partial x_i} = 0 \quad (1.57)$$

Using this condition the mass conservation equation

$$\frac{\partial\rho}{\partial t} + u_i \frac{\partial\rho}{\partial x_i} + \rho \frac{\partial u_i}{\partial x_i} = 0 \quad (1.58)$$

takes the simple form

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1.59)$$

which expresses that the rate of expansion is everywhere zero or, mathematically, that the velocity field is solenoidal. Since the incompressibility is a property of the flow and not of the fluid, we want to understand the conditions under which the flow can be considered incompressible; it can be done using dimensional analysis.

### 1.4.1 Dimensional Analysis

If a flow is incompressible we can also write that the density variation  $\Delta\rho$  experienced by any fluid element during its motion is small compared with the unperturbed value of the density  $\rho$ :

$$\left| \frac{\Delta\rho}{\rho} \right| \ll 1 \quad (1.60)$$

Let  $L$  and  $U$  denote respectively the characteristic length scale and the characteristic velocity of the flow, then the order of magnitude of the relative density variation is approximately

$$\frac{\Delta\rho}{\rho} \sim \frac{1}{\rho} \frac{D\rho}{Dt} \frac{L}{U} \quad (1.61)$$

since  $L/U$  expresses the characteristic time in which significant variations of flow quantities may occur. Thus the condition (1.60) can be written

$$\left| \frac{1}{\rho} \frac{D\rho}{Dt} \right| \ll \frac{U}{L} \quad (1.62)$$

If we choose density  $\rho$  and entropy  $S$  as the two independent thermodynamic state variables than we can express the pressure variation as follows

$$\frac{Dp(\rho, S)}{Dt} = \left( \frac{\partial p}{\partial \rho} \right)_S \frac{D\rho}{Dt} + \left( \frac{\partial p}{\partial S} \right)_\rho \frac{DS}{Dt} \quad (1.63)$$

Denoting with  $a^2$  the quantity  $(\partial p / \partial \rho)_S$  which is actually the square of the speed of sound, we may express the density variation as

$$\frac{D\rho}{Dt} = \frac{1}{a^2} \frac{Dp}{Dt} - \frac{1}{a^2} \left( \frac{\partial p}{\partial S} \right)_\rho \frac{DS}{Dt} \quad (1.64)$$

which substituted in the condition (1.62) gives

$$\left| \frac{1}{\rho a^2} \frac{Dp}{Dt} - \frac{1}{\rho a^2} \left( \frac{\partial p}{\partial S} \right)_\rho \frac{DS}{Dt} \right| \ll \frac{U}{L} \quad (1.65)$$

This condition is normally satisfied if each on the two terms on the left-hand side is small compared with  $U/L$ :

$$\left| \frac{1}{\rho a^2} \frac{Dp}{Dt} \right| \ll \frac{U}{L} \quad (1.66)$$

$$\left| \frac{1}{\rho a^2} \left( \frac{\partial p}{\partial S} \right)_\rho \frac{DS}{Dt} \right| \ll \frac{U}{L} \quad (1.67)$$

To estimate the order of magnitude of the term  $Dp/Dt$ , we can use the kinetic energy equation (1.45), in particular to express the pressure convection, and neglect the effect of viscosity which modifies the pressure distribution rather than the magnitude of the pressure variation  $Dp/Dt$ . The condition (1.66) can be rewritten as

$$\left| \frac{1}{\rho a^2} \frac{\partial p}{\partial t} - \frac{1}{2a^2} \frac{D\mathbf{u}^2}{Dt} + \frac{\mathbf{u} \cdot \mathbf{f}}{a^2} \right| \ll \frac{U}{L} \quad (1.68)$$

Again, this condition is satisfied if each of the terms is small in magnitude compared to the right-hand side:

$$\left| \frac{1}{2a^2} \frac{D\mathbf{u}^2}{Dt} \right| \ll \frac{U}{L} \quad (1.69)$$

$$\left| \frac{1}{\rho a^2} \frac{\partial p}{\partial t} \right| \ll \frac{U}{L} \quad (1.70)$$

$$\left| \frac{\mathbf{u} \cdot \mathbf{f}}{a^2} \right| \ll \frac{U}{L} \quad (1.71)$$

The order of magnitude of variation of  $\mathbf{u}^2$  is given by  $U^2/(L/U)$ , i.e.  $U^3/L$ , so that the first of these conditions becomes:

$$M^2 := \frac{U^2}{a^2} \ll 1 \quad (1.72)$$

where  $M$  is the Mach number characterising the flow. This condition is practically satisfied for Mach numbers lower than 0.3.

To estimate the time fluctuations of pressure contained in the second condition, we can use a simple case: an unidirectional flow with a velocity which is constant in space (over  $L$ ), but oscillates in time between opposite values of order  $U$  with the frequency  $f$ . In addition, without invalidating the analysis, we can neglect the effects of the body and the viscous forces. Using these assumptions and the momentum balance equation (1.32), one can express the pressure variation as  $\Delta p \approx \rho U L / \Delta t$  where the characteristic time of variation  $\Delta t$  is simply the reciprocal of the frequency  $f$ . Thus the condition

$$\left| \frac{1}{\rho a^2} \frac{\partial p}{\partial t} \right| \ll \frac{U}{L}$$

can be rewritten as follows

$$\left| \frac{1}{\rho a^2} \rho U L f^2 \right| = \frac{f^2 L^2}{a^2} \ll \frac{U}{L} \quad (1.73)$$

If the order of magnitude of the frequency  $f$  is  $U/L$ , this condition simply reduces to the previous condition ( $M \ll 1$ ). If the frequency of oscillations is instead high than the (1.73) represents and independent and more restrictive condition than  $M \ll 1$ . This explains why it is essential to take compressibility into account in acoustics even when Mach numbers are low.

The order of magnitude of the left-hand side in the last condition

$$\left| \frac{\mathbf{u} \cdot \mathbf{f}}{a^2} \right| \ll \frac{U}{L}$$

can be estimate supposing that the body forces arises from the gravitational acceleration  $g$  only. Thus the condition can be rewritten as follows

$$\left| \frac{gU}{a^2} \right| \ll \frac{U}{L} \quad \Rightarrow \quad \frac{gL}{a^2} \ll 1 \quad (1.74)$$

which implies that the typical length scale of motion  $L$  should be small compared to the characteristic length given by  $a^2/g$ .

For the remaining condition

$$\left| \frac{1}{\rho a^2} \left( \frac{\partial p}{\partial S} \right)_\rho \frac{DS}{Dt} \right| \ll \frac{U}{L} \quad (1.75)$$

it is possible to demonstrate using the entropy balance that it is satisfied in almost all cases of practical interest, provided that the Mach number is low and the externally imposed

temperature gradients are not significant. This condition is indeed almost irrelevant compared to the condition regarding  $Dp/Dt$ .

In conclusion it is possible to state that the fluid behaves as if it were incompressible when the following flow conditions are all satisfied:

$$M^2 = \frac{U^2}{a^2} \ll 1 \quad (1.76)$$

$$\frac{f^2 L^2}{a^2} \ll \frac{U}{L} \quad (1.77)$$

$$\frac{gL}{a^2} \ll 1 \quad (1.78)$$

### 1.4.2 Equations for incompressible flows

Explained the conditions under which the flow can be considered incompressible, we now want to know how equations of motion change. We have already seen that if the flow is incompressible then the velocity field is solenoidal ( $\nabla \cdot \mathbf{u} = 0$ ) because of the mass conservation; using this property of the velocity field in the internal energy balance (1.46) the contribution due to the pressure vanishes and the equation reduces to

$$\frac{DE}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} \quad (1.79)$$

in which we can assume that the internal energy is a function of the temperature  $T$  only since  $\rho$  is constant. In the internal energy balance the term containing the deviatoric part of stresses is usually referred to as *dissipation function* and denoted by  $\Phi$ :

$$\frac{DE}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \Phi \quad (1.80)$$

The set of equations of motion in the case of incompressible flow is then reduced to the following system

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1.81)$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (1.82)$$

$$\frac{DE}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \Phi \quad (1.83)$$

As will be seen later, in these equation  $\tau_{ij}$  can be considered as function of the velocity gradient only. Like in the case of generic compressible flows, the three components of velocity  $\mathbf{u}$  and the temperature  $T$  are still unknown functions. The density instead can no longer be an unknown since it does not change in the motion and is effectively constant in the whole field. The quantity which replaces the density as an unknown variable is the pressure  $p$  which, however, can no longer be considered a thermodynamic state function related to the density and the temperature by an equation of state. The pressure is purely a mechanical variable which adjusts itself instantaneously so that the velocity field can satisfies the divergence-free condition; in fact by applying the divergence operator to the momentum conservation equation and using  $\nabla \cdot \mathbf{u} = 0$ , it is possible to obtain a Poisson

equation for the pressure in which the source term is a known function of the derivatives in space of the velocity only:

$$\nabla^2 p = f(\mathbf{u}) \quad (1.84)$$

The pressure field is then completely defined by the velocity field and the satisfaction of the Poisson equation represents a necessary and sufficient condition for a solenoidal velocity field to remain solenoidal. Since the equation is not an evolution equation the pressure field has to change instantaneously to guarantee that the divergence-free condition is satisfied by the velocity.

From a mathematical point of view it can be observed that if one assumes that the density is constant and that the deviatoric stresses does not depend on the thermodynamic state, then the temperature, which represents the only thermodynamic variable, appears in the internal energy equation only. Consequently, the energy equation is decoupled from the other four scalar equations so that one could solve the system formed by mass conservation and momentum balance to obtain the velocity and the pressure fields and later, given the velocity field and a constitutive equation for  $k = k(T)$ , to solve the internal energy equation to obtain, if needed, the temperature field. When temperature field is not needed, in fact, the energy balance equation is not even written down and the problem reduces to the solution of the system given by equations (1.81) and (1.82) only.

# Chapter 2

## Viscous Stress Tensor

In the previous Chapter the following equations for compressible fluid motion have been derived

- Mass conservation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (2.1)$$

- Momentum conservation (for  $i = 1, 2, 3$ )

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.2)$$

- Energy conservation

$$\rho \frac{D}{Dt} \left( E + \frac{\mathbf{u}^2}{2} \right) = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j} - p \frac{\partial u_i}{\partial x_i} + \rho u_i f_i + u_i \frac{\partial \tau_{ij}}{\partial x_j} - u_i \frac{\partial p}{\partial x_i} \quad (2.3)$$

As explained, in these equations density, pressure, internal energy, thermal conductivity of the fluid and temperature are related through thermodynamic equations (the constitutive laws) proper of the fluid.

In order to carry out some considerations, we have previously assumed that the deviatoric part  $\tau_{ij}$  of the stress tensor was a function of the thermodynamic state and of the velocity gradient without clarifying these dependences; so far, an expression for  $\tau_{ij}$  is in fact missed. In order to derive an expression for  $\tau_{ij}$  it is essential to consider the molecular origin of the stresses and their relation with the local fluid properties.

### 2.1 Transport of momentum and stress tensor

When matter is in an equilibrium state the spatial distribution of each of the various properties of the material is uniform and each material element is in mechanical and thermal balance with near elements. If certain properties are not uniform it is observed that exchanges of mechanical and thermal properties occur between adjoining elements and tend to bring the material to an equilibrium state smoothing out the non-uniformities. These kind of exchanges occurring on molecular length scales are called *diffusive phenomena* and concern the transport on matter, energy and momentum. All molecules are in continual motion of a random kind because of thermal agitation and as consequence they tend to

migrate away from any initial position transporting their matter, energy and momentum. The transport of molecular momentum across an element surface occurs when molecules cross the surface and interact with each other; as consequence of this flux of molecular momentum in the fluid a local stress (a force per unit of surface) arises. The stress at any point is then a consequence of molecular motions and interactions around the point and if the fluid continuum velocity is uniform the stress is normal to the surface element for all orientation of the element. If the continuum velocity is not uniform crossing the surface then the tangential components of stress may not be zero since the net flux of molecular momentum in the direction of relative motion may not be zero. Tending to smooth out the non-uniformity these tangential stresses represent an internal friction and when a fluid shows this behavior is said to be *viscous*.

We have previously introduced the stress tensor  $\sigma_{ij}$  to represent the surface forces acting on a fluid element and we have decomposed it in isotropic and deviatoric parts. As explained, the isotropic part, invariant under any rotation of frame, is completely defined by a scalar quantity which represents the generalisation of the concept of pressure to fluid which are in non-equilibrium

$$\sigma_{ij}^0 = \frac{1}{3}\sigma_{ii}\delta_{ij} = -p\delta_{ij} \quad (2.4)$$

whereas an expression for the deviatoric part still misses. However, we now know that the deviatoric part  $\tau_{ij}$  of the stress tensor represents the viscous interaction between elements of fluid, it can be indeed named *viscous stress tensor*, and is entirely due to the diffusive transport of molecular momentum caused by non-uniformities in the continuum velocity field. Thus the local velocity gradient  $\partial u_i/\partial x_j$ , which expresses these non-uniformities, is the parameter of the flow with most relevance in the definition of viscous stresses.

## 2.2 Linear relation between viscous stress tensor and velocity gradient - Newtonian fluids

There is no rigorous way to deduce the dependence of  $\tau_{ij}$  on  $\partial u_i/\partial x_j$  for all the fluid in general, however it is possible to say that if the velocity gradient is sufficiently small in magnitude then  $\tau_{ij}$  is approximately a linear function of  $\partial u_i/\partial x_j$ :

$$\tau_{ij} = A_{ijkl} \frac{\partial u_k}{\partial x_l} \quad (2.5)$$

where  $A_{ijkl}$  is a fourth-order tensor of coefficients depending on the local state of the fluid, but not directly on the velocity gradient. Since  $\tau_{ij}$  is symmetrical, the tensor  $A_{ijkl}$  is necessarily symmetrical in the indices  $i$  and  $j$ . The velocity gradient can be written as the sum of a symmetric and antisymmetric tensor

$$\frac{\partial u_k}{\partial x_l} = D_{kl} + S_{kl} \quad (2.6)$$

where

$$D_{kl} = \frac{1}{2} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad (2.7)$$

is the symmetric *rate-of-strain* tensor, and

$$S_{kl} = \frac{1}{2} \left( \frac{\partial u_k}{\partial x_l} - \frac{\partial u_l}{\partial x_k} \right) \quad (2.8)$$

is the antisymmetric *rate-of-rotation* tensor. Using this decomposition, (2.5) becomes

$$\tau_{ij} = \frac{1}{2}A_{ijkl} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) + \frac{1}{2}A_{ijkl} \left( \frac{\partial u_k}{\partial x_l} - \frac{\partial u_l}{\partial x_k} \right) \quad (2.9)$$

If we suppose that the molecular structure of the fluid is statistically isotropic then the deviatoric stress generated in an element of fluid by a given velocity gradient is independent on the orientation of the element, i.e. the viscous response to a given gradient has not directional preferences. In general gases and simple liquids have this kind of isotropic structure because of the low number of atoms composing the molecules, however there exist some fluids, like solutions containing long-chain molecules (such as polymers), that may exhibit an anisotropic response to velocity gradient and for which this hypothesis is not valid. We now suppose to deal with the first category of fluids, for which the isotropic viscous response leads to the isotropy of the tensor of coefficients  $A_{ijkl}$  so that it can be written as follows

$$A_{ijkl} = \mu_0 \delta_{ik} \delta_{jl} + \mu_1 \delta_{il} \delta_{jk} + \mu_2 \delta_{ij} \delta_{kl} \quad (2.10)$$

where  $\mu_0$ ,  $\mu_1$  and  $\mu_2$  are scalar coefficients depending on the local state of the fluid, but not on the velocity gradient. Since  $A_{ijkl}$  is symmetrical in  $i$  and  $j$

$$A_{ijkl} = A_{jikl}$$

which is

$$\mu_0 \delta_{ik} \delta_{jl} + \mu_1 \delta_{il} \delta_{jk} + \mu_2 \delta_{ij} \delta_{kl} = \mu_0 \delta_{jk} \delta_{il} + \mu_1 \delta_{jl} \delta_{ik} + \mu_2 \delta_{ji} \delta_{kl}$$

Since  $\delta_{ij} = \delta_{ji}$  then

$$\mu_0 \delta_{ik} \delta_{jl} + \mu_1 \delta_{il} \delta_{jk} = \mu_0 \delta_{jk} \delta_{il} + \mu_1 \delta_{jl} \delta_{ik}$$

which reduces to

$$(\mu_0 - \mu_1) (\delta_{jl} \delta_{ik} - \delta_{il} \delta_{jk}) = 0$$

This relation is satisfied for each value of  $i, j, k$  and  $l$  if

$$\mu_1 = \mu_0 := \mu \quad (2.11)$$

so that

$$A_{ijkl} = \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \mu_2 \delta_{ij} \delta_{kl} \quad (2.12)$$

The relation (2.9) then becomes

$$\begin{aligned} \tau_{ij} = & \frac{1}{2} [\mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \mu_2 \delta_{ij} \delta_{kl}] \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) + \\ & + \frac{1}{2} [\mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \mu_2 \delta_{ij} \delta_{kl}] \left( \frac{\partial u_k}{\partial x_l} - \frac{\partial u_l}{\partial x_k} \right) \end{aligned} \quad (2.13)$$

It can be observed that  $\mu_0 = \mu_1$  implies that  $A_{ijkl}$  is also symmetrical in the indices  $k$  and  $l$  ( $A_{ijkl} = A_{ijlk}$ ) and as consequence its product with the antisymmetric part of the velocity gradient

$$[\mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \mu_2 \delta_{ij} \delta_{kl}] \left( \frac{\partial u_k}{\partial x_l} - \frac{\partial u_l}{\partial x_k} \right)$$

drops out leading to

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \mu_2 \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (2.14)$$



If we suppose that  $\tau_{ij}$  does not give contribution to the normal stress (*Stokes' hypothesis*) then

$$\tau_{ii} = (2\mu + 3\mu_2) \frac{\partial u_k}{\partial x_k} = 0 \quad (2.15)$$

for all the values of the velocity divergence  $\partial u_k / \partial x_k$ , implying that

$$\mu_2 = -\frac{2}{3}\mu \quad (2.16)$$

and leading to

$$\tau_{ij} = \mu \left[ \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] \quad (2.17)$$

where the quantity

$$\frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

represents the non-isotropic part of the rate of strain tensor

$$D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

If the incompressibility conditions previously presented are satisfied then  $\partial u_k / \partial x_k = 0$  and the viscous stress tensor reduces to

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = 2\mu D_{ij} \quad (2.18)$$

In the special case of simple shearing motion in which the fluid is moving along  $x_1$  with the velocity  $u_1$  which only varies along the direction  $x_2$  ( $u_1 = u_1(x_2)$ ) then all the components of  $\tau_{ij}$  are zero except the tangential stresses:

$$\tau_{12} = \tau_{21} = \mu \frac{\partial u_1}{\partial x_2} \quad (2.19)$$

Since this stress resulting from molecular momentum transport has to eliminate the non-uniformities in the velocity field, the scalar quantity  $\mu$  must be positive; thus  $\mu$  represents a measure of the internal friction opposing to shear deformation of the fluid, is called *dynamic viscosity* and may be function of the thermodynamic state of the fluid only.

The simple relation (2.19) states that the shear stress  $\tau_{12}$  is directly proportional to the shear rate of deformation  $\partial u_1 / \partial x_2$  (Figure 2.1); it was first formulated for simple shearing laminar motion by Sir Isaac Newton in his famous *Philosophiae Naturalis Principia Mathematica* (1686) in which he introduced the term *defectus lubricitatis* to express the concept of internal friction or viscosity in fluids. Fluids for which the linear relation between the non-isotropic part of the stress and the rate-of-strain tensor holds accurately are indeed called *Newtonian* after Isaac Newton's work. Only in 1845 Stokes was able to write Newton's simple relation in a three-dimensional form deriving the relation (2.17); few decades later Poiseuille and Couette proved Newton's relation experimentally. Today through experiments on a variety of fluids and flow fields we know that linear relation (2.17) is accurate for simple liquids and most gases over a wide range of values of the rate of strain despite the assumption of *sufficiently* small velocity gradient used to derived it. In general, the Newtonian constitutive equation (2.17) accurately describes the viscous

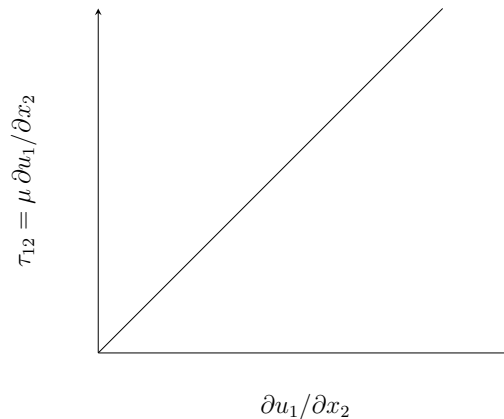


Figure 2.1: Linear relation between shear stress and velocity gradient for simple shearing motion

behavior of low molecular weight fluids. On the other hand, there exists a vast category of fluids, mainly of industrial importance, which show a behavior which differs from that shown in Figure 2.1, i.e. fluids for which the viscous stress tensor is not simply linearly related to the rate-of-strain. In the case of polymeric liquids, emulsions and concentrated suspension, for example, the viscosity  $\mu$  can be a strong function of the rate-of-strain. These kind of fluid are generally classified as *Non-Newtonian* to distinguish them from those which follow the simple relation (2.17).

## 2.3 Non-Newtonian fluids

We now consider fluids which still show an isotropic viscous response to imposed velocity gradients, but they are characterised by an *instantaneous* relation between the viscous stress tensor  $\boldsymbol{\tau}$  and the rate-of-strain tensor  $\mathbf{D}$  which is in general non-linear:

$$\boldsymbol{\tau} = f(2\mathbf{D}) \quad (2.20)$$

Since the isotropic behavior is still assumed, we can focus our attention to the simple case of shearing motion without loss of generality. In addition we assume that the flow is incompressible. Under these hypotheses, the principal departures from the Newtonian behavior of fluids, i.e. the principal non-Newtonian phenomena, can be summarised in:

- Dependence of the viscosity on the shear rate, also called **Shear thinning** or **shear thickening** behavior in which the shear stress  $\tau_{12}$  is respectively a sublinear or a superlinear function of the shear rate  $\partial u_1 / \partial x_2$ . For this kind of fluids a generalised viscosity  $\mu_g$ , which is function of the shear rate, can be defined

$$\mu_g = \mu_g \left( \frac{\partial u_1}{\partial x_2} \right) \quad (2.21)$$

If the fluid shows a shear thickening behavior is called *dilatant fluid* and its generalised viscosity is an increasing function of the shear rate (Figure 2.2); in general the generalised viscosity is positive for  $\partial u_1 / \partial x_2 = 0$ . On the other hand if the fluid shows a shear thinning behavior is called *pseudoplastic fluid* and its generalised viscosity is a decreasing function of the shear rate (Figure 2.3); in general the generalised viscosity is finite for  $\partial u_1 / \partial x_2 = 0$ . The Newtonian fluid is thus a very special

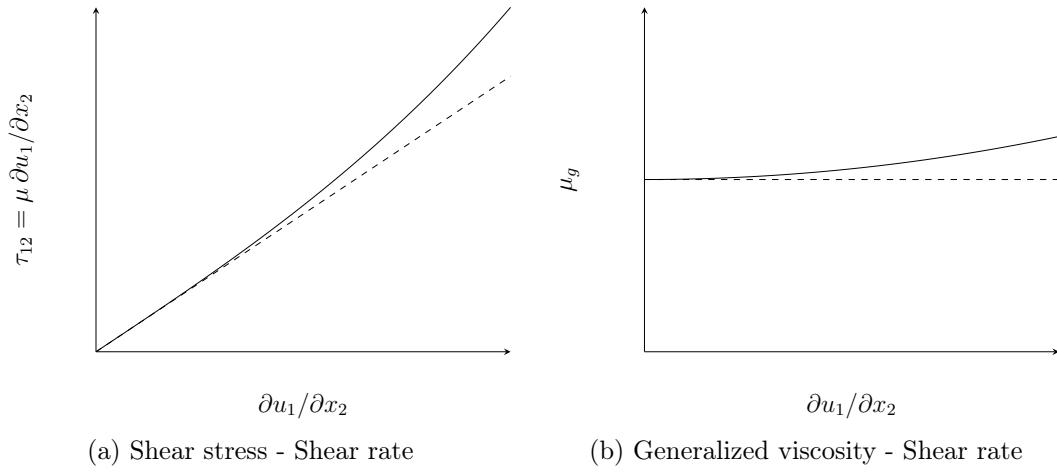


Figure 2.2: Shear Thickening behavior

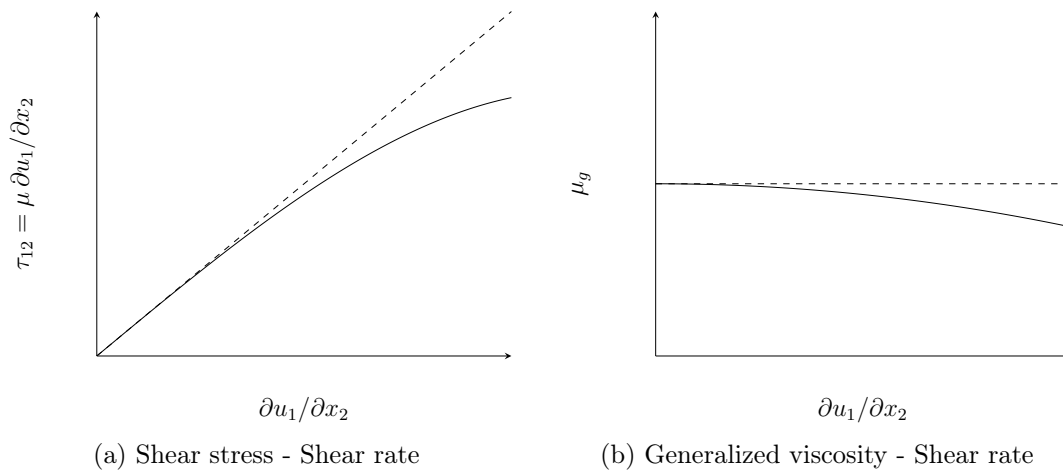


Figure 2.3: Shear Thinning behavior

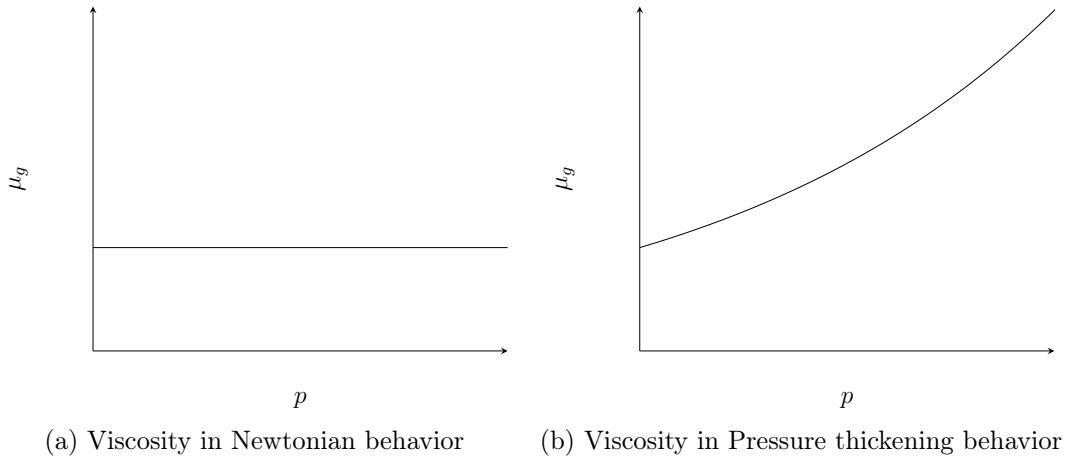


Figure 2.4: Viscosity - Pressure

fluid: it neither shear thins nor shear thickens. The models with shear dependent viscosity are used in many areas of engineering science such as geophysics, colloid mechanics, polymer mechanics, hemodynamics and food rheology, etc.

The simplest known model which describes these behaviors are the power-law models in which the viscous stress tensor is defined as

$$\tau_{ij} = 2K |4\Pi_{\mathbf{D}}|^{\frac{n-1}{2}} D_{ij} \quad (2.22)$$

where  $n$  is the power-law index,  $K$  is a constant called *consistency* and  $\Pi_{\mathbf{D}}$  is the second principal invariant of  $\mathbf{D}$  given by:

$$\Pi_{\mathbf{D}} = \frac{1}{2} [\text{tr}(\mathbf{D})]^2 - \frac{1}{2} \text{tr}(\mathbf{D}^2) \quad (2.23)$$

The generalised viscosity is then

$$\mu_g = K |4\Pi_{\mathbf{D}}|^{\frac{n-1}{2}} \quad (2.24)$$

When  $n = 1$  then the power-law reduces to the Newton constitutive law for incompressible fluids:

$$\tau_{ij} = 2K D_{ij} = 2\mu D_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.25)$$

When  $n$  is less than one, the constitutive equation describes the shear thinning, whereas when  $n$  is greater than one the equation describes the shear thickening.

- Dependence of the viscosity on the pressure, also called **Pressure thickening** behavior in which the generalised viscosity is not constant as in the case of the Newtonian fluids but it is a function of the pressure; in particular, experimental data show that viscosity is an increasing function of  $p$  (Figure 2.4). A famous relation which describes the generalised viscosity variation with pressure for such fluids is the exponential relation proposed by Barus [4] (1983):

$$\mu_g(p) = \mu_0 e^{\alpha p} \quad (2.26)$$

where  $\alpha$  is a constant pressure-viscosity coefficient characteristic for each fluid. The shear stresses are then

$$\tau_{ij} = 2\mu_0 e^{\alpha p} D_{ij} \quad (2.27)$$

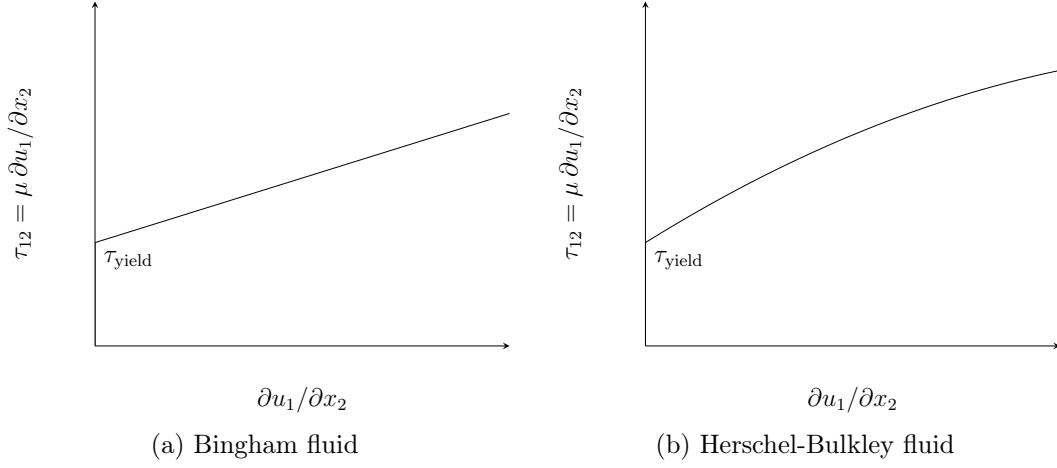


Figure 2.5: Fluids with yield stress

- The presence of activation/deactivation criteria (such as yield stress). There exists some fluids that start to flow when they reach a critical value of stress  $\tau$  which is called *yield stress*. Once the fluid is in motion, if the stress dependence on the shear rate is linear the fluid is called *Bingham fluid* (Figure 2.5.a), otherwise it is called *Herschel-Bulkley fluid* (Figure 2.5.b). For these kind of fluids the viscous stress is usually a non-continuous function of the shear rate.
- Time dependent phenomena in which viscous stresses are also function of the temporal variations of the rate-of-strain tensor  $\mathbf{D}$ .

A large number of models have been developed to cover the description of all the non-Newtonian behaviors. Most of these models, like the power-law fluid model, depends on the rate of deformation  $\mathbf{D}$  and they arise from a *general viscous* model. Let the stress tensor  $\boldsymbol{\sigma}$  depend only on the rate of deformation  $\mathbf{D}$ , i.e.  $\boldsymbol{\sigma} = f(2\mathbf{D})$ ; expanding the function in a power series gives

$$\boldsymbol{\sigma} = A_0 \mathbf{D}^0 + A_1 \mathbf{D}^1 + A_2 \mathbf{D}^2 + A_3 \mathbf{D}^3 + \dots \quad (2.28)$$

in which  $D_{ij}^0 = \delta_{ij}$  and, assuming that the flow is incompressible,  $A_0 = -p$ . The Cayley-Hamilton theorem states that any tensor  $T_{ij}$  (with  $i, j = 1, 2, 3$ ) satisfies its own characteristic equation

$$\det(\mathbf{T} - \lambda \mathbf{I}) = 0 \quad (2.29)$$

where  $\mathbf{I}$  is the identity matrix. Expanding the determinant, the characteristic equation can be rewritten as

$$\lambda^3 - \text{I}_{\mathbf{T}} \lambda^2 + \text{II}_{\mathbf{T}} \lambda - \text{III}_{\mathbf{T}} = 0 \quad (2.30)$$

where the coefficients are the three principal invariants of the tensor  $\mathbf{T}$  given by

$$\text{I}_{\mathbf{T}} = \text{tr}(\mathbf{T}) \quad (2.31)$$

$$\text{II}_{\mathbf{T}} = \frac{1}{2} [\text{tr}(\mathbf{T})]^2 - \frac{1}{2} \text{tr}(\mathbf{T}^2) \quad (2.32)$$

$$\text{III}_{\mathbf{T}} = \det(\mathbf{T}) \quad (2.33)$$

The symbol  $\text{tr}(\cdot)$  denotes the trace of the tensor. The theorem allows us to write

$$\mathbf{T}^3 - \text{I}_{\mathbf{T}} \mathbf{T}^2 + \text{II}_{\mathbf{T}} \mathbf{T} - \text{III}_{\mathbf{T}} \mathbf{I} = 0 \quad (2.34)$$

thus

$$\mathbf{T}^3 = \mathbf{I}_T \mathbf{T}^2 - \mathbf{II}_T \mathbf{T} + \mathbf{III}_T \mathbf{I} \quad (2.35)$$

Similarly higher power of  $\mathbf{T}$  can be expressed in terms of the lower powers and the invariants of  $\mathbf{T}$ . Using this results for the rate-of-strain tensor  $2\mathbf{D}$  and assuming that the flow is incompressible, i.e  $\mathbf{I}_{2\mathbf{D}} = \text{tr}(2\mathbf{D}) = 2 \nabla \cdot \mathbf{u} = 0$ , we can rewrite the (2.28) as follows

$$\boldsymbol{\sigma} = -p\mathbf{I} + \eta_1 2\mathbf{D} + \eta_2 (2\mathbf{D})^2 \quad (2.36)$$

in which  $\eta_1$  and  $\eta_2$  are scalar functions of the invariants  $\mathbf{II}_{2\mathbf{D}}$  and  $\mathbf{III}_{2\mathbf{D}}$ :

$$\eta_1 = \eta_1 (\mathbf{II}_{2\mathbf{D}}, \mathbf{III}_{2\mathbf{D}}) \quad (2.37)$$

$$\eta_2 = \eta_2 (\mathbf{II}_{2\mathbf{D}}, \mathbf{III}_{2\mathbf{D}}) \quad (2.38)$$

where, since  $\text{tr}(2\mathbf{D}) = 0$  and  $\mathbf{D}$  is symmetric, the second invariant is simply

$$\mathbf{II}_{2\mathbf{D}} = -\frac{1}{2} \sum_{i,j=1}^3 4D_{ij}^2 = -\frac{1}{2} \sum_{i,j=1}^3 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \quad (2.39)$$

It is related to the second main invariant as follows:

$$J_{2\mathbf{D}}^{(2)} = \mathbf{I}_{2\mathbf{D}}^2 - 2 \cdot \mathbf{II}_{2\mathbf{D}} = \sum_{i,j=1}^3 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \quad (2.40)$$

The constitutive equation (2.36) represents a general viscous model and describes what are called *Reiner-Rivlin fluids* or sometimes *Stokesian fluids*. More generally, a fluid is said to be Stokesian if it satisfies the following postulates:

1.  $\boldsymbol{\sigma}$  is a continuous function of the deformation tensor  $\mathbf{D}$ , and is independent of all other kinematic quantities.
2.  $\boldsymbol{\sigma}$  does not depend explicitly on the position  $\mathbf{x}$  (*spatial homogeneity*).
3. There is no preferred direction in space (*isotropy*).
4. When  $\mathbf{D} = 0$ ,  $\boldsymbol{\sigma}$  reduces to  $-p\mathbf{I}$

It can be noticed that the Newtonian fluid is a special case of the Reiner-Rivlin fluid in which  $\eta_1 (\mathbf{II}_{2\mathbf{D}}, \mathbf{III}_{2\mathbf{D}}) = \mu$  and  $\eta_2 = 0$ . The term containing  $\eta_2$  gives rise to some problems; it generates normal stresses in simple shearing flow that are not in qualitative agreement with experimental observations and for this reason it is usually discarded. The general viscous fluid equation reduces to

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2 \eta_1 (\mathbf{II}_{2\mathbf{D}}, \mathbf{III}_{2\mathbf{D}}) \mathbf{D} \quad (2.41)$$

for which several expressions of  $\eta_1$  can be found in rheology literature.

# Chapter 3

## Equations for viscous incompressible fluids

### 3.1 Incompressible Navier-Stokes Equations

Assuming that the fluid is Newtonian and that the flow is incompressible, it is possible to use the linear relation between the viscous stress tensor and the rate of strain

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = 2\mu D_{ij} \quad (3.1)$$

in equations (1.81) and (1.82) which describe incompressible flows, and to obtain

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (3.2)$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.3)$$

The momentum equation can be also written as follows

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j^2} + \mu \frac{\partial}{\partial x_i} \left( \frac{\partial u_j}{\partial x_j} \right)$$

and using the mass conservation  $\partial u_j / \partial x_j = 0$ :

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j^2} \quad (3.4)$$

or, alternatively, in vector notation

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \rho \mathbf{f} - \nabla p + \mu \nabla^2 \mathbf{u} \quad (3.5)$$

This vector equation is called *Navier-Stokes Equation*. It is a generalization of the equation devised in the 18th century (1757) by the Swiss mathematician Leonhard Euler to describe the flow of incompressible and non-viscous fluids. The first derivation of the Navier-Stokes equation appeared in two articles ([6],[7]) published by the French engineer Claude-Louis Navier (1785 - 1836). After some theoretical developments failed to include the effects of viscosity in the equations of motion of fluids, these publications formally introduced, for

the first time, friction in fluid motion. Even if it was known that the friction of fluids was the main cause for deviation of experiments from theory, no scientist but Navier formally tackled this problem and succeeded in solving it. Navier's publications and studies on the theory of elasticity encouraged other investigators, such as Cauchy (1828), Poisson (1829) and de Saint-Venant (1843), to derive equations for viscous fluid motion using their own equations of elasticity. All of these 19th century investigators tried to fill the gap between the rational fluid mechanics of the perfect non viscous fluid developed in the 18th century and the actual behavior of real viscous fluids.

In 1880 the British physicist and mathematician Sir George Gabriel Stokes carried out some experiments on pendulum [8] to investigate the departure of real fluids from perfect ones. He pointed out that friction in fluids is the main cause of this departure, but not the only one; he recognised other causes such as discontinuity of flow and instabilities that lead to a turbulent wake behind the pendulum. Since it was not possible to carry out accurate experiments to prove his insights, he decided to include internal fluid friction in the fundamental equations of hydrodynamics. By assuming that the stress tensor is proportional to the rate of deformation tensor, similarly to Cauchy and Poisson, he obtained the equation of motion for viscous fluids given by Navier. Stokes then made extensive comparisons of theory and experiments of different researchers. He succeeded in obtaining good agreement with the Navier-Stokes equation by comparing predictions with experimental data for oscillating pendula [9]. Similarly to Navier, Stokes had a very clear intention on the practicality of his efforts by confronting theory with experiments, and this may be a reason why he and Navier became associated with the equation of motion for viscous flows. Associated with the incompressibility condition  $\nabla \cdot \mathbf{u} = 0$ , the Navier-Stokes equation is recognised to be the model which best describes the motion of Newtonian and incompressible fluids.

### 3.1.1 Global regularity problem and partial results

From a mathematical point of view the incompressible Navier-Stokes equations

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \rho \mathbf{f} - \nabla p + \mu \nabla^2 \mathbf{u} \quad (3.6)$$

represent a system of non-linear evolution partial differential equations (PDEs). The unknowns are the velocity field  $\mathbf{u}(\mathbf{x}, t) : [0, T) \times \mathbb{R}^3 \rightarrow \mathbb{R}^3$  and the pressure field  $p(\mathbf{x}, t) : [0, T) \times \mathbb{R}^3 \rightarrow \mathbb{R}$ . In these equations the density  $\rho$  and the dynamic viscosity  $\mu$  are known constant, whereas  $\mathbf{f}$  is a known vector field representing the external volumetric force. Since in three dimensional space there are three equations and four unknowns, it is necessary another equation: the continuity equation  $\nabla \cdot \mathbf{u} = 0$ . The solution for the Navier-Stokes equations are then searched in the set of divergence-free functions.

The natural problem to solve in an evolution equation is the *initial value problem*, in which, given some initial data (at time  $t = 0$ ), it is required to construct a solution with this data for later times. For the Navier-Stokes equation one specifies an initial velocity field  $\mathbf{u}_0 : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  obeying the incompressibility condition  $\nabla \cdot \mathbf{u} = 0$ ; the initial pressure has not to be specified since it can be derived from the initial velocity. As explained in the Section 1.4.2, because of incompressibility the pressure instantly adjusts itself so that the velocity field is divergence-free. Applying Leray projection to the Navier-Stokes equation (projection onto the divergence-free vector fields), one can indeed eliminate both the pressure term and the continuity equation (Appendix A).



Solving partial differential equations is not an easy task, especially when the equations are non-linear. First of all, the problem for a given PDE has to be *well-posed*, which means that

1. the problem in fact has a solution
2. this solution is unique
3. the solution depends continuously on the data given in the problem

Then, once the well-posedness has been shown, one can try to construct a solution which is required to be smooth enough: if the PDE in the problem has order  $k$ , the solution has to be at least  $k$  times continuously differentiable. At least all the derivatives which appear in the statement of the PDE will exist and be continuous, although maybe certain higher derivatives will not exist. A solution with this smoothness is called *classical solution* of the PDE. Thus, solving an evolution PDE in the classical sense means, if possible, to write down a formula for a classical solution for all the times which is unique, which depends continuously on the initial data, which is smooth enough, or at least to show such solution exists, and deduce its properties. However, certain partial differential equations can not be solved in the classical sense. The structure of some equations may force to abandon the search for smooth, classical solutions and, instead, investigate a wider class of candidates for solution for which one requires less strict regularity properties. Even for those PDE which turn out to be classically solvable, it is often wiser to initially search for some kind of solutions which are called *generalized* or *weak solutions*. For this kind of solutions it may be easier to establish existence, uniqueness and continuous dependence on the given data and then to prove the well-posedness of the problem. For some equations a weak solution may turn out after all to be smooth enough to be considered as classical; thus, in solving PDE, existence problem and regularity (or smoothness) problem are usually tackled separately.

For the incompressible Navier-Stokes equations the global existence and smoothness problem is still open. For the three-dimensional system of equations, and given some initial conditions, mathematicians have not yet proved that smooth solutions always exist. In May 2000 this led the Clay Mathematics Institute to make this problem one of its seven *Millennium Prize* problems in mathematics, offering a one million dollar prize to the first person who proves or disproves the existence and the regularity of the Navier-Stokes solutions in the whole space  $\mathbb{R}^3$  or in the three-dimensional torus  $\mathbb{T}^3$ . The official statement of the problem in the whole space  $\mathbb{R}^3$  is the following [10]:

The *Navier-Stokes* equations are given by

$$\frac{\partial u_i}{\partial t} + \sum_{j=1}^n u_j \frac{\partial u_i}{\partial x_j} = \nu \Delta u_i - \frac{\partial p}{\partial x_i} + f_i(x, t) \quad (x \in \mathbb{R}^n, t \geq 0) \quad (3.7)$$

$$\sum_{i=1}^n \frac{\partial u_i}{\partial x_i} = 0 \quad (x \in \mathbb{R}^n, t \geq 0) \quad (3.8)$$

with initial conditions

$$u(x, 0) = u^0(x) \quad (x \in \mathbb{R}^n) \quad (3.9)$$

Here,  $u^\circ(x)$  is a given,  $C^\infty$  divergence-free vector field on  $\mathbb{R}^n$ ,  $f_i(x, t)$  are the components of a given, externally applied force,  $\nu$  is a positive coefficient (the viscosity), and  $\Delta$  is the Laplacian in the space variables. The *Euler equations* are equation (3.7), (3.8), (3.9) with  $\nu$  set equal to zero. [...] For physically reasonable solution, we want to make sure  $u(x, t)$  does not grow large as  $|x| \rightarrow \infty$ . Hence, we will restrict our attention to forces  $f$  and initial conditions  $u^\circ$  that satisfy

$$|\partial_x^\alpha u^\circ| \leq C_{\alpha K} (1 + |x|)^{-K} \quad \text{on } \mathbb{R}^n, \text{ for any } \alpha \text{ and } K \quad (3.10)$$

and

$$|\partial_x^\alpha \partial_t^m f(x, t)| \leq C_{\alpha m K} (1 + |x| + t)^{-K} \quad \text{on } \mathbb{R}^n \times [0, \infty), \text{ for any } \alpha, m, K \quad (3.11)$$

We accept a solution of (3.7), (3.8), (3.9) as physically reasonable only if it satisfies

$$p, u \in C^\infty(\mathbb{R}^3 \times [0, \infty)) \quad (3.12)$$

and

$$\int_{\mathbb{R}^n} |u(x, t)|^2 < C \quad \text{for all } t \geq 0 \text{ (bounded energy)}. \quad (3.13)$$

[...] A fundamental problem in analysis is to decide whether such smooth, physically reasonable solutions exist for the Navier–Stokes equations. To give reasonable leeway to solvers while retaining the heart of the problem, we ask for a proof of one of the following four statements.

**(A) Existence and smoothness of Navier–Stokes solutions on  $\mathbb{R}^3$ .** Take  $\nu > 0$  and  $n = 3$ . Let  $u^\circ(x)$  be any smooth, divergence-free vector field satisfying (3.10). Take  $f(x, t)$  to be identically zero. Then there exist smooth functions  $p(x, t)$ ,  $u_i(x, t)$  on  $\mathbb{R}^3 \times [0, \infty)$  that satisfy (3.7), (3.8), (3.9), (3.12), (3.13). [...]

**(C) Breakdown of Navier–Stokes solution on  $\mathbb{R}^3$ .** Take  $\nu > 0$  and  $n = 3$ . Then there exist a smooth, divergence-free vector field  $u^\circ(x)$  on  $\mathbb{R}^3$  and a smooth  $f(x, t)$  on  $\mathbb{R}^3 \times [0, \infty)$ , satisfying (3.10), (3.11), for which there exist no solutions of (3.7), (3.8), (3.9), (3.12), (3.13) on  $\mathbb{R}^3 \times [0, \infty)$ .

Even if the problem is still unsolved, some partial results have been achieved regarding the Navier–Stokes equations:

1. The Navier–Stokes problem in two dimensions has already been solved positively since the 1930s: there exist smooth and globally defined solutions.
2. In three dimensions, it is known that there exist smooth and globally defined solutions to the Navier–Stokes equation provided the initial velocity  $u^\circ(x)$  satisfies a smallness condition.
3. In three demensions, for initial data  $u^\circ(x)$  not assumed to be small, it is known that there exist smooth and globally defined solutions to the Navier–Stokes equation (also for  $\nu = 0$ , Euler equation) if the time interval  $[0, \infty)$  is replaced by a small time

interval  $[0, T)$ , with  $T$  depending on the initial data (*local existence*). For a given initial  $u^\circ(x)$ , the maximum allowable  $T$  is called the *blowup time*. The solution becomes unbounded ( $u \rightarrow \infty$ ) near the blowup time and it is not known if the solutions exist beyond the blowup time. It is not known if  $T$  is whether or not finite.

4. In 1934 Jean Leray [11] showed that the Navier–Stokes equations in three space dimensions always have a weak solution  $(p, u)$  with suitable growth properties. However uniqueness of weak solutions of the Navier–Stokes equation is not known.
5. In 1982 Caffarelli–Kohn–Nirenberg [12] proved a partial regularity theorem for suitable weak solutions of the Navier–Stokes equations.
6. In 2016 Terence Tao [13] published a finite time blowup result for an averaged version of the three-dimensional Navier–Stokes equation. For these averaged equations which satisfy the same energy identity of the original Navier–Stokes equation

$$\frac{1}{2} \frac{\partial}{\partial t} \int_{\mathbb{R}^3} |u|^2 \, dx = -\nu \int_{\mathbb{R}^3} |\nabla u|^2 \, dx$$

Tao has recognized a *supercriticality barrier* in the global regularity problem for which the boundedness of the energy does not seem to prevent the finite time blowup of the solution. Tao then claims that this result can be extended to the *true* Navier–Stokes equations and that the method of proof in fact hints at a possible route to establishing blowup for the true equations.

One may wonder why three-dimensional Navier–Stokes problem is so hard. According to Terence Tao [14]

the answer to this question is *Turbulence* - the behaviour of three-dimensional Navier–Stokes equations at fine scales is much more nonlinear (and hence unstable) than at coarse scales. I would phrase the obstruction slightly differently, as *supercriticality*. Or more precisely, all of the globally controlled quantities (such as the total energy) for Navier–Stokes evolution which we are aware of (and we are not aware of very many) are either *supercritical* with respect to scaling, which means that they are much weaker at controlling fine-scale behaviour than controlling coarse-scale behaviour, or they are *non-coercive*, which means that they do not really control the solution at all, either at coarse scales or at fine.

And then they can't be used to show the solution does not blow up. According to Tao one of the most promising strategies in tackling Navier–Stokes problem would be

Discover a new globally controlled quantity which is both coercive and either critical or subcritical; [...] but apart from the energy, it is not clear if there are any physical quantities of fluids which are deterministically monotone. [...] Given the turbulent, unstable, and chaotic nature of Navier–Stokes, it is quite conceivable that in fact no reasonable globally controlled quantities exist beyond that which arise from the energy.

### 3.2 Ladyzhenskaya's Equations

The Navier-Stokes equations are generally recognized as an accurate model for the incompressible motion of viscous fluids in many practical situations, and there are many who believe this is true even for turbulent flows since results from numerical simulations show turbulent behavior. However, the linear constitutive law used to express the viscous stress tensor in the Navier-Stokes presumes that derivatives of the components of the velocity are small. Moreover, as previously seen, the linear relation used to express the viscous stress tensor cannot describe the viscous behavior of the vast category of the non-Newtonian fluids. There are then various reasons why one could abandon the Navier-Stokes equation in favor of model employing nonlinear constitutive laws.

In *New equations for the description of the motions of viscous incompressible fluids, and global solvability for their boundary value problems* [15], the Russian mathematician Olga Ladyzhenskaya introduced some alternative models to describe the incompressible flow of viscous fluids which differ from the Navier-Stokes equations for the diffusive term only. The most interesting model is

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \mathcal{A}(\mathbf{u}) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + f_i \quad (3.14)$$

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (3.15)$$

where, in the three-dimensional space,  $i = 1, 2, 3$  and  $\mathcal{A}(\mathbf{u})$  is defined by

$$\mathcal{A}(\mathbf{u}) = \nu_0 + \nu_1 \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \right]^{\frac{r}{2}} \quad \text{with } r > 0 \quad (3.16)$$

In the equation (3.16)  $\nu_0$  and  $\nu_1$  are two positive constants, analogous to the kinematic viscosity ( $\nu = \mu/\rho$ ). The equation (3.15) is simply the divergence-free condition of the velocity field, whereas the vector equation (3.14) is a *momentum equation* which can be rewritten as follows:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \nu_0 \frac{\partial^2 u_i}{\partial x_j^2} + \boxed{\nu_1 \frac{\partial}{\partial x_j} \left[ \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \right]^{\frac{r}{2}} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right]} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + f_i \quad (3.17)$$

This form shows evidently that Ladyzhenskaya's equation is basically the Navier-Stokes equation with some additional non-linear diffusive terms (the boxed ones). Setting the parameter  $r$  to zero, one obtains the Navier-Stokes equation with  $\nu = \nu_0 + \nu_1$ ; thus, from a modeling stand point, the Navier-Stokes equation is a special case of the Ladyzhenskaya equation. Similarly to the Navier-Stokes equation, the Ladyzhenskaya equation can indeed be derived using the mass and the momentum conservation laws and supposing the fluid to be Stokesian (see Section 2.3), which means supposing that the stress tensor can be expressed by

$$\boldsymbol{\sigma} = -p\mathbf{I} + \eta_1 2\mathbf{D} + \eta_2 (2\mathbf{D})^2 \quad (3.18)$$

in which  $\eta_1$  and  $\eta_2$  are scalar functions of the principal invariants  $\text{II}_{2\mathbf{D}}$  and  $\text{III}_{2\mathbf{D}}$ :

$$\eta_1 = \eta_1(\text{II}_{2\mathbf{D}}, \text{III}_{2\mathbf{D}}) \quad (3.19)$$

$$\eta_2 = \eta_2 (\text{II}_{2\mathbf{D}}, \text{III}_{2\mathbf{D}}) \quad (3.20)$$

For incompressible flows

$$\text{I}_{2\mathbf{D}} = 2 \nabla \cdot \mathbf{u} = 0 \quad (3.21)$$

$$\text{II}_{2\mathbf{D}} = -\frac{1}{2} \sum_{k,l=1}^3 4D_{kl}^2 = -\frac{1}{2} \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 = -\frac{\widehat{d}^2}{2} \quad (3.22)$$

$$\text{III}_{2\mathbf{D}} = 2 \det(D) \quad (3.23)$$

In particular, the scalar quantity  $\widehat{d}^2$ , which is the second main invariant of  $2\mathbf{D}$ , is:

$$\begin{aligned} \widehat{d}^2 = & 4 \left[ \left( \frac{\partial u_1}{\partial x_1} \right)^2 + \left( \frac{\partial u_2}{\partial x_2} \right)^2 + \left( \frac{\partial u_3}{\partial x_3} \right)^2 \right] + 2 \left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)^2 + 2 \left( \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right)^2 + \\ & + 2 \left( \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)^2 \end{aligned} \quad (3.24)$$

Then the stress tensor can be rewritten as follows:

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta_1 \left( \widehat{d}^2, \det(D) \right) \mathbf{D} + 4\eta_2 \left( \widehat{d}^2, \det(D) \right) \mathbf{D}^2 \quad (3.25)$$

If one retains some of the nonlinear terms of this constitutive law then arrives at the Ladyzhenskaya models. In fact, if one assume that  $\eta_2 = 0$  and

$$\eta_1 \left( \widehat{d}^2 \right) = \nu_0 \left( 1 + \varepsilon \widehat{d}^2 \right) \quad (3.26)$$

it is possible to obtain

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\nu_0 \mathbf{D} + 2\varepsilon \nu_0 \widehat{d}^2 \mathbf{D} \quad (3.27)$$

or

$$\sigma_{ij} = -p\delta_{ij} + \nu_0 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \varepsilon \nu_0 \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \right] \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.28)$$

which is exactly the stress tensor provided by the Ladyzhenskaya model [16] with  $r = 2$  and  $\nu_1 = \varepsilon \nu_0$ . Ladyzhenskaya also gives a partial justification, based on kinetic theory arguments, for why one should retain the nonlinear terms she chooses to include in the constitutive relation. Information about the constant  $\nu_1$  and the parameter  $r$  may be derived from the kinetic theory of gases and the Stokes hypotheses; however, generally one can assume  $\nu_1 \ll \nu_0$ , whereas two natural choices for  $r$  are  $r = 1$  and  $r = 2$ .

The most interesting feature of these sets of equations is that Olga Ladyzhenskaya has proven in [15] and [16] that weak solutions to the initial values problem for these equations are globally unique in time for any Reynolds number and parameter  $r \geq 1/2$ . In 1989 [17] this results has been extended to  $r \geq 1/5$ .

# Chapter 4

## Turbulence

Chaos: When the present determines the future, but the approximate present does not approximately determine the future.

---

- Edward Norton Lorenz, 2005.

*Turbulence is a chaotic motion of real fluids that are subject to shearing forces* [18]. It can be regarded as an example of *deterministic chaos*: classical events which are described by deterministic equations and appear to be *random*. Dynamical systems whose apparently random states and irregularities are actually governed by deterministic laws that are highly sensitive to initial conditions, are said to be *Chaotic*. Two other famous examples of such systems are the double pendulum (Figure 4.1) and the Lorenz attractor [28] (Figure 4.2).

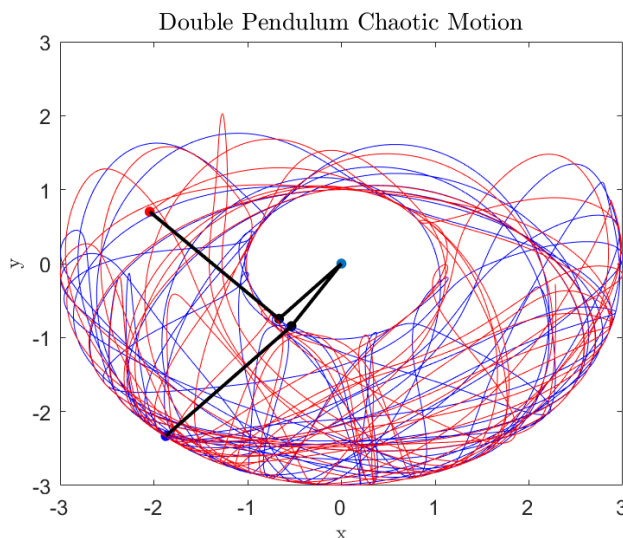


Figure 4.1: Double Pendulum - Chaotic Motion and sensitivity to initial conditions: solutions obtained for two identical double pendula with slightly different initial positions.

A rigorous definition of turbulence does not exist and would not be useful without describing its characteristics. Some of the known characteristic features of fluid turbulence are the following:

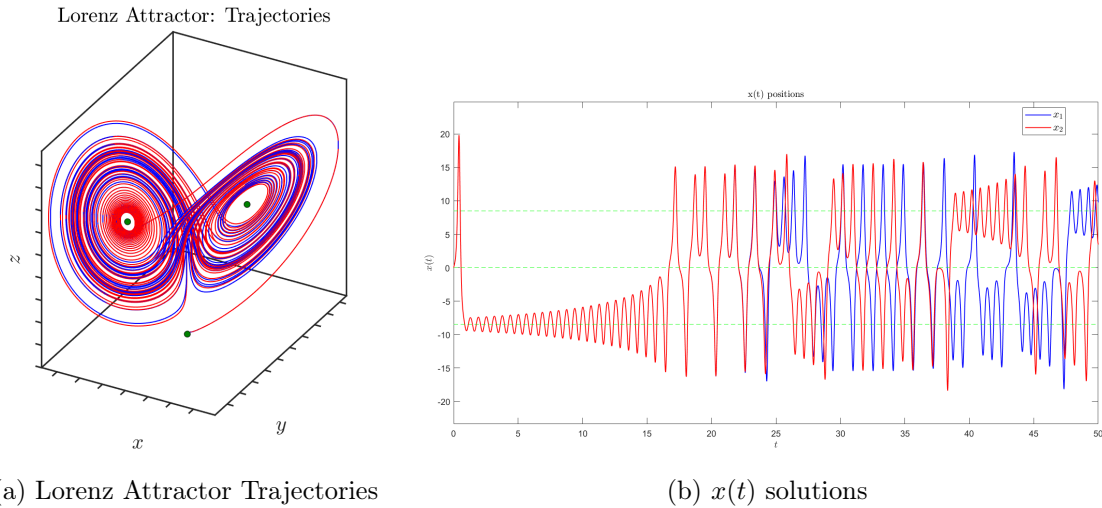


Figure 4.2: Solutions of Lorenz System (Attractor): solutions obtained for two identical systems ( $\rho = 28$ ,  $\sigma = 10$ ,  $\beta = 8/3$ ) which have slightly different initial positions  $\mathbf{x}^\circ$  ( $\mathbf{x}_1^\circ = \{0, 1, 0\}$  and  $\mathbf{x}_2^\circ = \{0, 1.001, 0\}$ ). Solutions show chaotic behaviour and extreme sensitivity to initial conditions.

- Turbulent flows are irregular and chaotic. Fluid velocity is a random function of space and time, with a non-Gaussian probability distribution. Even if equations of fluid motion are deterministic, solutions may be random because in real flows there are, unavoidably, perturbations in initial conditions, boundary conditions and material properties and, moreover, turbulent flows display an extreme sensitivity to such perturbations.
- Turbulent flows occur when Reynolds number is sufficiently high. Below critical Reynolds numbers, disturbances cannot generate flow instabilities and turbulent flows cannot exist.
- Turbulence consists of many eddying motions, of various sizes and speeds which define the so-called length and velocity scales. Turbulence contains in fact a wide and continuous range of space and time scales. The different scales coexist superimposed in the flow, with the smaller ones living inside the larger ones. The largest eddies are of the order of the flow geometry and may break up into smaller eddies.
- Turbulent flows are unsteady and three-dimensional in nature. However, for Navier-Stokes equations has been proved in [29] that Leray-Hopf weak solutions of the equations preserve initially imposed symmetry or two-dimensionality and that such two-dimensional or symmetric flows are stable under general three-dimensional perturbations, globally in time. Thus if the initial velocity field is two-dimensional or, for example, axisymmetric, then Leray-Hopf weak solution of three-dimensional incompressible Navier-Stokes remains two-dimensional or axisymmetric.
- Turbulent flows are highly dissipative; kinetic energy is transferred from largest scales to smaller scales in a *cascade* process, then the smallest eddies dissipate this energy into thermal energy. The rate at which kinetic energy is dissipated is usually denoted by  $\varepsilon$ .

- Turbulent flows are strongly *mixing* in nature; turbulent velocity fluctuations results in an eddying motion which enhances diffusivity and mixing.

In 1922 Lewis Fry Richardson [30] recognized maybe the main phenomenology of turbulence: the *energy cascade* process. The largest eddies, whose length and velocity scales are comparable to the flow ones, are characterized by large Reynolds numbers and their dynamic is essentially inviscid; because of the large Reynolds number, they are unstable and break-up, transferring their energy to somewhat smaller eddies. These smaller eddies undergo similar break-up processes transferring their energy to yet smaller eddies. This process goes on until the Reynolds number is sufficiently small that eddy motion is stable, and molecular viscosity is effective in dissipating kinetic energy. The smallest eddy motion is usually referred to as *dissipative* or *Kolmogorov scale*, after the Soviet mathematician Andrey Nikolaevich Kolmogorov who proposed in 1941 the first statistical theory of turbulence based on the Richardson's notion of the energy cascade. Kolmogorov stated that for very high Reynolds numbers the small-scale turbulent motions are statistically isotropic, i. e. velocity statistics are invariant under rotations and reflections of the coordinate system. This means that, while the scale is reduced, the directional information is lost, and turbulence at small scales has a universal character which does not depend on the type of flow. He then postulated that in every turbulent flow at sufficiently high Reynolds number, the statistics of the motions of small scale have a universal form that is uniquely determined by the kinematic viscosity  $\nu$  and the energy dissipation rate  $\varepsilon$ . With only these two parameters, the unique length, velocity and time scales that can be formed by dimensional analysis are respectively

$$\begin{aligned}\eta &= \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \\ v_\eta &= (\nu\varepsilon)^{1/4} \\ \tau_\eta &= \left(\frac{\nu}{\varepsilon}\right)^{1/2}\end{aligned}\tag{4.1}$$

which are called Kolmogorov or dissipative scales. Assuming that the rate of dissipation  $\varepsilon$  is entirely determined by characteristics of the large eddies (the velocity  $U$ , the length  $L$  and the time  $\Theta$ )

$$\varepsilon = \frac{U^3}{L}\tag{4.2}$$

it is possible to write the ratio between Kolmogorov and flow scales as function of the Reynolds number  $\text{Re}_L = UL/\nu$

$$\begin{aligned}\frac{\eta}{L} &= \text{Re}_L^{-3/4} \\ \frac{v_\eta}{U} &= \text{Re}_L^{-1/4} \\ \frac{\tau_\eta}{\Theta} &= \text{Re}_L^{-1/2}\end{aligned}\tag{4.3}$$

which show that as the Reynolds number increases the gap between the large and the small structure increases, and for very high Reynolds numbers the small scale motions are independent of the largest structures.

It is then possible to recognize in turbulence three ranges (Figure 4.3 ):

1. the *energy containing range* corresponding to the largest eddy motion which produces turbulence kinetic energy from the flow and which contains most of this energy;



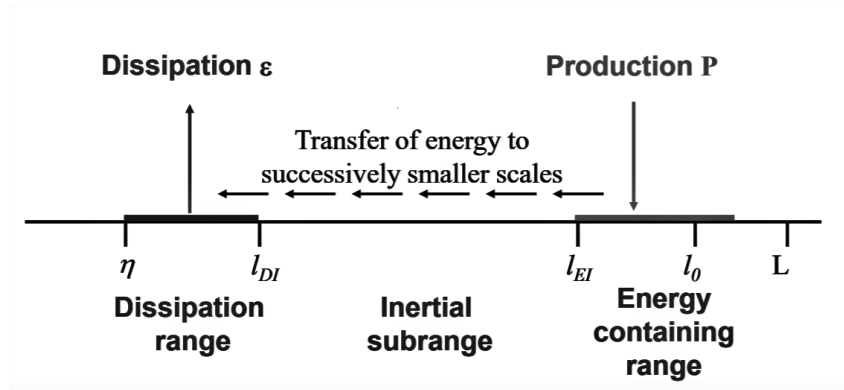


Figure 4.3: Turbulence length scales

2. the *dissipation range* corresponding to the small scale motion in which viscosity is effective in dissipating kinetic energy;
3. the *inertial subrange* corresponding to the intermediate scales in which energy cascade process takes place, transferring energy to smaller and smaller scales. The extension of this intermediate range depends on the Reynolds number according to the expressions (4.3). As the Reynolds number increases the inertial subrange becomes wider.

## 4.1 Statistical description of turbulence and mean flow equations

In a turbulent flow, the velocity field  $\mathbf{u}(\mathbf{x}, t)$  is a time-dependent *random vector field* and its values are inherently unpredictable. It is possible, however, to determine the *probability* that the value of a random variable  $U$ , or a random field  $\mathbf{u}(\mathbf{x}, t)$ , is within a certain interval. A random variable  $U$  can be in fact completely characterized by its *probability density function* (PDF). Introducing an independent velocity variable  $V$ , referred to as the *sample-space* variable corresponding to  $U$ , it is possible to define the *cumulative distribution function* (CDF) as

$$F(V) := P\{U < V\} \quad (4.4)$$

which represents the probability  $p$  of the event  $\{U < V\}$ . The probability  $p$  of an event is a real number, such that  $0 \leq p \leq 1$ , indicating the likelihood of the occurrence of the event. If  $p = 0$  the event cannot occur, if instead  $p = 1$  the event certainly occurs. The higher the probability of an event, the more likely it is that the event will occur.

The *probability density function* (PDF) is defined to be the derivative of the cumulative distribution function:

$$f(V) := \frac{dF(V)}{dV} \quad (4.5)$$

The cumulative distribution function has the following properties:

- since  $\{U < -\infty\}$  is impossible,  $F(-\infty) = 0$ ;
- since  $\{U < \infty\}$  is certain,  $F(\infty) = 1$ ;

- since the probability  $p$  is non-negative,  $F(V_b) \geq F(V_a)$  for  $V_b > V_a$ . Thus, the CDF is a non-decreasing function.

From this last CDF property follows that the PDF is non-negative:  $f(V) \geq 0$ . Moreover, the PDF satisfies the condition

$$\int_{-\infty}^{\infty} f(V) dV = 1 \quad (4.6)$$

and  $f(-\infty) = f(\infty) = 0$ .

Using the PDF it is possible to define the *mean* (or *expectation*) of the random variable  $U$  as

$$\langle U \rangle = \int_{-\infty}^{\infty} V f(V) dV. \quad (4.7)$$

It represents the first-order moment of  $U$ . The *fluctuating* in  $U$  is

$$U' = U - \langle U \rangle. \quad (4.8)$$

The *variance* is defined to be the mean-square fluctuation:

$$\text{var}(U) = \langle U'^2 \rangle = \int_{-\infty}^{\infty} (V - \langle U \rangle)^2 f(V) dV \quad (4.9)$$

and represents the second-order central moment of  $U$ . The square-root of the variance defines the *standard deviation*:

$$\text{sdev}(U) = \sigma_U = \sqrt{\text{var}(U)} = \langle U'^2 \rangle^{\frac{1}{2}} \quad (4.10)$$

which is a *measure* of the random fluctuations. In general the *n*th central moment is

$$\mu_n := \langle U'^n \rangle = \int_{-\infty}^{\infty} (V - \langle U \rangle)^n f(V) dV \quad (4.11)$$

The moments can be *standardized* to have zero mean (*central moment*) and unit variance as follows:

$$\hat{\mu}_n := \frac{\mu_n}{\sigma_U^n} \quad (4.12)$$

The third and fourth order standardized central moments are called respectively *skewness* ( $\hat{\mu}_3$ ) and *kurtosis* ( $\hat{\mu}_4$ ).

Having two joint random variables  $(U_1, U_2)$  the CDF is defined by

$$F_{12}(V_1, V_2) := P\{U_1 < V_1, U_2 < V_2\} \quad (4.13)$$

The joint PDF is then

$$f_{12}(V_1, V_2) := \frac{\partial^2}{\partial V_1 \partial V_2} F_{12}(V_1, V_2) \quad (4.14)$$

The *covariance* of  $U_1$  and  $U_2$  is the mixed second moment

$$\text{cov}(U_1, U_2) = \langle U_1' U_2' \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (V_1 - \langle U_1 \rangle) (V_2 - \langle U_2 \rangle) f_{12}(V_1, V_2) dV_1 dV_2 \quad (4.15)$$

These notions can be extended to time-dependent random vector fields  $\mathbf{u}(\mathbf{x}, t) = \{u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)\}^T$ ; the one-point and one-time joint CDF of velocity is

$$F(\mathbf{v}, \mathbf{x}, t) := P\{u_i(\mathbf{x}, t) < v_i, i = 1, 2, 3\} \quad (4.16)$$

and then the joint PDF is

$$f(\mathbf{v}; \mathbf{x}, t) := \frac{\partial^3}{\partial v_1 \partial v_2 \partial v_3} F(\mathbf{v}, \mathbf{x}, t) \quad (4.17)$$

The mean velocity field is

$$\langle \mathbf{u}(\mathbf{x}, t) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathbf{v} f(\mathbf{v}; \mathbf{x}, t) \, dv_1 \, dv_2 \, dv_3 \quad (4.18)$$

then the fluctuating field is defined as follows

$$\mathbf{u}'(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}, t) - \langle \mathbf{u}(\mathbf{x}, t) \rangle \quad (4.19)$$

The simplest statistic which contains information on the spatial structure of the field  $\mathbf{u}(\mathbf{x}, t)$  is the two-point, one-time *autocovariance* (also named *two-point correlation*):

$$R_{ij}(\mathbf{r}, \mathbf{x}, t) = \langle u'_i(\mathbf{x}, t) u'_j(\mathbf{x} + \mathbf{r}, t) \rangle \quad (4.20)$$

which integrated in any direction and divided by  $R_{ij}(0, \mathbf{x}, t)$ , gives the integral lengthscale in that direction; for example, the integral lengthscale in direction  $\mathbf{e}_1$  is

$$L_{ij}^{(1)}(\mathbf{x}, t) = \frac{1}{R_{ij}(0, x_1, t)} \int_{-\infty}^{\infty} R_{ij}(\mathbf{e}_1 r, \mathbf{x}, t) \, dr \quad (4.21)$$

The integral lengthscale provides a quantitative measure of the correlation length scale at the time  $t$ .

Random processes whose multi-time statistics are invariant under a shift in time are said to be *statistically stationary*; for such processes the simplest multi-time statistic is the autocovariance (a one-point two-time covariance):

$$R_{ij}^{(t)}(\mathbf{x}, \tau) = \langle u'_i(\mathbf{x}, t) u'_j(\mathbf{x}, t + \tau) \rangle \quad (4.22)$$

or, in normalized form, the autocovariance function

$$\rho_{ij}^{(t)}(\mathbf{x}, \tau) = \frac{R_{ij}^{(t)}(\mathbf{x}, \tau)}{R_{ij}^{(t)}(\mathbf{x}, 0)} \quad (4.23)$$

which integrated in  $\tau$  gives the integral timescale of the process:

$$\Theta_{ij}(\mathbf{x}) = \int_0^{\infty} \rho_{ij}^{(t)}(\mathbf{x}, \tau) \, d\tau \quad (4.24)$$

which provides a quantitative measure of the correlation timescale in the point  $\mathbf{x}$ . For turbulent flows the integral length and time scales are the characteristic length and time of the largest eddies; moreover, their ratio defines the velocity scale  $U = L/\Theta$  which is comparable to the flow velocity.

### 4.1.1 Reynolds-averaged equations

According to the *Reynolds decomposition* for turbulent flows one can decompose the velocity and the pressure fields in the sum of a time-averaged field and a fluctuating field associated with turbulence:

$$\begin{aligned} u_i(\mathbf{x}, t) &= \overline{u_i} + u'_i \\ p(\mathbf{x}, t) &= \overline{p} + p' \end{aligned} \quad (4.25)$$

The time-averaged field is denoted by the overbar, whereas the apex denotes the turbulent fluctuating field. Mathematically, the time average can be defined as follows.

**Time Average.** Let  $u(\mathbf{x}, t)$  be an integrable function with respect to  $t$  for  $t \rightarrow \infty$  and defined for any desired  $\mathbf{x} \in \mathbb{R}^d$ ,  $d = 1, 2, 3$ . Then the time average of  $u$  at the point  $\mathbf{x}$  is defined as

$$\bar{u}(\mathbf{x}) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T u(\mathbf{x}, t) dt \quad (4.26)$$

It is clear that the average cannot be a function of time, and it follows that all time derivatives of  $\bar{u}(\mathbf{x})$  are identically zero. It is possible another operation of average, the *ensemble average*, defined as follows.

**Ensemble Average.** Let  $\{u^{(i)}(\mathbf{x}, t)\}_{i=1}^N$  be a sequence of realizations of a function  $u(\mathbf{x}, t)$  defined for  $\mathbf{x} \in \mathbb{R}^d$  and  $t \in [0, t_f]$ . Then the *ensemble average* of  $u$  is defined as

$$\langle u(\mathbf{x}, t) \rangle := \frac{1}{N} \sum_{i=1}^N u^{(i)}(\mathbf{x}, t) \quad (4.27)$$

and it is formally a time-dependent quantity. For *ergodic processes*, i.e. stochastic processes whose statistical properties can be deduced from a single, sufficiently long, random sample of the process, time averages and ensemble averages are equivalent as the number of realizations  $N$  tends to infinity. Thus assuming that the turbulence is ergodic, one can use ensemble averages instead of time averages and formally keep the time dependence in the averaged fields.

Introducing the Reynolds decomposition with ensemble averages in the Navier-Stokes equations and taking the average of the resulting equations, one obtains the *Reynolds-averaged Navier-Stokes equations* (RANS):

$$\begin{cases} \rho \frac{\partial \langle u_i \rangle}{\partial t} + \rho \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{\partial \langle p \rangle}{\partial x_i} + \mu \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \rho \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} \\ \frac{\partial \langle u_j \rangle}{\partial x_j} = 0 \end{cases} \quad (4.28)$$

The momentum equation in the RANS is formally the Navier-Stokes equation for the mean flow with some additional terms arising from averaging the original nonlinear term. These additional terms have the physical dimensions of a stress and form a symmetric tensor

$$R_{ij} = -\rho \langle u'_i u'_j \rangle \quad (4.29)$$

called *Reynolds stress tensor*. The mean velocity depends on the covariance of the fluctuating velocities and this introduces the closure problem for the set of RANS.

It is possible to introduce the Reynolds decomposition in the Ladyzhenskaya equations as well. The Reynolds-averaged Ladyzhenskaya equations will be similar to the RANS with some additional terms deriving from the nonlinear diffusive terms (Appendix B):

$$\begin{cases} \rho \frac{\partial \langle u_i \rangle}{\partial t} + \rho \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = -\frac{\partial \langle p \rangle}{\partial x_i} + \mu_0 \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \rho \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} + \\ + \mu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} + \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \right] + \mu_1 \frac{\partial Z_{ij}}{\partial x_j} \\ \frac{\partial \langle u_j \rangle}{\partial x_j} = 0 \end{cases} \quad (4.30)$$

where

$$Z_{ij} = \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_k}{\partial x_l} + \frac{\partial u'_l}{\partial x_k} \right)^2 \right\rangle \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) + \sum_{k,l=1}^3 \left\langle \left[ \left( \frac{\partial u'_k}{\partial x_l} \right)^2 + \left( \frac{\partial u'_l}{\partial x_k} \right)^2 \right] d'_{ij} \right\rangle +$$

$$+ 2 \sum_{k,l=1}^3 \left[ \frac{\partial \langle u_k \rangle}{\partial x_l} \left\langle \frac{\partial u'_k}{\partial x_l} d'_{ij} \right\rangle + \frac{\partial \langle u_l \rangle}{\partial x_k} \left\langle \frac{\partial u'_l}{\partial x_k} d'_{ij} \right\rangle \right]$$

and

$$d'_{ij} = \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}$$

### 4.1.2 Homogeneous Isotropic Turbulence (HIT)

A random field  $\mathbf{u}(\mathbf{x}, t)$  is *statistically homogenous* if all statistics (moments and mixed moments) are invariant under a shift in position, i. e. under any translation. Turbulence, instead, is said to be *homogeneous* if its fluctuating velocity field  $\mathbf{u}'(\mathbf{x}, t)$  is statistically homogeneous. If an homogeneous random field  $\mathbf{u}(\mathbf{x}, t)$  is also statistically invariant under rotations and reflections of the coordinate system, then it is said to be *statistically isotropic*.

In general real turbulent flows are not homogeneous because the presence of boundaries and other physical constraints results in spatial variation of flow statistical properties; real fluids are not generally isotropic neither, since the simple idea of a flow direction is incompatible with isotropy. However there exist some flows in which some regions can be considered as characterized by homogeneity and isotropy in a *local sense*; examples are those regions in large-scale flows which are far from boundaries.

By definition, for homogeneous turbulence the two-point correlation (4.20) is independent of  $\mathbf{x}$ :  $R_{ij}(\mathbf{r}, t)$ . Using the Fourier's Transform it is then possible to transform the two-point correlation from the physical space to the wavenumber space  $\mathbf{k}$  obtaining the *velocity spectrum* tensor:

$$\Phi_{ij}(\mathbf{k}, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R_{ij}(\mathbf{r}, t) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \quad (4.31)$$

thus, one can obtain the *energy spectrum function*:

$$E(k, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2} \Phi_{ii}(\mathbf{k}, t) \delta(|\mathbf{k}| - k) d\mathbf{k} \quad (4.32)$$

which shows, for every time, how turbulent kinetic energy  $\Phi_{ii}(\mathbf{k}, t)/2$  is distributed among the different wavenumbers.

**Energy Equation.** Ladyzhenskaya equations with  $r = 2$  are

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + \nu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \quad (4.33)$$

along with the mass conservation

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (4.34)$$

Multiplying (4.33) by  $u_i$ , summing over  $i$  and taking the ensemble average over space one obtains

$$\begin{aligned} \frac{1}{2} \frac{\partial \langle u_i^2 \rangle}{\partial t} + \left\langle u_i \frac{\partial (u_i u_j)}{\partial x_j} \right\rangle &= -\frac{1}{\rho} \left\langle u_i \frac{\partial p}{\partial x_i} \right\rangle + \nu \left\langle u_i \frac{\partial^2 u_i}{\partial x_j^2} \right\rangle + \\ &+ \nu_1 \left\langle u_i \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \right\rangle \end{aligned} \quad (4.35)$$

The convective and the pressure term vanish. In fact the convective term can be rewritten as

$$2 \left\langle u_i \frac{\partial (u_i u_j)}{\partial x_j} \right\rangle = \frac{\partial}{\partial x_j} \langle u_i^2 u_j \rangle - \left\langle u_i^2 \frac{\partial u_j}{\partial x_j} \right\rangle \quad (4.36)$$

The first term on right-hand side is zero because, by homogeneity, the average is constant and its derivative is zero, whereas the second term vanishes thanks to continuity  $\partial u_j / \partial x_j = 0$ . Similarly the pressure term can be rewritten as

$$\left\langle u_i \frac{\partial p}{\partial x_i} \right\rangle = \frac{\partial}{\partial x_i} \langle u_i p \rangle - \left\langle \frac{1}{\rho} \frac{\partial u_i}{\partial x_i} \right\rangle \quad (4.37)$$

and the two terms on the right-hand side vanish for the same reasons: homogeneity and continuity respectively.

The Newtonian viscous term becomes

$$\nu \left\langle u_i \frac{\partial^2 u_i}{\partial x_j^2} \right\rangle = \nu \left\langle u_i \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} \right) \right\rangle = \nu \frac{\partial}{\partial x_j} \left\langle u_j \frac{\partial u_i}{\partial x_j} \right\rangle - \nu \left\langle \left( \frac{\partial u_i}{\partial x_j} \right)^2 \right\rangle \quad (4.38)$$

and thanks to homogeneity

$$\nu \left\langle u_i \frac{\partial^2 u_i}{\partial x_j^2} \right\rangle = -\nu \left\langle \left( \frac{\partial u_i}{\partial x_j} \right)^2 \right\rangle \quad (4.39)$$

The nonlinear viscous term contribution is

$$\nu_1 \left\langle u_i \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \right\rangle \quad (4.40)$$

or alternatively

$$\nu_1 \left\langle u_i \frac{\partial}{\partial x_j} \left[ \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \right\rangle \quad (4.41)$$

where  $\widehat{d}^2$  is the scalar quantity

$$\widehat{d}^2 = \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \quad (4.42)$$

This contribution can be rewritten as

$$\nu_1 \left\langle u_i \frac{\partial}{\partial x_j} \left[ \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \right\rangle = \nu_1 \left\langle \frac{\partial}{\partial x_j} \left[ \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) u_i \right] \right\rangle - \nu_1 \left\langle \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \right\rangle \quad (4.43)$$

The first term on right-hand side vanishes because average and derivative can commute and thanks to homogeneity the derivative of the ensemble average is zero, thus

$$\nu_1 \left\langle u_i \frac{\partial}{\partial x_j} \left[ \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \right\rangle = -\nu_1 \left\langle \widehat{d}^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \right\rangle \quad (4.44)$$

Finally, energy balance is

$$\frac{1}{2} \frac{\partial \langle u_i^2 \rangle}{\partial t} = -\nu \left\langle \left( \frac{\partial u_i}{\partial x_j} \right)^2 \right\rangle - \nu_1 \sum_{i,j=1}^3 \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \right\rangle \quad (4.45)$$

or, compactly,

$$\frac{\partial E}{\partial t} = -\varepsilon - \varepsilon^{\text{lad}} \quad (4.46)$$

where

$$E = \frac{1}{2} \sum_{i=1}^3 \langle u_i^2 \rangle \quad (4.47)$$

is the kinetic energy,

$$\varepsilon = \nu \sum_{i,j=1}^3 \left\langle \left( \frac{\partial u_i}{\partial x_j} \right)^2 \right\rangle \quad (4.48)$$

is the *viscous Newtonian dissipation*, and

$$\varepsilon^{\text{lad}} = \nu_1 \sum_{i,j=1}^3 \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \right\rangle \quad (4.49)$$

is the *viscous dissipation* due to the nonlinear additional term in Ladyzhenskaya equations. Navier-Stokes energy equation can be simply obtained, as particular case, by setting the nonlinear viscous contribution to zero:

$$\frac{\partial E}{\partial t} = -\varepsilon \quad (4.50)$$

If one rewrites the additional dissipation as follows

$$\varepsilon^{\text{lad}} = \nu_1 \sum_{i,j=1}^3 \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left[ \left( \frac{\partial u_i}{\partial x_j} \right)^2 + \left( \frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} \right) \right] \right\rangle \quad (4.51)$$

one can observe that  $\widehat{d}^2$  and  $(\partial u_i / \partial x_j)^2$  are certainly positive, whereas the product

$$\frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j}, \quad (4.52)$$

which is basically the velocity gradient tensor multiplied by its transpose, might have negative off-diagonal entries.

# Concluding Remarks

The laws of conservation of mass, momentum and energy, which no one questions, provide a system of partial differential equations in which one has to model the viscous stress tensor  $\tau$  through a constitutive law which depends on the kind of fluid one is dealing with. As previously seen, the Navier-Stokes equations are based on the assumption of small velocity gradient so that a linear relation between the viscous stress tensor and the rate of deformation could hold. However, there exist many reasons why one should investigate new fluid dynamic models in which nonlinearities are included in the viscous stress tensor, such as better mathematical properties of solutions and the extension of the model to very large velocity gradient or to non-Newtonian fluids. From a mathematical standing point, studying some slightly modified Navier-Stokes equations could help in better understanding the behavior of the original ones, of their possible solutions and maybe Turbulence. The Navier-Stokes equations have smooth and globally defined solution in the two-dimensional space; the problem of global regularity is instead still unsolved for the three-dimensional space and many blame Turbulence, the random, chaotic and multi-scale fluid motion which, up to date, has no rigorous definition. One may then wonder if this kind of motion, whose characteristics are partially known, results also from other sets of equations for viscous incompressible fluids for which better mathematical results have been proved. In this sense, the Ladyzhenskaya equations with  $r = 2$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \nu_0 \frac{\partial^2 u_i}{\partial x_j^2} + \nu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{1}{\rho} \frac{\partial p}{\partial x_i}$$

$$\frac{\partial u_j}{\partial x_j} = 0$$

represent an useful tool for this kind of research. The basic idea of the present study is then to investigate numerically how the solutions of the Ladyzhenskaya equations differ from those of Navier-Stokes for a test case: free-decaying of Taylor-Green Vortex assuming the Turbulence to be homogeneous and isotropic. The additional diffusive term

$$\nu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right]$$

has clearly a *stabilizing* effect by strengthening the viscous term so that one should expect solutions which are more damped then those of the Navier-Stokes equations, but obviously it is not the same kind of damping which one achieves by simply increasing the viscosity. It is interesting to understand if Ladyzhenskaya equations develop Turbulence, similarly to other non-Newtonian viscous models, and eventually how turbulent solutions differ from those of the Navier-Stokes equations.



## Part II

# Numerical Investigation: Homogeneous Isotropic Turbulence

# Chapter 5

## Mathematical Problems

For our purposes, the two sets of equations we want to solve numerically are the previously presented:

- three-dimensional incompressible Navier-Stokes equations ( $i = 1, 2, 3$ )

$$\begin{cases} \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j^2} \\ \frac{\partial u_j}{\partial x_j} = 0 \end{cases} \quad (\text{NS})$$

- three-dimensional Ladyzhenskaya equations ( $i = 1, 2, 3$ ) with  $r = 2$

$$\begin{cases} \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho f_i - \frac{\partial p}{\partial x_i} + \mu_0 \frac{\partial^2 u_i}{\partial x_j^2} + \mu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \\ \frac{\partial u_j}{\partial x_j} = 0 \end{cases} \quad (\text{Lr2})$$

where  $\mathbf{u}(\mathbf{x}, t) = (u_1, u_2, u_3)$  and  $p(\mathbf{x}, t)$  are respectively the unknown velocity and pressure fields,  $\rho$  is the constant fluid density,  $\mu$  and  $\mu_0$  are the constant *Newtonian* dynamic viscosities and  $\mu_1$  is the additional constant *viscosity* appearing in the Ladyzhenskaya models (generally  $\mu_1 \ll \mu_0$ ); it is important to note that  $\mu_1$  actually has not the physical dimension of a viscosity, in fact

$$\mu_1 = [M] \cdot [T] \cdot [L]^{-1}$$

whereas

$$\mu = [M] \cdot [T]^{-1} \cdot [L]^{-1}$$

For simplicity we set the volumetric forces  $\mathbf{f}(\mathbf{x}, t)$  to zero; then, given an initial solenoidal velocity field  $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}^\circ(\mathbf{x})$ , we want to solve the systems (NS) and (Lr2) for the velocity field  $\mathbf{u}(\mathbf{x}, t)$  in the whole space  $\mathbb{R}^3$  (unbounded flow).

In the  $\mathbb{R}^3$  space we can assume that the turbulence arising in the flow is homogeneous and isotropic, which means that turbulent statistical properties are respectively invariant under any translation and under any rotation. Thanks to homogeneity we look for solutions  $\mathbf{u}(\mathbf{x}, t)$  which are space-periodic, therefore for simplicity we assume the periodicity is  $L = 2\pi$  in each direction:

$$\mathbf{u}(\mathbf{x} + 2\pi n \mathbf{e}_j, t) = \mathbf{u}(\mathbf{x}, t) \quad j = 1, 2, 3 \quad (5.1)$$

where  $\mathbf{e}_j$  is a unit vector in the  $j^{\text{th}}$  direction and  $n$  is an integer. Thus the space domain on which we solve the equations can be reduced to the box  $\Omega_b = [0, 2\pi] \times [0, 2\pi] \times [0, 2\pi]$  (Figure 5.1) by assuming periodic boundary conditions (for  $j = 1, 2, 3$ ):

$$\mathbf{u}(\mathbf{x} + 2\pi\mathbf{e}_j, t) = \mathbf{u}(\mathbf{x}, t) \quad (5.2)$$

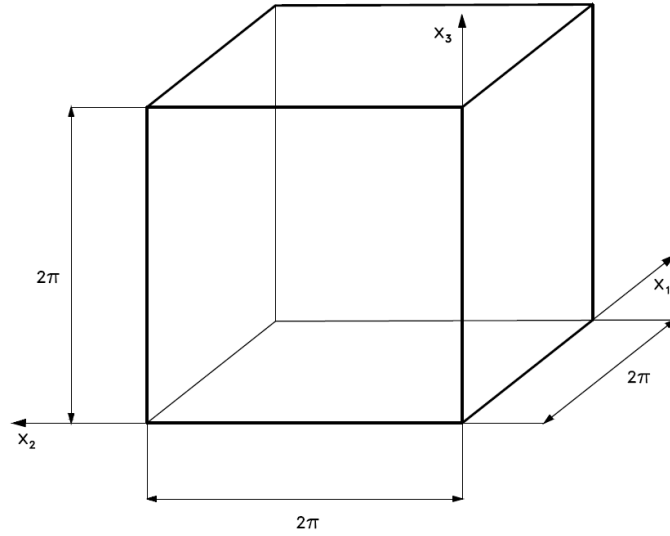


Figure 5.1: Domain Geometry  $\Omega_b$

The two problems can be then formally rewritten as follows (for  $i = 1, 2, 3$ ):

$$\begin{cases} \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \mu \frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i} & \text{in } \Omega_b \times [0, T] \\ \frac{\partial u_j}{\partial x_j} = 0 & \text{in } \Omega_b \times [0, T] \\ u_i(\mathbf{x}, 0) = u_i^\circ(\mathbf{x}) & \text{in } \Omega_b \times \{0\} \\ u_i(\mathbf{x} + 2\pi\mathbf{e}_j, t) = u_i(\mathbf{x}, t) & \text{on } \partial\Omega_b \times [0, T] \end{cases} \quad (\text{NS hit})$$

and

$$\begin{cases} \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \mu_0 \frac{\partial^2 u_i}{\partial x_j^2} - \frac{\partial p}{\partial x_i} + \mu_1 \frac{\partial}{\partial x_j} \left( 2\widehat{d}^2 D_{ij} \right) & \text{in } \Omega_b \times [0, T] \\ \frac{\partial u_j}{\partial x_j} = 0 & \text{in } \Omega_b \times [0, T] \\ u_i(\mathbf{x}, 0) = u_i^\circ(\mathbf{x}) & \text{in } \Omega_b \times \{0\} \\ u_i(\mathbf{x} + 2\pi\mathbf{e}_j, t) = u_i(\mathbf{x}, t) & \text{on } \partial\Omega_b \times [0, T] \end{cases} \quad (\text{Lr2 hit})$$

in which  $\widehat{d}^2$  is the scalar quantity

$$\widehat{d}^2 = \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \quad (5.3)$$

and  $D_{ij}$  is the rate of strain tensor

$$D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (5.4)$$

## 5.1 Initial conditions - Taylor-Green Vortex

For the problems (NS hit) and (Lr2 hit) - where *hit* stands for *homogeneous isotropic turbulence problem* - it is possible to use as initial conditions the three-dimensional velocity field devised by Sir Geoffrey Ingram Taylor and Albert Edward Green in [19] *to illustrate the process of grinding down of large eddies into smaller ones*. The Taylor-Green Vortex (TGV) is a synthetic flow field that fulfills the time-dependent incompressible Navier-Stokes equations. In two dimensions the vortex is stable and keeps its shape, while dissipating energy; in three dimension vortex stretching occurs and energy is transported from large scales to smaller scales: small vortices are generated while the base vortex decays. The three-dimensional TGV has the following form:

$$\mathbf{u}(\mathbf{x}) = \begin{Bmatrix} u_1(x_1, x_2, x_3) \\ u_2(x_1, x_2, x_3) \\ u_3(x_1, x_2, x_3) \end{Bmatrix} = \begin{Bmatrix} A \cos(ax_1) \sin(bx_2) \sin(cx_3) \\ B \sin(ax_1) \cos(bx_2) \sin(cx_3) \\ C \sin(ax_1) \sin(bx_2) \cos(cx_3) \end{Bmatrix} \quad (5.5)$$

and it is divergence-free if the constants  $A$ ,  $B$ ,  $C$ ,  $a$ ,  $b$  and  $c$  satisfy the following condition:

$$Aa + Bb + Cc = 0 \quad (5.6)$$

Since we want the initial velocity field to be  $2\pi$ -periodic in  $x_1$ ,  $x_2$  and  $x_3$ , we set  $a = b = c = 1$ . The condition (5.6) reduces to

$$A + B + C = 0 \quad (5.7)$$

Setting  $C = 0$  and  $A$  equal to the velocity scale  $U_0$ , one obtains  $B = -U_0$  from (5.7). Thus the initial velocity field can be written as

$$\mathbf{u}^\circ(\mathbf{x}) = \begin{Bmatrix} u_1^\circ(x_1, x_2, x_3) \\ u_2^\circ(x_1, x_2, x_3) \\ u_3^\circ(x_1, x_2, x_3) \end{Bmatrix} = \begin{Bmatrix} U_0 \cos(x_1) \sin(x_2) \sin(x_3) \\ -U_0 \sin(x_1) \cos(x_2) \sin(x_3) \\ 0 \end{Bmatrix} \quad (5.8)$$

## 5.2 Non-dimensional equations

Equations (NS) and (Lr2) can be non-dimensionalized using the velocity scale  $U_0$  for the velocities,  $L = L_b/(2\pi)$  for the space variables  $\mathbf{x}$ , where  $L_b$  is the physical domain size, the dynamic pressure  $\rho U_0^2$  for the pressure and the characteristic time  $L/U_0$  for the time variable; therefore the non-dimensionalized variables are

$$\begin{aligned} \tilde{u}_i &= \frac{u_i}{U_0} \\ \tilde{x}_i &= \frac{x_i}{L} \\ \tilde{p} &= \frac{p}{\rho U_0^2} \\ \tilde{t} &= t \cdot \frac{U_0}{L} \end{aligned} \quad (5.9)$$

Introducing this non-dimensionalization the equations (NS) and (Lr2) become

$$\begin{cases} \frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j^2} \\ \frac{\partial \tilde{u}_j}{\partial \tilde{x}_j} = 0 \end{cases} \quad (\text{NS nd})$$

and

$$\begin{cases} \frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j^2} + \frac{1}{\text{La}_2} \cdot \frac{\partial}{\partial \tilde{x}_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial \tilde{u}_k}{\partial \tilde{x}_l} + \frac{\partial \tilde{u}_l}{\partial \tilde{x}_k} \right)^2 \left( \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} + \frac{\partial \tilde{u}_j}{\partial \tilde{x}_i} \right) \right] \\ \frac{\partial \tilde{u}_j}{\partial \tilde{x}_j} = 0 \end{cases} \quad (\text{Lr2 nd})$$

where Re is the Reynolds number

$$\text{Re} = \frac{\rho L U_0}{\mu} \quad (5.10)$$

and La<sub>2</sub> is the non-dimensional parameter defined by

$$\text{La}_2 = \frac{\rho L^3}{\mu_1 U_0} \quad (5.11)$$

which arises from non-dimensionalization of the Ladyzhenskaya equations with  $r = 2$  and may be called *Ladyzhenskaya number*. For a generic  $r$  this parameter can be defined by

$$\text{La}_r = \frac{\rho L^{r+1} U_0^{1-r}}{\mu_1} \quad (5.12)$$

with

$$\mu_1 = [M] \cdot [T]^{r-1} [L]^{-1}$$

The problems can be then rewritten in non-dimensional form as follows

$$\begin{cases} \frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j^2} & \text{in } \tilde{\Omega}_b \times [0, \tilde{T}] \\ \frac{\partial \tilde{u}_j}{\partial \tilde{x}_j} = 0 & \text{in } \tilde{\Omega}_b \times [0, \tilde{T}] \\ \tilde{u}_i(\tilde{\mathbf{x}}, 0) = \tilde{u}_i^\circ(\tilde{\mathbf{x}}) & \text{in } \tilde{\Omega}_b \times \{0\} \\ \tilde{u}_i(\tilde{\mathbf{x}} + 2\pi/L\mathbf{e}_j, \tilde{t}) = \tilde{u}_i(\tilde{\mathbf{x}}, \tilde{t}) & \text{on } \partial\tilde{\Omega}_b \times [0, \tilde{T}] \end{cases} \quad (5.13)$$

and

$$\begin{cases} \frac{\partial \tilde{u}_i}{\partial \tilde{t}} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} = -\frac{\partial \tilde{p}}{\partial \tilde{x}_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 \tilde{u}_i}{\partial \tilde{x}_j^2} + \frac{1}{\text{La}_2} \cdot \frac{\partial}{\partial \tilde{x}_j} \left( 2\hat{d}^2 \tilde{D}_{ij} \right) & \text{in } \tilde{\Omega}_b \times [0, \tilde{T}] \\ \frac{\partial \tilde{u}_j}{\partial \tilde{x}_j} = 0 & \text{in } \tilde{\Omega}_b \times [0, \tilde{T}] \\ \tilde{u}_i(\tilde{\mathbf{x}}, 0) = \tilde{u}_i^\circ(\tilde{\mathbf{x}}) & \text{in } \tilde{\Omega}_b \times \{0\} \\ \tilde{u}_i(\tilde{\mathbf{x}} + 2\pi/L\mathbf{e}_j, \tilde{t}) = \tilde{u}_i(\tilde{\mathbf{x}}, \tilde{t}) & \text{on } \partial\tilde{\Omega}_b \times [0, \tilde{T}] \end{cases} \quad (5.14)$$

in which  $\widehat{d}^2$  is the scalar quantity

$$\widehat{d}^2 = \sum_{k,l=1}^3 \left( \frac{\partial \tilde{u}_k}{\partial \tilde{x}_l} + \frac{\partial \tilde{u}_l}{\partial \tilde{x}_k} \right)^2 \quad (5.15)$$

and  $\tilde{D}_{ij}$  is the non-dimensional rate of strain tensor

$$\tilde{D}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial \tilde{x}_j} + \frac{\partial \tilde{u}_j}{\partial \tilde{x}_i} \right) \quad (5.16)$$

The non-dimensional domain is simply  $\tilde{\Omega}_b = [0, 2\pi] \times [0, 2\pi] \times [0, 2\pi]$  since  $L = 1$  and the time  $\tilde{T}$  equals  $TU_0$ . The non-dimensional initial condition instead is

$$\tilde{\mathbf{u}}^\circ(\tilde{\mathbf{x}}) = \begin{Bmatrix} \cos(\tilde{x}_1) \sin(\tilde{x}_2) \sin(\tilde{x}_3) \\ -\sin(\tilde{x}_1) \cos(\tilde{x}_2) \sin(\tilde{x}_3) \\ 0 \end{Bmatrix} \quad (5.17)$$

# Chapter 6

## Numerical methods and implementation

The problems presented in the previous Chapter can be numerically solved using different methods, such as those which employ finite differences, finite elements or spectral approximations. Because of their ability to achieve moderately accurate solutions with less dense grids, over the past sixty years spectral methods have gained a lot of popularity in solving fluid dynamic problems and seem to be the natural choice when dealing with turbulent flows.

### 6.1 Spectral methods

Spectral methods belong to a class of discretization schemes for differential equations known generically as *methods of weighted residuals*. In this kind of methods one uses some functions called *trial functions*  $\{\phi_k\}$  as basis to approximate the solution  $u$  in a truncated series expansion

$$u_N(x) = \sum_{k=0}^N \hat{u}_k \phi_k(x) \quad \text{with } x \in \Omega \subseteq \mathbb{R}^d, d \in \mathbb{Z}^+ \quad (6.1)$$

and some other functions called *test function*  $\{\psi_k\}$  to ensure that the differential equation is satisfied as closely as possible by the approximating expansion. In fact if one uses the truncated expansion instead of the exact solution in the differential equation, say generically

$$\mathcal{F}(u) - g = 0 \quad \text{in } \Omega \subseteq \mathbb{R}^d, d \in \mathbb{Z}^+, \quad (6.2)$$

produces an error called *residual*

$$R_N(x) = \mathcal{F}(u_N) - g \quad (6.3)$$

which can be minimized by imposing an orthogonality condition with respect to each of the test functions:

$$(R_N, \psi_i)_{w_*} = \int_{\Omega} R_N \psi_i w_* dx = 0 \quad i \in I_N \quad (6.4)$$

where  $w_*$  is the weight associated with the method and the trial functions, and the dimension of the discrete set  $I_N$  depends on the problem under consideration. For complex

functions,  $\psi_i$  in the integral is replaced by its complex conjugate  $\overline{\psi_i}$

$$(R_N, \psi_i)_{w_*} = \int_{\Omega} R_N \overline{\psi_i} w_* dx = 0 \quad i \in I_N \quad (6.5)$$

Spectral methods are distinguished from the other methods of weighted residuals, such as the finite elements methods, for the type of trial functions used and the extension of the domain on which they are specified. Unlike finite elements methods in which the domain  $\Omega$  is divided into small elements and a trial function is specified in each element, for spectral methods the trial functions are infinitely differentiable global functions, i. e. they are defined over the whole domain of the problem. The trial functions are generally orthogonal with respect to some weight  $w(x)$  such that

$$(\phi_k, \phi_l)_w = \int_{\Omega} \phi_k \phi_l w dx = c_k \delta_{kl} = \begin{cases} c_k & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases} \quad (6.6)$$

where  $c_k$  are constants and  $\delta_{kl}$  is the Kronecker delta. The most frequently used trial functions are trigonometric polynomials (for periodic problems), Chebyshev polynomials  $T_k(x)$  and Legendre polynomials  $L_k(x)$  (for nonperiodic problems).

The most popular and commonly used spectral scheme are the *Galerkin*, the *collocation* and the *tau* schemes. They differ for the choice of the test functions and the weight  $w_*$

- in the Galerkin method the test function are the same as the trial functions; they are infinitely smooth functions which individually satisfy the boundary conditions. The weight  $w_*$  is the weight associated with the orthogonality of the trial functions (6.6):

$$\psi_k = \phi_k \quad \text{and} \quad w_* = w$$

- in the collocation method the test functions are translated Dirac functions centered at special points  $x_k$  called *collocation points*

$$\psi_k = \delta(x - x_k)$$

and the weight is  $w_* = 1$ . For this method the residual minimization condition (6.4) simply gives

$$(R_N, \psi_i)_{w_*} = \int_{\Omega} R_N \delta(x - x_k) dx = 0$$

$$R_N(x_k) = 0$$

Therefore in the collocation method the residual is exactly zero at certain points, whereas in the Galerkin method the residual is zero in the mean.

- the tau method is similar to the Galerkin method but none of the test functions has to satisfy the boundary conditions and a supplementary set of equations is needed to enforce boundary conditions. The tau approach is a modification of the Galerkin method that is applicable to problem with nonperiodic boundary conditions.

From a numerical point of view, Galerkin and tau methods are implemented in terms of the coefficients  $\{\hat{u}_k\}$  of the expansion which approximates the solution, whereas collocation methods are implemented in terms of the physical space values of the unknown solution. The key feature of the Galerkin method is that the trial functions must individually satisfy



the boundary condition; thus, if the boundary conditions are periodic the Galerkin method with the Fourier series approximating the solution, called *Fourier-Galerkin method*, is the most obvious and simple way to follow since the trigonometric functions with an appropriate periodicity will automatically satisfy the boundary conditions. If boundary conditions are not periodic, instead, one has to choose different trial functions, like for example Chebyshev and Legendre polynomials, or alternatively use a different method, like the tau method, for which the trial functions are not supposed to satisfy the boundary conditions.

### 6.1.1 Spectral approximation of a function

One of the main ideas on which many numerical methods are based is the approximation of the unknown function in term of an infinite sequence of orthogonal functions  $\{\phi_k\}$ :

$$u = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k(x) \quad \text{with } x \in \Omega \subseteq \mathbb{R}^d, d \in \mathbb{Z}^+ \quad (6.7)$$

The expansion in term of an orthogonal system introduces a linear transformation between  $u$  and the sequence of its expansion coefficients  $\{\hat{u}_k\}$ . If the expansion functions are chosen properly it is possible to obtain series for which the  $k$ -th coefficient decays faster than any inverse power of  $k$ . This rapid decay of the coefficients implies that the series truncated after just few terms represents a good approximation of the function. This characteristic is referred to as *spectral accuracy* of the series. This property can be obtained for periodic functions expanded in Fourier series and for smooth nonperiodic functions as well using the eigenfunctions of a singular Sturm-Liouville problem (see Appendix C), namely Chebyshev or Legendre polynomials.

As will be seen later, we are interested in approximating our solutions through spectral methods supposing the solution to be periodic in all directions; therefore we focus our attention on the Fourier system.

#### Continuous Fourier expansion

The set of trigonometric functions

$$\phi_k(x) = e^{ikx} = \cos(kx) + i \sin(kx) \quad (6.8)$$

is an orthogonal system for  $x \in [0, 2\pi]$ , that is

$$\int_0^{2\pi} \phi_k(x) \overline{\phi_l(x)} dx = \int_0^{2\pi} e^{ikx} e^{-ilx} dx = 2\pi \delta_{kl} = \begin{cases} 2\pi & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases} \quad (6.9)$$

where  $i$  is the imaginary unit and  $\overline{\phi_k(x)}$  denotes the complex conjugate of  $\phi_k(x)$ . One can then use this system as basis to expand a complex-valued function  $u(x)$  defined on  $(0, 2\pi)$  as follows

$$Su = \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ikx} \quad (6.10)$$

This expansion is called *Fourier series* of the function  $u$  and  $\hat{u}_k$ , named *Fourier coefficients* of  $u$ , are defined by

$$\hat{u}_k = \frac{1}{2\pi} \int_0^{2\pi} u(x) e^{-ikx} dx \quad k = 0, \pm 1, \pm 2, \dots \quad (6.11)$$

This relation associates with  $u$  a sequence of complex number called *Fourier transform* of  $u$ . The function  $u$  is transformed from the physical space to the space of (angular) wavenumbers  $k$ , called *transform space*. The Fourier series of  $u$  truncated to a sequence of  $N$  trigonometric polynomials is

$$P_N u(x) = \sum_{k=-N/2}^{N/2-1} \hat{u}_k e^{ikx} \quad (6.12)$$

The most important convergence property of the Fourier series is the following: for a function  $u(x)$ , periodic, continuous on  $[0, 2\pi]$  as well as its derivative to the order  $m-1$  included and with the  $m$ -th derivative absolutely integrable, the Fourier coefficients behave like

$$\hat{u}_k = \mathcal{O}(|k|^{-m}) \quad \text{for } k \rightarrow \infty \quad (6.13)$$

As corollary of this property one can conclude that *the  $k$ -th Fourier coefficient of a function which is infinitely differentiable and periodic with all its derivatives on  $[0, 2\pi]$  decays faster than any negative power of  $k$* . In conclusion, for smooth periodic functions the Fourier series ensures the so-called spectral accuracy. This behavior has to be compared to the  $\mathcal{O}(N^{-p})$  error of a finite-difference approximation, where  $N$  is the mesh size and  $p$ , which depends on the particular scheme, is a relatively small order.

These results can be extended to smooth functions  $u(x)$  defined on  $[0, L]$  which are  $L$ -periodic ( $u(0^+) = u(L^-)$ ) assuming as basis the set of functions

$$\phi_k(x) = e^{ik\frac{2\pi}{L}x} = \cos\left(k\frac{2\pi}{L}x\right) + i\sin\left(k\frac{2\pi}{L}x\right) \quad (6.14)$$

which are the trigonometric polynomials with periodicity equal to  $L$ . These functions form a orthogonal system over  $[0, L]$

$$\int_0^L \phi_k(x) \overline{\phi_l(x)} dx = \int_0^L e^{ik\frac{2\pi}{L}x} e^{-il\frac{2\pi}{L}x} dx = L\delta_{kl} = \begin{cases} L & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases} \quad (6.15)$$

Thus the function  $u(x)$  can be approximated by

$$u \approx \sum_{k=-\infty}^{\infty} \hat{u}_k \phi_k(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ik\frac{2\pi}{L}x} \quad (6.16)$$

and the Fourier coefficients are

$$\hat{u}_k = \frac{1}{L} \int_0^L u(x) e^{-ik\frac{2\pi}{L}x} dx \quad k = 0, \pm 1, \pm 2, \dots \quad (6.17)$$

### Discrete Fourier expansion

In many numerical applications the continuous Fourier series cannot be precisely implemented because of some difficulties, such as the fact that the Fourier coefficients of an arbitrary function are not known in closed form and must be approximated in some way. To overcome this kind of problems discrete Fourier transform and discrete Fourier series are used.

The discrete Fourier coefficients of a complex-valued function  $u(x)$  in  $[0, 2\pi]$  with respect to the points  $x_j = 2\pi j/N$  (with  $j = 0, \dots, N-1$  and  $N \in \mathbb{Z}^+$ ) are

$$\tilde{u}_k = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j} \quad -N/2 \leq k \leq N/2 - 1 \quad (6.18)$$

Thanks to the orthonormality

$$\frac{1}{N} \sum_{j=0}^{N-1} e^{ipx_j} = \begin{cases} 1 & \text{if } p = Nm, m = 0, \pm 1, \pm 2, \dots \\ 0 & \text{otherwise} \end{cases} \quad (6.19)$$

one can write the inversion formula

$$u(x_j) = \sum_{k=-N/2}^{N/2-1} \tilde{u}_k e^{ikx_j} \quad j = 0, \dots, N-1 \quad (6.20)$$

which is the interpolation of  $u$  at the nodes  $x_j$  also known as discrete Fourier series of  $u$ . The discrete Fourier Transform (DFT) is the mapping between the  $N$  complex numbers  $u(x_j)$ , the values of the function at the nodes, and the  $N$  complex numbers  $\tilde{u}_k$ , the discrete Fourier coefficients. From a numerical point of view, the discrete Fourier transform can be easily calculated using the computationally cheap Fast Fourier Transform (FFT) algorithms. By far the most commonly used FFT algorithm is the Cooley–Tukey algorithm [22].

### 6.1.2 Fourier-Galerkin method for space discretization

For our purposes we are interested in the Galerkin scheme coupled with the Fourier's approximation on the unknown solution; the resulting method is called *Fourier-Galerkin method*.

We want to approximate the solution  $u(x, t)$  of the evolution equation

$$\frac{\partial u}{\partial t} = \mathcal{L}(u) \quad (6.21)$$

where  $\mathcal{L}$  is a linear operator which contains all the spatial derivatives of  $u(x, t)$  up to the finite order  $M$ . The problem must include an initial condition  $u(x, 0)$  and suitable boundary conditions. We suppose that the problem is one dimensional, that the spatial domain is  $(0, 2\pi)$  and that the boundary conditions are periodic:

$$u(0, t) = u(2\pi, t) \quad (6.22)$$

Moreover, we assume  $\mathcal{L}$  to be

$$\mathcal{L}(u) = \sum_{m=0}^M c_m \frac{\partial^m u}{\partial x^m} \quad (6.23)$$

where  $c_m$  are known real constants. The approximated solution is represented as

$$u_N(x, t) = \sum_{k=-N/2}^{N/2} a_k(t) \phi_k(x) \quad (6.24)$$

where  $\phi_k$  are the trial functions and  $a_k$  are the expansion coefficients. Thanks to periodic boundary conditions we can approximate the solution using the trigonometric polynomials with periodicity  $L = 2\pi$

$$u_N(x, t) = \sum_{k=-N/2}^{N/2} a_k(t) \phi_k(x) = \sum_{k=-N/2}^{N/2} \hat{u}_k(t) e^{ikx} \quad (6.25)$$

In general, being an approximation,  $u_N$  will not satisfy the equation

$$\frac{\partial u}{\partial t} = \mathcal{L}(u)$$

so that the residual

$$R_N(x) = \frac{\partial u_N}{\partial t} - \mathcal{L}(u_N) \quad (6.26)$$

will not vanish everywhere. However, using the weighted residual method we can minimize the residual by imposing its orthogonality with respect to the test functions

$$(R_N, \psi_l)_{w_*} = \int_{\Omega} R_N \bar{\psi}_l w_* dx = 0 \quad l = -N/2, \dots, N/2 \quad (6.27)$$

We now decide to employ the Galerkin scheme for which we have already seen that

$$\psi_k = \phi_k \quad \text{and} \quad w_* = w$$

Having chosen as trial functions the trigonometric polynomial

$$\phi_k(x) = e^{ikx} \quad (6.28)$$

and knowing that they form a orthogonal system over  $[0, 2\pi]$

$$\int_0^{2\pi} \phi_k(x) \overline{\phi_l(x)} dx = \int_0^{2\pi} e^{ikx} e^{-ilx} dx = 2\pi \delta_{kl} = \begin{cases} 2\pi & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases} \quad (6.29)$$

we conclude that, for the Fourier-Galerkin scheme,  $w_* = \frac{1}{2\pi}$  such that

$$\int_0^{2\pi} R_N(x) \bar{\psi}_k w_* dx = \frac{1}{2\pi} \int_0^{2\pi} \left[ \frac{\partial u_N}{\partial t} - \mathcal{L}(u_N) \right] e^{-ilx} dx = 0 \quad (6.30)$$

for  $l = -N/2, \dots, N/2$ . Introducing the approximation (6.25) in this condition one obtains

$$\int_0^{2\pi} \left[ \left( \frac{\partial}{\partial t} - \mathcal{L} \right) \left( \sum_{k=-N/2}^{N/2} \hat{u}_k(t) e^{ikx} \right) \right] e^{-ilx} dx = 0 \quad l = -N/2, \dots, N/2$$

We have assumed  $\mathcal{L}$  to be a linear operator containing all the spatial derivatives of  $u(x, t)$  up to the order  $M$  such that

$$\int_0^{2\pi} \left[ \left( \frac{\partial}{\partial t} - \sum_{m=0}^M c_m \frac{\partial^m}{\partial x^m} \right) \left( \sum_{k=-N/2}^{N/2} \hat{u}_k(t) e^{ikx} \right) \right] e^{-ilx} dx = 0$$

We can now analytically space differentiate the trial functions

$$\int_0^{2\pi} \left[ \sum_{k=-N/2}^{N/2} \left( \frac{d\hat{u}_k}{dt} - \sum_{m=0}^M c_m i^m k^m \hat{u}_k \right) e^{ikx} \right] e^{-ilx} dx = 0$$

and exploit the orthogonality between the trial and the test functions, obtaining the following system of ODEs in the transform space

$$\frac{d\hat{u}_k}{dt} - \sum_{m=0}^M c_m i^m k^m \hat{u}_k = 0 \quad \text{for } k = -N/2, \dots, N/2$$

For example, if  $\mathcal{L}$  is the second-order derivative in space  $\partial^2/\partial x^2$  only, one obtains

$$\frac{d\hat{u}_k}{dt} - i^2 k^2 \hat{u}_k = 0 \quad \text{for } k = -N/2, \dots, N/2$$

The problem then reduces to the solution of a set of ODEs in the transform space for which one assumes as initial conditions the coefficients for the expansion of the initial physical condition, namely

$$\hat{u}_k(0) = \frac{1}{2\pi} \int_0^{2\pi} u(x, 0) e^{-ikx} dx \quad \text{for } k = -N/2, \dots, N/2$$

In order to solve this problem, a stable scheme for the temporal discretization is required.

### Application - Burgers Equation

In order to understand how nonlinearities can be treated within this method, we now apply the Fourier-Galerkin method to the viscous Burgers equation; this raises issues that occur also for much complicated equations like those we intend to solve.

The viscous Burgers equation is the following nonlinear PDE

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0 \quad (6.31)$$

where  $\nu$  is a positive constant. The nonlinearity is due to the term  $u(\partial u/\partial x)$ . Given an initial condition  $u(0, x) = u^o(x)$ , we want to solve the equation (6.31) over  $[0, 2\pi]$  with periodic boundary conditions. We can approximate the solution  $u$  in a truncated Fourier series

$$u_N(x, t) = \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx} \quad (6.32)$$

and, using the Galerkin scheme, require that the residual of the equation due to this approximation is orthogonal to all the test functions:

$$\int_0^{2\pi} \left( \frac{\partial u_N}{\partial t} + u_N \frac{\partial u_N}{\partial x} - \nu \frac{\partial^2 u_N}{\partial x^2} \right) e^{-ilx} dx = 0 \quad l = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (6.33)$$

Due to the orthogonality property of the test and the trial functions one obtains the following system of  $N$  ordinary differential equations:

$$\frac{d\hat{u}_k}{dt} + \left\langle u_N \frac{\partial u_N}{\partial x} \right\rangle_k + \nu k^2 \hat{u}_k = 0 \quad k = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (6.34)$$

with initial conditions

$$\hat{u}_k(0) = \frac{1}{2\pi} \int_0^{2\pi} u^\circ(x) e^{-ikx} dx \quad \text{for } k = -N/2, \dots, N/2$$

where the  $N$  terms due to the nonlinearity  $u(\partial u/\partial x)$  have the implicit expression

$$\left\langle u_N \frac{\partial u_N}{\partial x} \right\rangle_l = \frac{1}{2\pi} \int_0^{2\pi} u_N \frac{\partial u_N}{\partial x} e^{-ilx} dx \quad l = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (6.35)$$

In fact, the nonlinearity does not allow to use the orthogonality property of the trial and the test functions directly, and we have to find a different way to evaluate the  $N$  terms given by (6.35). It can be noted however that (6.35) is actually a particular case of the general quadratic nonlinear term

$$\langle uv \rangle_l = \frac{1}{2\pi} \int_0^{2\pi} uv e^{-ilx} dx \quad (6.36)$$

where  $u$  e  $v$  are generic trigonometric polynomials which can be expanded in

$$u(x, t) = \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx}$$

$$v(x, t) = \sum_{k=-N/2}^{N/2-1} \hat{v}_k(t) e^{ikx}$$

Substituting these expressions in the (6.36) and invoking the orthogonality property of the trigonometric basis (see [20]), one obtains the convolution sum

$$\langle uv \rangle_k = \hat{w}_k = \sum_{\substack{p+q=k \\ |p|, |q| \leq N/2}} \hat{u}_p \hat{v}_q \quad (6.37)$$

Since the numerical evaluation of this convolution is prohibitively expensive (in three dimensions the cost is  $\mathcal{O}(N^4)$ ) one can decide to use the so-called *transform method*. In order to evaluate the convolution, we may introduce the inverse discrete Fourier transform with respect to the points  $x_j = 2\pi j/N$  (with  $j = 0, \dots, N-1$  and  $N \in \mathbb{Z}^+$ ) of  $u$  and  $v$ :

$$u(x_j) = U_j = \sum_{k=-N/2}^{N/2-1} \hat{u}_k e^{ikx_j} \quad j = 0, 1, \dots, N-1 \quad (6.38)$$

$$v(x_j) = V_j = \sum_{k=-N/2}^{N/2-1} \hat{v}_k e^{ikx_j}$$

and define

$$W_j = U_j V_j \quad j = 0, 1, \dots, N-1$$

and

$$\hat{W}_k = \frac{1}{N} \sum_{j=0}^{N-1} W_j e^{-ikx_j} \quad k = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (6.39)$$

Therefore

$$\hat{W}_k = \frac{1}{N} \sum_{j=0}^{N-1} U_j V_j e^{-ikx_j} \quad k = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (6.40)$$

Using the orthonormality relation

$$\frac{1}{N} \sum_{j=0}^{N-1} e^{ipx_j} = \begin{cases} 1 & \text{if } p = Nm, m = 0, \pm 1, \pm 2, \dots \\ 0 & \text{otherwise} \end{cases} \quad (6.41)$$

one finds

$$\hat{W}_k = \sum_{m+n=k} \hat{u}_m \hat{v}_n + \sum_{m+n=k \pm N} \hat{u}_m \hat{v}_n = \hat{w}_k + \sum_{m+n=k \pm N} \hat{u}_m \hat{v}_n \quad (6.42)$$

In conclusion, approximating the convolution  $\hat{w}_k = \langle uv \rangle_k$  with  $\hat{W}_j$ , which is defined by the (6.40) and the evaluations (6.38) of  $U_j$  and  $V_j$ , produces an error equal to

$$\sum_{m+n=k \pm N} \hat{u}_m \hat{v}_n \quad (6.43)$$

which is called *aliasing error*. However, on the upside, if one uses FFT algorithms for the discrete Fourier transforms in this *transform* method, the number of operations needed to evaluate the convolution is reduced to  $\mathcal{O}(N \log_2 N)$  multiplications. A spectral method which employs this transform method for treating nonlinearities is said *pseudospectral*. The idea of the pseudospectral transform method is basically to evaluate the product  $uv$  in the physical space and then transform the product's result in the wavenumbers' space, introducing however an error which depends on the mode  $k$  and the total number  $N$  of modes.

**Padding/Truncation technique for de-aliasing.** A technique for removing the aliasing error from the (6.42) is the *Padding/Truncation* technique, also called *3/2-rule*. The basic idea in this *de-aliasing* technique is to use the discrete transforms of  $u$  and  $v$  with respect to  $M$  nodes instead of  $N$  with  $M \geq 3N/2$ .

Let

$$\begin{aligned} y_j &= 2\pi j/M \\ U_j &= \sum_{k=-M/2}^{M/2-1} \tilde{u}_k e^{iky_j} \\ V_j &= \sum_{k=-M/2}^{M/2-1} \tilde{v}_k e^{iky_j} \\ W_j &= U_j V_j \end{aligned} \quad j = 0, 1, \dots, M-1$$

where

$$\tilde{u}_k = \begin{cases} \hat{u} & \text{for } |k| \leq N/2 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\tilde{v}_k = \begin{cases} \hat{v} & \text{for } |k| \leq N/2 \\ 0 & \text{otherwise} \end{cases}$$

Thus the coefficients  $\tilde{u}$  and  $\tilde{v}$  are basically the coefficients  $\hat{u}$  and  $\hat{v}$  padded with zeros for the additional wavenumbers, namely  $N/2 < |k| \leq M/2$ . Let

$$\widetilde{W}_k = \frac{1}{M} \sum_{j=0}^{M-1} W_j e^{-iky_j} \quad k = -\frac{M}{2}, \dots, \frac{M}{2} - 1 \quad (6.44)$$

then

$$\widetilde{W}_k = \sum_{m+n=k} \tilde{u}_m \tilde{v}_n + \sum_{m+n=k \pm M} \tilde{u}_m \tilde{v}_n \quad (6.45)$$

It can be shown that for  $M \geq 3N/2$  the aliasing error (the second term on the right-hand side) vanishes for the wavenumbers we are interested in, i. e.  $|k| \leq N/2$ .

In conclusion, the  $N$  terms resulting from the nonlinearity, which are

$$\begin{aligned} \left\langle u_N \frac{\partial u_N}{\partial x} \right\rangle_l &= \frac{1}{2\pi} \int_0^{2\pi} u_N \frac{\partial u_N}{\partial x} e^{-ilx} dx = \\ &= \frac{1}{2\pi} \int_0^{2\pi} \left( \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx} \right) \left( \sum_{k=-N/2}^{N/2-1} ik \hat{u}_k(t) e^{ikx} \right) e^{-ilx} dx, \end{aligned}$$

find a *pseudospectral* evaluation in

$$\left\langle u_N \frac{\partial u_N}{\partial x} \right\rangle_l = \frac{1}{M} \sum_{j=0}^{M-1} U_j V_j e^{-ily_j} \quad l = -\frac{M}{2}, \dots, \frac{M}{2} - 1, \quad (6.46)$$

with

$$\begin{aligned} M &\geq 3N/2 \\ y_j &= 2\pi j/M \\ U_j &= \sum_{k=-M/2}^{M/2-1} \tilde{u}_k e^{iky_j} \quad j = 0, 1, \dots, M-1 \\ V_j &= \sum_{k=-M/2}^{M/2-1} ik \tilde{u}_k e^{iky_j} \end{aligned}$$

reduced to the wavenumbers of interest  $l = -N/2, \dots, N/2 - 1$ .

From a numerical point of view this technique can be implemented in another equivalent way called *2/3-rule*: products are calculated over  $N$  nodes instead of  $M \geq 3N/2$  and then the values corresponding to the aliased  $N/3$  *central* (with greatest absolute value) modes are set to zero, avoiding padding-truncation operations. This however means to solve equations over  $2N/3$  nodes, i. e.  $2N/3$  modes, instead of  $N$ , because the remaining  $N/3$  modes are used to remove aliasing error only.

## 6.2 Numerical scheme for HIT problem

For the problems (NS hit) and (Lr2 hit) we want to solve, space-periodic solutions along the three directions are assumed thanks to the homogeneity and the isotropy of the turbulence. Consequently, the natural choice for the discretization scheme is the Fourier-Galerkin method.



We recall the two problems presented in the Chapter 5 (for  $i = 1, 2, 3$ ) in non-dimensional form dropping out the *tilde* to denote the non-dimensional variables for simplicity:

$$\begin{cases} \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 u_i}{\partial x_j^2} & \text{in } \Omega_b \times [0, T] \\ \frac{\partial u_j}{\partial x_j} = 0 & \text{in } \Omega_b \times [0, T] \\ u_i(\mathbf{x}, 0) = u_i^\circ(\mathbf{x}) & \text{in } \Omega_b \times \{0\} \\ u_i(\mathbf{x} + 2\pi \mathbf{e}_j, t) = u_i(\mathbf{x}, t) & \text{on } \partial\Omega_b \times [0, T] \end{cases} \quad (6.47)$$

and

$$\begin{cases} \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\text{Re}} \cdot \frac{\partial^2 u_i}{\partial x_j^2} + \frac{1}{\text{La}_2} \cdot \frac{\partial}{\partial x_j} \left( 2\widehat{d^2} D_{ij} \right) & \text{in } \Omega_b \times [0, T] \\ \frac{\partial u_j}{\partial x_j} = 0 & \text{in } \Omega_b \times [0, T] \\ u_i(\mathbf{x}, 0) = u_i^\circ(\mathbf{x}) & \text{in } \Omega_b \times \{0\} \\ u_i(\mathbf{x} + 2\pi \mathbf{e}_j, t) = u_i(\mathbf{x}, t) & \text{on } \partial\Omega_b \times [0, T] \end{cases} \quad (6.48)$$

in which  $\widehat{d^2}$  is the scalar quantity

$$\widehat{d^2} = \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \quad (6.49)$$

$D_{ij}$  is the non-dimensional rate of strain tensor

$$D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (6.50)$$

and  $\mathbf{u}^\circ(\mathbf{x})$  is the non-dimensional initial condition

$$\mathbf{u}^\circ(\mathbf{x}) = \begin{pmatrix} \cos(x_1) \sin(x_2) \sin(x_3) \\ -\sin(x_1) \cos(x_2) \sin(x_3) \\ 0 \end{pmatrix} \quad (6.51)$$

Since periodic boundary conditions are assumed in all directions we can approximate the velocity and the pressure field in term of trigonometric polynomials with periodicity  $2\pi$ :

$$u_i(\mathbf{x}, t) = \sum_{h=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \hat{u}_{klh}^{(i)}(t) e^{ikx_1} e^{ilx_2} e^{ihx_3} \quad (6.52)$$

$$p(\mathbf{x}, t) = \sum_{h=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \hat{p}_{klh}(t) e^{ikx_1} e^{ilx_2} e^{ihx_3} \quad (6.53)$$

Truncating the expansions to  $N_1$  terms in  $x_1$ ,  $N_2$  terms in  $x_2$  and  $N_3$  terms in  $x_3$ :

$$u_N^{(i)}(\mathbf{x}, t) = \sum_{h=-N_3/2}^{N_3/2-1} \sum_{l=-N_2/2}^{N_2/2-1} \sum_{k=-N_1/2}^{N_1/2-1} \hat{u}_{klh}^{(i)}(t) e^{ikx_1} e^{ilx_2} e^{ihx_3} \quad (6.54)$$

$$p_N(\mathbf{x}, t) = \sum_{h=-N_3/2}^{N_3/2-1} \sum_{l=-N_2/2}^{N_2/2-1} \sum_{k=-N_1/2}^{N_1/2-1} \hat{p}_{klh}(t) e^{ikx_1} e^{ilx_2} e^{ihx_3} \quad (6.55)$$

In order to simplify the notation we rewrite these last two expressions as follows

$$u_N^{(i)}(\mathbf{x}, t) = \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \phi_k(x_1) \phi_l(x_2) \phi_h(x_3) \quad (6.56)$$

$$p_N(\mathbf{x}, t) = \sum_h \sum_l \sum_k \hat{p}_{klh} \phi_k(x_1) \phi_l(x_2) \phi_h(x_3) \quad (6.57)$$

with  $h = -N_3/2, \dots, N_3/2 - 1$ ,  $l = -N_2/2, \dots, N_2/2 - 1$ ,  $k = -N_1/2, \dots, N_1/2 - 1$  and

$$\phi_k(x_i) = e^{ikx_i}$$

We then note that the trial functions form three orthonormal systems over  $[0, 2\pi]$  in each direction

$$\frac{1}{2\pi} \int_0^{2\pi} \phi_k(x) \overline{\phi_l(x)} dx = \frac{1}{2\pi} \int_0^{2\pi} e^{ikx} e^{-ilx} dx = \delta_{kl} = \begin{cases} 1 & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases}$$

We then apply the Galerkin method for the space discretization to the Navier-Stokes and the Ladyzhenskaya equations obtaining respectively (for  $n = -N_1/2, \dots, N_1/2 - 1$ ,  $m = -N_2/2, \dots, N_2/2 - 1$ ,  $s = -N_3/2, \dots, N_3/2 - 1$ )

$$\begin{aligned} \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \left[ \frac{\partial u_N^{(i)}}{\partial t} + u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} - \frac{1}{\text{Re}} \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} + \frac{\partial p_N}{\partial x_i} \right] e^{-inx_1} e^{-imx_2} e^{-isx_3} dx_1 dx_2 dx_3 = 0 \\ \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \left[ \frac{\partial u_N^{(i)}}{\partial t} + u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} - \frac{1}{\text{Re}} \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} + \frac{\partial p_N}{\partial x_i} - \frac{1}{\text{La}_2} \frac{\partial}{\partial x_j} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(i)}}{\partial x_j} + \frac{\partial u_N^{(j)}}{\partial x_i} \right) \right] \right] \\ \cdot e^{-inx_1} e^{-imx_2} e^{-isx_3} dx_1 dx_2 dx_3 = 0 \end{aligned}$$

where

$$\widehat{d_N^2} = \sum_{k,l=1}^3 \left( \frac{\partial u_N^{(k)}}{\partial x_l} + \frac{\partial u_N^{(l)}}{\partial x_k} \right)^2$$

If we denote with  $\langle \cdot \rangle_{nms}$  the Galerkin projection

$$\begin{aligned} \langle \cdot \rangle_{nms} &= \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} (\cdot) e^{-inx_1} e^{-imx_2} e^{-isx_3} dx_1 dx_2 dx_3 = \\ &= \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} (\cdot) \bar{\phi}_n(x_1) \bar{\phi}_m(x_2) \bar{\phi}_s(x_3) dx_1 dx_2 dx_3 = \\ &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} (\cdot) \bar{\psi}_{nms}(x_1, x_2, x_3) d\Omega_b \end{aligned} \quad (6.58)$$

for  $n = -N_1/2, \dots, N_1/2 - 1$ ,  $m = -N_2/2, \dots, N_2/2 - 1$  and  $s = -N_3/2, \dots, N_3/2 - 1$ , we can rewrite the schemes as follows

$$\left\langle \frac{\partial u_N^{(i)}}{\partial t} \right\rangle_{nms} + \left\langle u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} \right\rangle_{nms} - \frac{1}{\text{Re}} \left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} \right\rangle_{nms} + \left\langle \frac{\partial p_N}{\partial x_i} \right\rangle_{nms} = 0 \quad (6.59)$$

and

$$\begin{aligned} & \left\langle \frac{\partial u_N^{(i)}}{\partial t} \right\rangle_{nms} + \left\langle u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} \right\rangle_{nms} - \frac{1}{\text{Re}} \left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} \right\rangle_{nms} + \left\langle \frac{\partial p_N}{\partial x_i} \right\rangle_{nms} + \\ & - \frac{1}{\text{La}_2} \left\langle \frac{\partial}{\partial x_j} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(i)}}{\partial x_j} + \frac{\partial u_N^{(j)}}{\partial x_i} \right) \right] \right\rangle_{nms} = 0 \end{aligned} \quad (6.60)$$

We now consider term by term the second of these two systems, namely the Galerkin approximation of the Ladyzhenskaya equations; that for the Navier-Stokes equations can be obtained by setting to zero the additional nonlinear viscous terms.

**Local time variation.** The projection of the local time-variation of the velocity field is simply

$$\begin{aligned} \left\langle \frac{\partial u_N^{(i)}}{\partial t} \right\rangle_{nms} &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \frac{\partial}{\partial t} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = \\ &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \frac{d\hat{u}_{klh}^{(i)}}{dt} \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b \end{aligned}$$

and using the orthogonality property of the test and the trial functions it becomes

$$\left\langle \frac{\partial u_N^{(i)}}{\partial t} \right\rangle_{nms} = \frac{d\hat{u}_{nms}^{(i)}}{dt} \quad (6.61)$$

**Linear viscous term.** The projection of the linear viscous term is the tensor

$$-\frac{1}{\text{Re}} \left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} \right\rangle_{nms} = -\frac{1}{\text{Re}} \left\{ \begin{aligned} & \left\langle \frac{\partial^2 u_N^{(1)}}{\partial x_1^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(1)}}{\partial x_2^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(1)}}{\partial x_3^2} \right\rangle_{nms} \\ & \left\langle \frac{\partial^2 u_N^{(2)}}{\partial x_1^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(2)}}{\partial x_2^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(2)}}{\partial x_3^2} \right\rangle_{nms} \\ & \left\langle \frac{\partial^2 u_N^{(3)}}{\partial x_1^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(3)}}{\partial x_2^2} \right\rangle_{nms} + \left\langle \frac{\partial^2 u_N^{(3)}}{\partial x_3^2} \right\rangle_{nms} \end{aligned} \right\} \quad (6.62)$$

Differentiating with respect to the space variables and using the orthogonality properties, the terms in (6.62) which contain the derivatives with respect to  $x_1$ ,  $x_2$  and  $x_3$  become respectively

$$\begin{aligned} \left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_1^2} \right\rangle_{nms} &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \frac{\partial^2}{\partial x_1^2} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = \\ &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \frac{\partial^2 \psi_{klh}}{\partial x_1^2} \right) \bar{\psi}_{nms} d\Omega_b = \\ &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} (ik)^2 \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = -n^2 \hat{u}_{nms}^{(i)} \end{aligned}$$

$$\begin{aligned}
\left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_2^2} \right\rangle_{nms} &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \frac{\partial^2}{\partial x_2^2} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = \\
&= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \frac{\partial^2 \psi_{klh}}{\partial x_2^2} \right) \bar{\psi}_{nms} d\Omega_b = \\
&= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} (il)^2 \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = -m^2 \hat{u}_{nms}^{(i)} \\
\left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_3^2} \right\rangle_{nms} &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \frac{\partial^2}{\partial x_3^2} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = \\
&= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} \frac{\partial^2 \psi_{klh}}{\partial x_3^2} \right) \bar{\psi}_{nms} d\Omega_b = \\
&= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(i)} (ih)^2 \psi_{klh} \right) \bar{\psi}_{nms} d\Omega_b = -s^2 \hat{u}_{nms}^{(i)}
\end{aligned}$$

The resulting discretized linear viscous term (6.62) thus is

$$-\frac{1}{\text{Re}} \left\langle \frac{\partial^2 u_N^{(i)}}{\partial x_j^2} \right\rangle_{nms} = \frac{1}{\text{Re}} \begin{Bmatrix} (n^2 + m^2 + s^2) \hat{u}_{nms}^{(1)} \\ (n^2 + m^2 + s^2) \hat{u}_{nms}^{(2)} \\ (n^2 + m^2 + s^2) \hat{u}_{nms}^{(3)} \end{Bmatrix} \quad (6.63)$$

**Pressure term.** Similarly to the linear viscous term, the following Galerkin projection of the pressure term can be obtained

$$\left\langle \frac{\partial p_N}{\partial x_i} \right\rangle_{nms} = \begin{Bmatrix} \left\langle \frac{\partial p_N}{\partial x_1} \right\rangle_{nms} \\ \left\langle \frac{\partial p_N}{\partial x_2} \right\rangle_{nms} \\ \left\langle \frac{\partial p_N}{\partial x_3} \right\rangle_{nms} \end{Bmatrix} = \begin{Bmatrix} in \hat{p}_{nms} \\ im \hat{p}_{nms} \\ is \hat{p}_{nms} \end{Bmatrix} \quad (6.64)$$

**Convective term.** The discretized nonlinear convective term is

$$\left\langle u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} \right\rangle_{nms} = \begin{Bmatrix} \left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} + \left\langle u_N^{(2)} \frac{\partial u_N^{(1)}}{\partial x_2} \right\rangle_{nms} + \left\langle u_N^{(3)} \frac{\partial u_N^{(1)}}{\partial x_3} \right\rangle_{nms} \\ \left\langle u_N^{(1)} \frac{\partial u_N^{(2)}}{\partial x_1} \right\rangle_{nms} + \left\langle u_N^{(2)} \frac{\partial u_N^{(2)}}{\partial x_2} \right\rangle_{nms} + \left\langle u_N^{(3)} \frac{\partial u_N^{(2)}}{\partial x_3} \right\rangle_{nms} \\ \left\langle u_N^{(1)} \frac{\partial u_N^{(3)}}{\partial x_1} \right\rangle_{nms} + \left\langle u_N^{(2)} \frac{\partial u_N^{(3)}}{\partial x_2} \right\rangle_{nms} + \left\langle u_N^{(3)} \frac{\partial u_N^{(3)}}{\partial x_3} \right\rangle_{nms} \end{Bmatrix} \quad (6.65)$$

Unlike the linear terms, which can be easily obtained, it needs to be considered carefully. As previously seen for the Burgers equation, the terms resulting from the nonlinearity  $(\mathbf{u} \cdot \nabla) \mathbf{u}$  contained in the (6.65) can be expressed as convolution sums. Let focus for the moment on some representative terms. For example, for the first term one can write

$$\begin{aligned} \left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left[ \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} \psi_{klh} \right) \frac{\partial}{\partial x_1} \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} \psi_{klh} \right) \right] \bar{\psi}_{nms} d\Omega_b = \\ &= \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left[ \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} \psi_{klh} \right) \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} \frac{\partial \psi_{klh}}{\partial x_1} \right) \right] \bar{\psi}_{nms} d\Omega_b \end{aligned} \quad (6.66)$$

Differentiating  $\psi_{klh}(x_1, x_2, x_3) = e^{ikx_1 + ilx_2 + ihx_3}$  with respect to  $x_1$  one obtains

$$\left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} = \frac{1}{\dim(\Omega_b)} \int_{\Omega_b} \left[ \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} \psi_{klh} \right) \left( \sum_h \sum_l \sum_k \hat{u}_{klh}^{(1)} ik \psi_{klh} \right) \right] \bar{\psi}_{nms} d\Omega_b \quad (6.67)$$

or, alternatively

$$\left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} = in \left\langle u_N^{(1)} u_N^{(1)} \right\rangle_{nms}, \quad (6.68)$$

then invoking the orthogonality property leads to the convolution sum

$$\left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} = in \sum_{\substack{p+r=n \\ |p|, |r| \leq N_1/2}} \sum_{\substack{q+f=m \\ |q|, |f| \leq N_2/2}} \sum_{\substack{e+y=s \\ |e|, |y| \leq N_3/2}} \hat{u}_{pqe}^{(1)} \hat{u}_{rfy}^{(1)} \quad (6.69)$$

Since the numerical evaluation of these convolution sums is prohibitively expensive, we decide to evaluate the convolution integral

$$\left\langle u_N^{(1)} \frac{\partial u_N^{(1)}}{\partial x_1} \right\rangle_{nms} = in \left\langle u_N^{(1)} u_N^{(1)} \right\rangle_{nms}, \quad (6.70)$$

employing the pseudospectral transform method coupled with the 2/3-rule for the de-aliasing, as explained in the previous Section for the Burgers equation. The other terms of (6.65) can be treated exactly like the term (6.66) obtaining

$$\left\langle u_N^{(j)} \frac{\partial u_N^{(i)}}{\partial x_j} \right\rangle_{nms} = \left\{ \begin{aligned} &in \left\langle u_N^{(1)} u_N^{(1)} \right\rangle_{nms} + im \left\langle u_N^{(2)} u_N^{(1)} \right\rangle_{nms} + is \left\langle u_N^{(3)} u_N^{(1)} \right\rangle_{nms} \\ &in \left\langle u_N^{(1)} u_N^{(2)} \right\rangle_{nms} + im \left\langle u_N^{(2)} u_N^{(2)} \right\rangle_{nms} + is \left\langle u_N^{(3)} u_N^{(2)} \right\rangle_{nms} \\ &in \left\langle u_N^{(1)} u_N^{(3)} \right\rangle_{nms} + im \left\langle u_N^{(2)} u_N^{(3)} \right\rangle_{nms} + is \left\langle u_N^{(3)} u_N^{(3)} \right\rangle_{nms} \end{aligned} \right\} \quad (6.71)$$

**Nonlinear viscous term.** The Galerkin projection of the nonlinear viscous term associated with the Ladyzhenskaya equations is

$$\begin{aligned}
& -\frac{1}{\text{La}_2} \left\langle \frac{\partial}{\partial x_j} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(i)}}{\partial x_j} + \frac{\partial u_N^{(j)}}{\partial x_i} \right) \right] \right\rangle_{nms} = \\
& = -\frac{1}{\text{La}_2} \left\{ \left\langle \frac{\partial}{\partial x_1} \left[ 2\widehat{d_N^2} \frac{\partial u_N^{(1)}}{\partial x_1} \right] + \frac{\partial}{\partial x_2} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(1)}}{\partial x_2} + \frac{\partial u_N^{(2)}}{\partial x_1} \right) \right] + \frac{\partial}{\partial x_3} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(1)}}{\partial x_3} + \frac{\partial u_N^{(3)}}{\partial x_1} \right) \right] \right\rangle_{nms} \right. \\
& \quad \left. \left\langle \frac{\partial}{\partial x_1} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(2)}}{\partial x_1} + \frac{\partial u_N^{(1)}}{\partial x_2} \right) \right] + \frac{\partial}{\partial x_2} \left[ 2\widehat{d_N^2} \frac{\partial u_N^{(2)}}{\partial x_2} \right] + \frac{\partial}{\partial x_3} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(2)}}{\partial x_3} + \frac{\partial u_N^{(3)}}{\partial x_2} \right) \right] \right\rangle_{nms} \right. \\
& \quad \left. \left\langle \frac{\partial}{\partial x_1} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(3)}}{\partial x_1} + \frac{\partial u_N^{(1)}}{\partial x_3} \right) \right] + \frac{\partial}{\partial x_2} \left[ \widehat{d_N^2} \left( \frac{\partial u_N^{(3)}}{\partial x_2} + \frac{\partial u_N^{(2)}}{\partial x_3} \right) \right] + \frac{\partial}{\partial x_3} \left[ 2\widehat{d_N^2} \frac{\partial u_N^{(3)}}{\partial x_3} \right] \right\rangle_{nms} \right\} \quad (6.72)
\end{aligned}$$

This term is strongly nonlinear since  $\widehat{d^2}$ , which contains the square of the components of the rate-of-strain tensor

$$\begin{aligned}
\widehat{d^2} &= \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 = 4 \left[ \left( \frac{\partial u_1}{\partial x_1} \right)^2 + \left( \frac{\partial u_2}{\partial x_2} \right)^2 + \left( \frac{\partial u_3}{\partial x_3} \right)^2 \right] + \\
&+ 2 \left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)^2 + 2 \left( \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right)^2 + 2 \left( \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)^2, \quad (6.73)
\end{aligned}$$

is multiplied by the rate-of-strain tensor  $D_{ij}$  itself. We want to evaluate these terms in the space of wavenumbers; we know that in this space, at given time, our solution is defined by the Fourier's coefficients

$$\hat{u}_{nms}^{(i)}(t) \quad (6.74)$$

for  $n = -N_1/2, \dots, N_1/2 - 1$ ,  $m = -N_2/2, \dots, N_2/2 - 1$  and  $s = -N_3/2, \dots, N_3/2 - 1$ . Moreover, we also know that in this space the derivatives of the solution with respect to  $x_1$  are

$$\frac{\partial u_i}{\partial x_1} \rightarrow in \hat{u}_{nms}^{(i)} \quad (6.75)$$

the derivatives with respect to  $x_2$  are

$$\frac{\partial u_i}{\partial x_2} \rightarrow im \hat{u}_{nms}^{(i)} \quad (6.76)$$

and the derivatives with respect to  $x_3$  are

$$\frac{\partial u_i}{\partial x_3} \rightarrow is \hat{u}_{nms}^{(i)} \quad (6.77)$$

If we suppose to know the coefficients  $\hat{u}_{nms}^{(i)}$ , we can numerically evaluate the derivatives in the transform space directly like in the expressions (6.75), (6.76) and (6.77). In order to evaluate the nonlinear viscous term, then, we can adopt this evaluation of the derivatives in the transform space and proceed as follows:

- transform the value of the derivatives from the wavenumbers' space to the physical space obtaining the values of the derivative of  $u_i$  on the  $N_1$ ,  $N_2$  and  $N_3$  points along  $x_1$ ,  $x_2$  and  $x_3$  respectively.

- use the values of the physical derivatives to evaluate the term  $\widehat{d}^2$  and the rate-of-strain tensor  $D_{ij}$  in physical space;
- compute the products  $\widehat{d}^2 D_{ij}$  in the physical space;
- transform the product's results from the physical space back to the space of wavenumbers and set to zero the values corresponding to the aliased modes; thus one has the Ladyzhenskaya nonlinear viscous stress tensor in the transform space;
- compute in the transform space the divergence of the tensor adopting the same differentiation technique expressed by (6.75), (6.76) and (6.77).

This procedure is basically the application of the transform method, coupled with the de-aliasing 2/3-rule, used for the evaluation of the convective nonlinear term; products, which provide the nonlinear stress tensor, are in fact solved in the physical space and then transformed back to the transform space. The divergence of the nonlinear viscous tensor is then calculated in the transform space.

In conclusion, the results obtained in (6.61), (6.63), (6.64) and (6.71) allow to rewrite the Navier-Stokes equations in the transform space as follows

$$\left\{ \begin{array}{l} \frac{d\hat{u}_{nms}^{(1)}}{dt} + in \langle u_N^{(1)} u_N^{(1)} \rangle_{nms} + im \langle u_N^{(2)} u_N^{(1)} \rangle_{nms} + is \langle u_N^{(3)} u_N^{(1)} \rangle_{nms} + \frac{1}{\text{Re}} (n^2 + m^2 + s^2) \hat{u}_{nms}^{(1)} + in \hat{p}_{nms} = 0 \\ \frac{d\hat{u}_{nms}^{(2)}}{dt} + in \langle u_N^{(1)} u_N^{(2)} \rangle_{nms} + im \langle u_N^{(2)} u_N^{(2)} \rangle_{nms} + is \langle u_N^{(3)} u_N^{(2)} \rangle_{nms} + \frac{1}{\text{Re}} (n^2 + m^2 + s^2) \hat{u}_{nms}^{(2)} + im \hat{p}_{nms} = 0 \\ \frac{d\hat{u}_{nms}^{(3)}}{dt} + in \langle u_N^{(1)} u_N^{(3)} \rangle_{nms} + im \langle u_N^{(2)} u_N^{(3)} \rangle_{nms} + is \langle u_N^{(3)} u_N^{(3)} \rangle_{nms} + \frac{1}{\text{Re}} (n^2 + m^2 + s^2) \hat{u}_{nms}^{(3)} + is \hat{p}_{nms} = 0 \end{array} \right. \quad (6.78)$$

In order to simplify the notation, we set for the moment

$$\begin{aligned} (x_1, x_2, z_3) &= (x, y, z) \\ (u_N^{(1)}, u_N^{(2)}, u_N^{(3)}) &= (u, v, w) \\ (\hat{u}_{nms}^{(1)}, \hat{u}_{nms}^{(2)}, \hat{u}_{nms}^{(3)}) &= (\hat{u}, \hat{v}, \hat{w}) \\ k_x &= n, \quad k_y = m, \quad k_z = s \\ k^2 &= k_x^2 + k_y^2 + k_z^2 = n^2 + m^2 + s^2 \\ \langle \cdot \rangle_{nms} &= \langle \cdot \rangle \end{aligned}$$

thus we can rewrite the (6.78) as follows

$$\left\{ \begin{array}{l} \frac{d\hat{u}}{dt} + ik_x \langle uu \rangle + ik_y \langle uv \rangle + ik_z \langle wu \rangle + \frac{1}{\text{Re}} k^2 \hat{u} + ik_x \hat{p} = 0 \\ \frac{d\hat{v}}{dt} + ik_x \langle uv \rangle + ik_y \langle vv \rangle + ik_z \langle wv \rangle + \frac{1}{\text{Re}} k^2 \hat{v} + ik_y \hat{p} = 0 \\ \frac{d\hat{w}}{dt} + ik_x \langle uw \rangle + ik_y \langle vw \rangle + ik_z \langle ww \rangle + \frac{1}{\text{Re}} k^2 \hat{w} + ik_z \hat{p} = 0 \end{array} \right. \quad (6.79)$$

Consequently, adding the nonlinear viscous term to this scheme, the Ladyzhenskaya equations can be rewritten in the transform space as follows

$$\left\{ \begin{aligned} & \frac{d\hat{u}}{dt} + ik_x \langle uv \rangle + ik_y \langle uv \rangle + ik_z \langle uv \rangle + \frac{1}{\text{Re}} k^2 \hat{u} + ik_x \hat{p} - \frac{1}{\text{La}_2} \left\langle \frac{\partial}{\partial x} \left( 2\hat{d}^2 \frac{\partial u}{\partial x} \right) + \right. \\ & \left. \frac{\partial}{\partial y} \left[ \hat{d}^2 \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \hat{d}^2 \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \right\rangle = 0 \\ & \frac{d\hat{v}}{dt} + ik_x \langle uv \rangle + ik_y \langle vv \rangle + ik_z \langle vw \rangle + \frac{1}{\text{Re}} k^2 \hat{v} + ik_y \hat{p} - \frac{1}{\text{La}_2} \left\langle \frac{\partial}{\partial x} \left[ \hat{d}^2 \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] + \right. \\ & \left. + \frac{\partial}{\partial y} \left( 2\hat{d}^2 \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left[ \hat{d}^2 \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] \right\rangle = 0 \\ & \frac{d\hat{w}}{dt} + ik_x \langle uw \rangle + ik_y \langle vw \rangle + ik_z \langle ww \rangle + \frac{1}{\text{Re}} k^2 \hat{w} + ik_z \hat{p} - \frac{1}{\text{La}_2} \left\langle \frac{\partial}{\partial x} \left[ \hat{d}^2 \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] + \right. \\ & \left. + \frac{\partial}{\partial y} \left[ \hat{d}^2 \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left( 2\hat{d}^2 \frac{\partial w}{\partial z} \right) \right\rangle = 0 \end{aligned} \right. \quad (6.80)$$

in which the nonlinear viscous term are computed using the procedure previously explained. It is important to remember that these equations must hold for all the wavenumbers associated with the spectral approximation; every equation in (6.79) and (6.80) forms indeed a system of  $n \times m \times s$  differential equations for which discretization in time has not yet been realized.

The velocity divergence-free condition can be simply discretized, since the divergence is a linear operator. The Galerkin projection of  $\nabla \cdot \mathbf{u} = 0$  is in fact

$$ik_x \hat{u} + ik_y \hat{v} + ik_z \hat{w} = 0 \quad (6.81)$$

In Fourier space, Navier-Stokes and Ladyzhenskaya systems can be written in a even more compact way denoting with  $\hat{\mathbf{c}}_{\mathbf{k}} = -\langle \mathbf{u} \cdot \nabla \mathbf{u} \rangle_{\mathbf{k}}$  the non-linear convective term, and with  $\hat{\mathbf{g}}_{\mathbf{k}} = \langle \nabla \cdot (\hat{d}^2 \mathbf{D}) \rangle_{\mathbf{k}}$  the non-linear diffusive term:

$$\left\{ \begin{aligned} & \frac{d\hat{\mathbf{u}}_{\mathbf{k}}}{dt} = -\frac{1}{\text{Re}} |\mathbf{k}|^2 \hat{\mathbf{u}}_{\mathbf{k}} - i\mathbf{k} \hat{p}_{\mathbf{k}} + \hat{\mathbf{c}}_{\mathbf{k}} \\ & i\mathbf{k} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = 0 \end{aligned} \right. \quad (6.82)$$

$$\left\{ \begin{aligned} & \frac{d\hat{\mathbf{u}}_{\mathbf{k}}}{dt} = -\frac{1}{\text{Re}} |\mathbf{k}|^2 \hat{\mathbf{u}}_{\mathbf{k}} - i\mathbf{k} \hat{p}_{\mathbf{k}} + \hat{\mathbf{c}}_{\mathbf{k}} + \frac{1}{\text{La}_2} \hat{\mathbf{g}}_{\mathbf{k}} \\ & i\mathbf{k} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = 0 \end{aligned} \right. \quad (6.83)$$

The pressure may be eliminated by taking  $i\mathbf{k}$  dotted with the momentum equations and using the mass conservation  $i\mathbf{k} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = 0$ . Hence, for Navier-Stokes system one obtains

$$\hat{p}_{\mathbf{k}} = -\frac{1}{|\mathbf{k}|^2} i\mathbf{k} \cdot \hat{\mathbf{c}}_{\mathbf{k}} \quad (6.84)$$

and then

$$\frac{d\hat{\mathbf{u}}_{\mathbf{k}}}{dt} = -\frac{1}{\text{Re}} |\mathbf{k}|^2 \hat{\mathbf{u}}_{\mathbf{k}} + \hat{\mathbf{c}}_{\mathbf{k}} - \mathbf{k} \frac{\mathbf{k} \cdot \hat{\mathbf{c}}_{\mathbf{k}}}{|\mathbf{k}|^2} \quad (6.85)$$



whereas for Ladyzhenskaya system one obtains

$$\hat{p}_{\mathbf{k}} = -\frac{1}{|\mathbf{k}|^2} i\mathbf{k} \cdot \hat{\mathbf{c}}_{\mathbf{k}} - \frac{1}{\text{La}_2 |\mathbf{k}|^2} i\mathbf{k} \cdot \hat{\mathbf{g}}_{\mathbf{k}} \quad (6.86)$$

and then

$$\frac{d\hat{\mathbf{u}}_{\mathbf{k}}}{dt} = -\frac{1}{\text{Re}} |\mathbf{k}|^2 \hat{\mathbf{u}}_{\mathbf{k}} + \hat{\mathbf{c}}_{\mathbf{k}} + \frac{1}{\text{La}_2} \hat{\mathbf{g}}_{\mathbf{k}} - \mathbf{k} \frac{\mathbf{k} \cdot \hat{\mathbf{c}}_{\mathbf{k}}}{|\mathbf{k}|^2} - \mathbf{k} \frac{\mathbf{k} \cdot \hat{\mathbf{g}}_{\mathbf{k}}}{\text{La}_2 |\mathbf{k}|^2} \quad (6.87)$$

This is equivalent to evaluating, in every sub-step of the time advancement scheme (Section 6.2.1), the space operators without the pressure term to calculate an intermediate velocity  $\mathbf{u}^*$  which does not satisfy the incompressibility condition  $\nabla \cdot \mathbf{u}^* = 0$ , then taking the divergence of  $\mathbf{u}^*$ , solving the following Poisson equation for the *pressure correction*  $\varphi$

$$\nabla^2 \varphi = \nabla \cdot \mathbf{u}^* \quad (6.88)$$

which, in the Fourier's space, is simply

$$\hat{\varphi}_{\mathbf{k}} = -\frac{1}{|\mathbf{k}|^2} i\mathbf{k} \cdot \hat{\mathbf{u}}^* \quad (6.89)$$

and correcting the field  $\mathbf{u}^*$  with the gradient  $\nabla \varphi$  to obtain  $\mathbf{u}$  which satisfies the incompressibility condition, enforced implicitly by the Poisson equation (6.88).

### 6.2.1 Temporal discretization

For time advancement, the fourth-order explicit Runge-Kutta method has been used.

#### Fourth-order Runge Kutta scheme

Typical problems for evolution equations can be written in the general form

$$\begin{aligned} \frac{\partial u}{\partial t} &= \mathcal{F}(u, t) \quad t > 0 \\ u(0) &= u^0 \end{aligned} \quad (6.90)$$

where the generally nonlinear operator  $\mathcal{F}$  contains the spatial part of the PDE. Given an initial condition, a time integration scheme can be applied to find the solution at later times. For this problem the generic explicit Runge-Kutta scheme of  $s$ -th order has the form

$$u^{(n+1)} = u^{(n)} + \Delta t \sum_{j=1}^s b_j k_j \quad (6.91)$$

where  $\Delta t = t^{(n+1)} - t^{(n)}$  is the constant integration step and, for  $j = 1, 2, \dots, s$ ,  $k_j$  are

$$k_j = \mathcal{F} \left( u^{(n)} + \Delta t \sum_{l=1}^{j-1} a_{jl} k_l, t^{(n)} + c_j \Delta t \right) \quad (6.92)$$

In the scheme  $a_{jl}$ ,  $c_j$  and  $b_j$  are coefficients which depends on the order  $s$ . For the fourth order scheme  $s = 4$  and

$$u^{(n+1)} = u^{(n)} + \Delta t (b_1 k_1 + b_2 k_2 + b_3 k_3 + b_4 k_4) = u^{(n)} + \Delta t \left( \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \right) \quad (6.93)$$

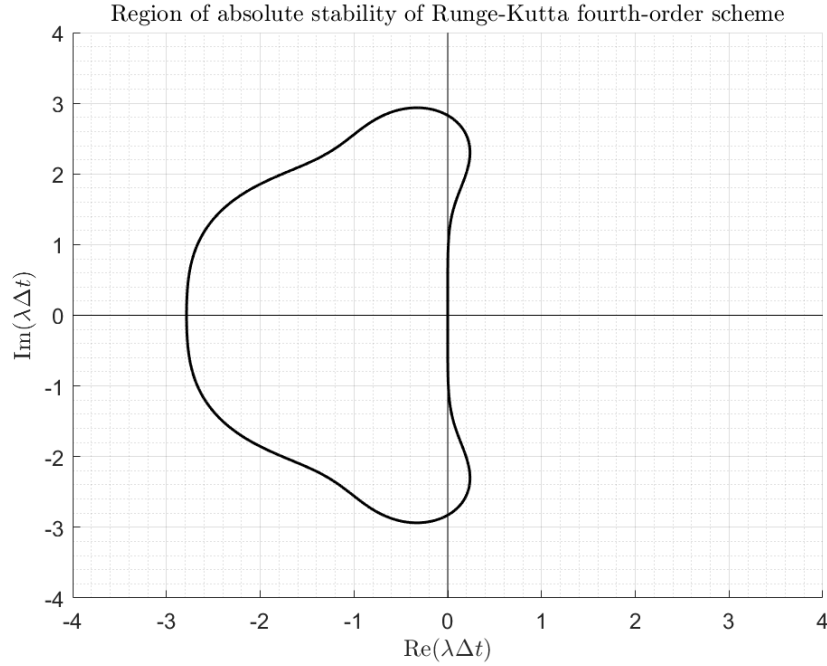


Figure 6.1: Region of absolute stability of Runge-Kutta fourth-order scheme.

with

$$\begin{aligned}
 k_1 &= \mathcal{F}(u^{(n)}, t^{(n)}) \\
 k_2 &= \mathcal{F}\left(u^{(n)} + \Delta t \frac{k_1}{2}, t^{(n)} + \frac{\Delta t}{2}\right) \\
 k_3 &= \mathcal{F}\left(u^{(n)} + \Delta t \frac{k_2}{2}, t^{(n)} + \frac{\Delta t}{2}\right) \\
 k_4 &= \mathcal{F}(u^{(n)} + \Delta t k_3, t^{(n)} + \Delta t)
 \end{aligned}$$

This explicit method computes the value of  $u$  at the time  $t^{(n+1)}$  adding four weighted increments to the value  $u$  assumes at the previous time  $t^{(n)}$ :

- $k_1$  is the increment based on the slope of  $u$  at the beginning of the interval  $[t^{(n)}, t^{(n+1)}]$ ;
- $k_2$  and  $k_3$  are two different increments based on the slope of  $u$  at the midpoint of the interval  $[t^{(n)}, t^{(n+1)}]$ ;
- $k_4$  is the increment based on the slope of  $u$  at the end of the interval  $[t^{(n)}, t^{(n+1)}]$ .

The method is fourth-order accurate: the local truncation error in (6.93) is on the order of  $\mathcal{O}(h^5)$ , while the total accumulated error (the cumulative error caused by many iterations) is on the order of  $\mathcal{O}(h^4)$ . The region of absolute stability of this method is given in Figure 6.1.

Note that the systems we are solving are autonomous, i. e. the function  $\mathcal{F}$  is independent of  $t$ . The scheme can be divided into four steps, in fact one can write  $u^{(0)} = u^{(n)}$  and implement the scheme as follows:

- sub-step 1

$$u^{(1)} = u^{(0)} + \Delta t \frac{k_1}{2} = u^{(0)} + \frac{\Delta t}{2} \mathcal{F}(u^{(0)})$$

- sub-step 2

$$u^{(2)} = u^{(0)} + \Delta t \frac{k_2}{2} = u^{(0)} + \frac{\Delta t}{2} \mathcal{F}(u^{(1)})$$

- sub-step 3

$$u^{(3)} = u^{(0)} + \Delta t k_3 = u^{(0)} + \Delta t \mathcal{F}(u^{(2)})$$

- sub-step 4

$$\begin{aligned} u^{(n+1)} = u^{(4)} &= u^{(0)} + \Delta t \left( \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \right) = \\ &= u^{(0)} + \frac{\Delta t}{6} \mathcal{F}(u^{(0)}) + \frac{\Delta t}{3} \mathcal{F}(u^{(1)}) + \frac{\Delta t}{3} \mathcal{F}(u^{(2)}) + \frac{\Delta t}{6} \mathcal{F}(u^{(3)}) \end{aligned}$$

The fourth-order Runge Kutta scheme requires at least five levels of storage:  $u^{(n)}$ ,  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_4$ ; then  $u^{(n+1)}$  may be overwritten in  $u^{(n)}$ .

## 6.2.2 Computational cost

The computational cost is mainly due to the resolution requirements: the domain size  $\mathcal{L}$  must be large enough to catch the energy-containing motions (largest structures) and, on the other side, the grid spacing has to be small enough to resolve the smallest scales, namely the *dissipative scale*  $\eta$ . Moreover, the time step  $\Delta t$  used in the time advancement scheme is limited by numerical accuracy and stability requirements proper of the scheme. The resolution of the smallest scales requires a small grid spacing  $\Delta x/\eta$  which corresponds, for spectral methods, to sufficiently large maximum wavenumber  $k_{\max}\eta = \eta\pi/\Delta x$ . Since experience shows that *dissipation* is small for  $k\eta \geq 1.5$ , the criterion  $k_{\max}\eta \geq 1.5$  can be used to guarantee the resolution of the smallest scales. It corresponds to the grid spacing requirement

$$\frac{\Delta x}{\eta} \leq \frac{\pi}{1.5} \simeq 2.1 \quad (6.94)$$

A reasonable minimum limit for the domain's size  $\mathcal{L}$  is  $\mathcal{L} = 8L_{11}$  which, in terms of wavenumber, implies that

$$k_0 L_{11} = \frac{\pi}{4} \simeq 0.8 \quad (6.95)$$

for which almost all energy (95%) is resolved. The necessary number of modes is then a function of the Reynolds number, since the ratio between the largest and the smallest length scales depends on  $Re$  according to (4.3). Approximatively this dependence is

$$N^3 \sim 4.4 \cdot Re_L^{9/4}. \quad (6.96)$$

For time advancement it is necessary to chose a time step  $\Delta t$  which allows to catch the diffusive and the convective phenomena at small scales. In practice, the following condition for the Courant number is required

$$C = k_e^{1/2} \frac{\Delta t}{\Delta x} \leq \frac{1}{20} \quad (6.97)$$

where  $k_e$  is turbulent kinetic energy. In order to obtain valid statistics in time is then necessary to simulate at least for four times the turbulence time scale:  $\tau = k_e/\varepsilon$ . Thus, using also the limit in (6.97), the number of steps required is at least

$$n_{\text{steps}} = \frac{4\tau}{\Delta t} = 80 \frac{k_e^{3/2}}{\varepsilon \Delta x}$$

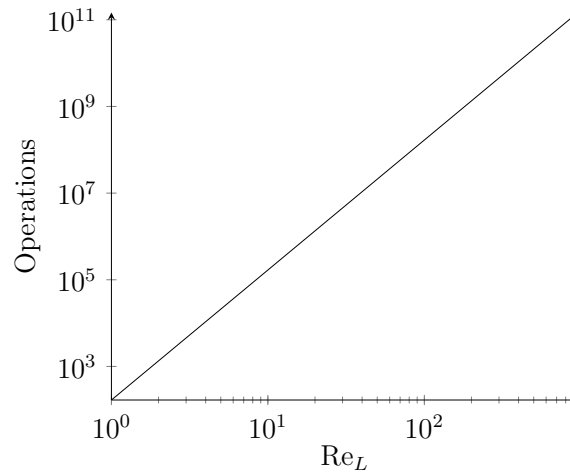


Figure 6.2: Total number of operations growth with Reynolds number per simulation

Since the integral lengthscale is on the order of  $L = k^{3/2}/\varepsilon$  and, according to (6.94),  $\Delta x$  has to be at most equal to  $2.1\eta$ , the total number of steps required is

$$n_{\text{steps}} \simeq 38 \cdot \frac{L}{\eta}$$

Thus using  $L/\eta = \text{Re}_L^{3/4}$  from (4.3) one finds

$$n_{\text{steps}} \simeq 38 \cdot \text{Re}_L^{3/4} \quad (6.98)$$

The number of operations required to perform a simulation is approximatively proportional to the product of the number of modes and the number of steps:

$$N^3 \cdot n_{\text{steps}} \sim 4.4 \cdot \text{Re}_L^{9/4} \cdot 38 \cdot \text{Re}_L^{3/4} \simeq 168 \cdot \text{Re}_L^3 \quad (6.99)$$

which shows how the number of operations rapidly grows with the Reynolds number (Figure 6.2).

## 6.3 Fortran Program

The schemes presented in the previous Section (Fourier-Galerkin method coupled with the fourth-order Runge-Kutta time advancement) have been implemented in a program named *dns\_hit\_mpi* written in Fortran language; the program implements a parallel algorithm, using Message Passing Interface (MPI), decomposing the physical domain into slices parallel to the plane  $(x_1, x_2)$ , i. e. *parallelizing* the third direction  $x_3$  (Figure 6.3). The program's structure is based on *DNS-TurIsMi* (version 1.4), developed by Professor Michele Iovieno (see [24], [25], [26] and [27] as references), which can solve three-dimensional Navier-Stokes equations and the passive scalar transport equation assuming turbulence to be homogeneous and isotropic.

```

1 program dns_hit_mpi
2 !developed and written by Domenico Zaza
3 !Subroutines for data transposition are taken from
4 !DNS-TurIsMi (v1.4) developed by Professor Michele Iovieno

```

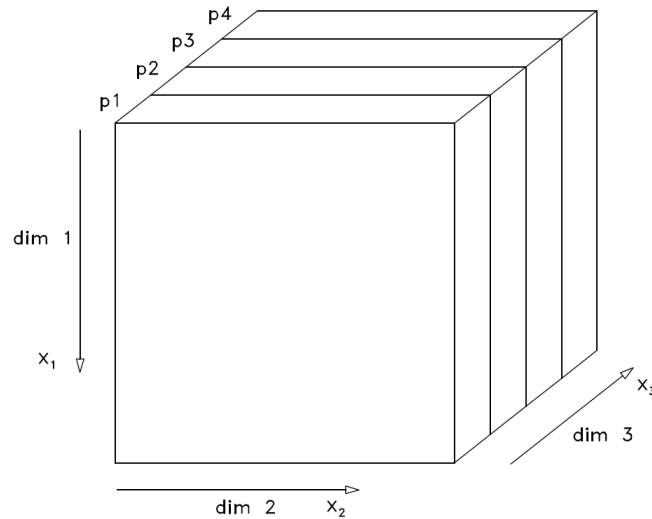


Figure 6.3: Parallelization - Decomposition of the computational domain ( $p_n$  denotes the  $n$ -th process)

```

5  include 'mpif.h'
6  common nid,noprocs,n1,nloc,n3,n3loc
7  double precision::deltat,pi,sim_time
8  double precision::Re, La
9  integer:: model,nsalva,ntot
10 integer:: m1,m2,m3,m4
11 double precision,allocatable, dimension(:):: xx,xx3loc
12 double precision,allocatable, dimension(:):: k,k3,k3loc
13 double precision,allocatable, dimension(:,:,:):: kk1,kk2,kk3loc,...
    kk_quad,kk_quadnz
14 double complex,allocatable, dimension(:,:,:):: u0,u1
15 double precision,allocatable,dimension(:)::deal1,deal3,deal3loc
16 double precision,allocatable, dimension(:,:,:)::deal
17 double complex,allocatable, dimension(:,:,:):: HH1,HH2,HH3,HH4
18 double precision,allocatable, dimension(:,:,:):: u0real
19 integer,allocatable,dimension(:)::inds,inds3
20 character*20, allocatable:: nomefile(:)
21 character(len=10)::snapshot
22
23 !.....Variables for parallelization:
24 integer status(MPI_Status_size)
25 !.....Parallel initialization:
26 call MPI_Init(ierr)
27 call MPI_Comm_size(MPI_COMM_WORLD,noprocs,ierr) !noprocs=number...
    of processors
28 call MPI_Comm_rank(MPI_COMM_WORLD,nid,ierr) !nid=rank of each ...
    processor
29 !.....End of initialization...
30 call MPI_BARRIER(MPI_Comm_World,ierr)
31 !.....Parameters definition:
32
33 pi=4.0*atan(1.0d0)
34
35 !.....parameter are read by processor 0 from file in_dns.txt...
36 if(nid.eq.0)then
37 open(1,file='in_dns.txt')

```

```

38  read(1,*)n1
39  read(1,*)n3
40  read(1,*)deltat
41  read(1,*)ntot
42  read(1,*)nsalva
43  read(1,*)model
44  read(1,*)Re
45  read(1,*)La
46  close(1)
47
48  sim_time=deltat*ntot
49
50  WRITE(*,*) '                                dns_hit_mpi PROGRAM ...
51
52  WRITE(*,*)
53  WRITE(*,*) '***** INPUT DATA ...
54  WRITE(*,*) '...
55  WRITE(*,*) '***** '
56  WRITE(*,*) 'Number of points in x1 and x2:', n1
57  WRITE(*,*) 'Number of points in x3:', n3
58  WRITE(*,*) 'Reynolds number:', RE
59  if(model.eq.1) then
60  WRITE(*,*) 'Model: Navier-Stokes equations'
61  elseif(model.eq.2) then
62  WRITE(*,*) 'Model: Ladyzhenskaya equations with r=2'
63  WRITE(*,*) 'Ladyzhenskaya number: ', La
64  else
65  WRITE(*,*) 'ERROR IN FLUID DYNAMIC MODEL SELECTION'
66  end if
67  WRITE(*,*) 'Integration Step: ',deltat
68  WRITE(*,*) 'Number of steps: ',ntot
69  WRITE(*,*) 'Simulation Time: ',sim_time
70  WRITE(*,*) 'Steps for saving: ',nsalva
71  WRITE(*,*) '...
72  WRITE(*,*) '***** '
73
74  end if
75  !.....and spread to all processors...
76  call MPI_Bcast(n1,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierror)
77  call MPI_Bcast(n3,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierror)
78  call MPI_Bcast(ntot,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierror)
79  call MPI_Bcast(nsalva,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierror)
80  call MPI_Bcast(model,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierror)
81
82  call MPI_Bcast(Re,1,MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,ierror...)
83  call MPI_Bcast(La,1,MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,ierror...)
84  call MPI_Bcast(deltat,1,MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,...
85  ierror)
86  call MPI_Bcast(sim_time,1,MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,...
87  ierror)

```

```

87  n3loc=n3/noprocs
88  nloc=n1/noprocs
89
90  !.....Points for de-aliasing
91  m1=CEILING(n1/3.D0)
92  m2=n1+3-2*m1
93
94  m3=CEILING(n3/3.D0)
95  m4=n3+3-2*m3
96
97  !.....wavenumbers
98  allocate(k(0:n1-1),k3(0:n3-1),k3loc(0:n3loc-1))
99  allocate(deal1(0:n1-1),deal3(0:n3-1),deal3loc(0:n3loc-1))
100 allocate(deal(0:n1-1,0:n1-1,0:n3loc-1))
101 allocate(inds(0:m2-1),inds3(0:m4-1))
102
103 do ii=0,n1/2
104   k(ii)=dfloat(ii)
105 end do
106 do ii=1,n1/2-1
107   k(n1-ii)=-dfloat(ii)
108 end do
109 do ii=0,n3/2
110   k3(ii)=dfloat(ii)
111 end do
112 do ii=1,n3/2-1
113   k3(n3-ii)=-dfloat(ii)
114 end do
115
116 do ii=0,n1-1
117   deal1(ii)=1.0d0
118 end do
119 do ii=0,n1-1
120   deal3(ii)=1.0d0
121 end do
122
123 !.....deactivating aliased modes
124 do ii=0,m2-1
125   inds(ii)=m1+ii
126 end do
127 do ii=0,m4-1
128   inds3(ii)=m3+ii
129 end do
130
131 k(inds)=0.0d0
132 k3(inds3)=0.0d0
133 deal1(inds)=0.0d0
134 deal3(inds)=0.0d0
135
136 do ii=0,n3loc-1
137   k3loc(ii)=k3(nid*n3loc+ii)
138   deal3loc(ii)=deal3(nid*n3loc+ii)
139 end do
140 deallocate(k3)
141 deallocate(deal3)
142
143 allocate(kk1(0:n1-1,0:n1-1,0:n3loc-1),kk2(0:n1-1,0:n1-1,0:n3loc-1)...
      ,kk3loc(0:n1-1,0:n1-1,0:n3loc-1),kk_quad(0:n1-1,0:n1-1,0:n3loc-1)...)

```

```

-1))
144 allocate(kk_quadnz(0:n1-1,0:n1-1,0:n3loc-1))
145
146 do ll=0,n3loc-1
147 do jj=0,n1-1
148 do ii=0,n1-1
149   kk1(ii,jj,ll)=k(ii)
150   kk2(ii,jj,ll)=k(jj)
151   kk3loc(ii,jj,ll)=k3loc(ll)
152   kk_quad(ii,jj,ll)=k(ii)**2+k(jj)**2+k3loc(ll)**2
153   deal(ii,jj,ll)=deal1(ii)*deal1(jj)*deal3loc(ll)
154   if(kk_quad(ii,jj,ll).eq.0.0D0)then
155     kk_quadnz(ii,jj,ll)=0.0d0
156   else
157     kk_quadnz(ii,jj,ll)=(1.0d0)/kk_quad(ii,jj,ll)
158   end if
159 end do
160 end do
161 end do
162 deallocate(k,k3loc)
163
164 allocate(u0real(0:n1-1,0:n1-1,0:n3loc-1,1:3))
165 allocate(u0(0:n1-1,0:n1-1,0:n3loc-1,1:3))
166 allocate(xx(0:n1-1),xx3loc(0:n3loc-1))
167
168 do i1=0,n1-1
169 do i2=0,n1-1
170 do i3=0,n3loc-1
171 do j=1,3
172   u0(i1,i2,i3,j)=(0.0d0,0.0d0)
173   u0real(i1,i2,i3,j)=0.0d0
174 end do
175 end do
176 end do
177 end do
178
179 !.....space variables
180 do ii=0,n1-1
181   xx(ii)=ii*2.d0*pi/n1
182 end do
183 do ii=0,n3loc-1
184   xx3loc(ii)=(nid*n3loc+ii)*2.d0*pi/n3
185 end do
186
187 call MPI_BARRIER(MPI_Comm_World,ierror)
188 !.....initial condition: Taylor-Green Vortex
189 do i1=0,n1-1
190 do i2=0,n1-1
191 do i3=0,n3loc-1
192   u0real(i1,i2,i3,1)=sin(xx(i1))*cos(xx(i2))*cos(xx3loc(i3)) ! ...
193     u0
194   u0real(i1,i2,i3,2)=-cos(xx(i1))*sin(xx(i2))*cos(xx3loc(i3)) ! ...
195     v0
196   u0real(i1,i2,i3,3)=0.0d0 ! w0
197 end do
198 end do
199 end do

```



```

199 deallocate(xx,xx3loc)
200
201 if(nid.eq.0)then
202     write(*,*)'Saving Initial Velocity Field'
203 end if
204
205 !.....saving initial field
206 allocate(nomefile(1:3))
207 nomefile(1)='u_0.bin'
208 nomefile(2)='v_0.bin'
209 nomefile(3)='w_0.bin'
210 call MPI_Barrier(MPI_COMM_WORLD,ierror)
211 !.....Data storage.....
212 do jcomp=1,3
213     call saveres(u0real,jcomp,nomefile(jcomp))
214 end do
215
216
217 if(nid.eq.0)then
218     write(*,*)'Flow initialised and saved in:'
219     do ii=1,3
220         write(*,*)nomefile(ii)
221     end do
222     WRITE(*,*)'...'
223     !*****
224     WRITE(*,*)'...'
225     !*****
226     WRITE(*,*)'Starting Solver...'
227     WRITE(*,*)
228     WRITE(*,*)'***** TIME INTEGRATION ...'
229     !*****
230 end if
231
232 call MPI_BARRIER(MPI_Comm_World,ierror)
233 call transform_notr(u0,u0real)
234
235 !....March in time:Fourth Order Runge-Kutta scheme
236 ncicli=ntot/nsalva
237
238 allocate(HH1(0:n1-1,0:n1-1,0:n3loc-1,1:3),HH2(0:n1-1,0:n1-1,0:...
239           n3loc-1,1:3))
240 allocate(HH3(0:n1-1,0:n1-1,0:n3loc-1,1:3),HH4(0:n1-1,0:n1-1,0:...
241           n3loc-1,1:3))
242 allocate(u1(0:n1-1,0:n1-1,0:n3loc-1,1:3))
243 call MPI_BARRIER(MPI_Comm_World,ierror)
244 call projection(u0,kk1,kk2,kk3loc,kk_quadnz)
245
246 if(model.eq.1) then !Navier-Stokes equations
247 !.....External loop = save results
248 do iext=1,ncicli
249 !.....Inner loop= time integration with Runge-Kutta 4th
250 do int=0,nsalva-1
251
252     CALL SPACE_OP(HH1,u0,kk1,kk2,kk3loc,kk_quad,Re,deal)
253     u1=u0+0.5d0*deltat*HH1
254     call projection(u1,kk1,kk2,kk3loc,kk_quadnz)
255
256     CALL SPACE_OP(HH2,u1,kk1,kk2,kk3loc,kk_quad,Re,deal)

```

```

252     u1=u0+0.5d0*deltat*HH2
253     call projection(u1, kk1, kk2, kk3loc, kk_quadnz)
254
255     CALL SPACE_OP(HH3, u1, kk1, kk2, kk3loc, kk_quad, Re, deal)
256     u1=u0+deltat*HH3
257     call projection(u1, kk1, kk2, kk3loc, kk_quadnz)
258
259     CALL SPACE_OP(HH4, u1, kk1, kk2, kk3loc, kk_quad, Re, deal)
260     u0=u0+deltat*(HH1/(6.0d0)+HH2/(3.0d0)+HH3/(3.0d0)+HH4/(6.0d0...
        ))
261     call projection(u0, kk1, kk2, kk3loc, kk_quadnz)
262
263     write(*,*) 'End of cicle ', int+1, '/', iext
264     end do
265     !.....End of inner loop (RK4)
266
267     call MPI_BARRIER(MPI_Comm_World, ierror)
268
269     !.....Data storage.....
270     call transforminv_notr(u0real, u0)
271
272     write(snapshot, '(i8)') (iext)
273     nomefile(1)='u_'//trim(adjustl(snapshot))//'.bin'
274     nomefile(2)='v_'//trim(adjustl(snapshot))//'.bin'
275     nomefile(3)='w_'//trim(adjustl(snapshot))//'.bin'
276
277     write(*,*) 'Saving results'
278     do jcomp=1,3
279         call saveres(u0real, jcomp, nomefile(jcomp))
280     end do
281
282     call MPI_Barrier(MPI_COMM_WORLD, ierror)
283 end do
284 !.....End of external loop
285
286 elseif(model.eq.2) then !Ladyzhenskaya equations with r=2
287 !.....External loop = save results
288     do iext=1, ncicli
289 !.....Inner loop= time integration with Runge-Kutta 4th
290         do int=0, nsalva-1
291
292             CALL SPACE_OP_LAD(HH1, u0, kk1, kk2, kk3loc, kk_quad, Re, La, deal)
293             u1=u0+0.5d0*deltat*HH1
294             call projection(u1, kk1, kk2, kk3loc, kk_quadnz)
295
296             CALL SPACE_OP_LAD(HH2, u1, kk1, kk2, kk3loc, kk_quad, Re, La, deal)
297             u1=u0+0.5d0*deltat*HH2
298             call projection(u1, kk1, kk2, kk3loc, kk_quadnz)
299
300             CALL SPACE_OP_LAD(HH3, u1, kk1, kk2, kk3loc, kk_quad, Re, La, deal)
301             u1=u0+deltat*HH3
302             call projection(u1, kk1, kk2, kk3loc, kk_quadnz)
303
304             CALL SPACE_OP_LAD(HH4, u1, kk1, kk2, kk3loc, kk_quad, Re, La, deal)
305             u0=u0+deltat*(HH1/(6.0d0)+HH2/(3.0d0)+HH3/(3.0d0)+HH4/(6.0d0...
                ))
306             call projection(u0, kk1, kk2, kk3loc, kk_quadnz)
307

```

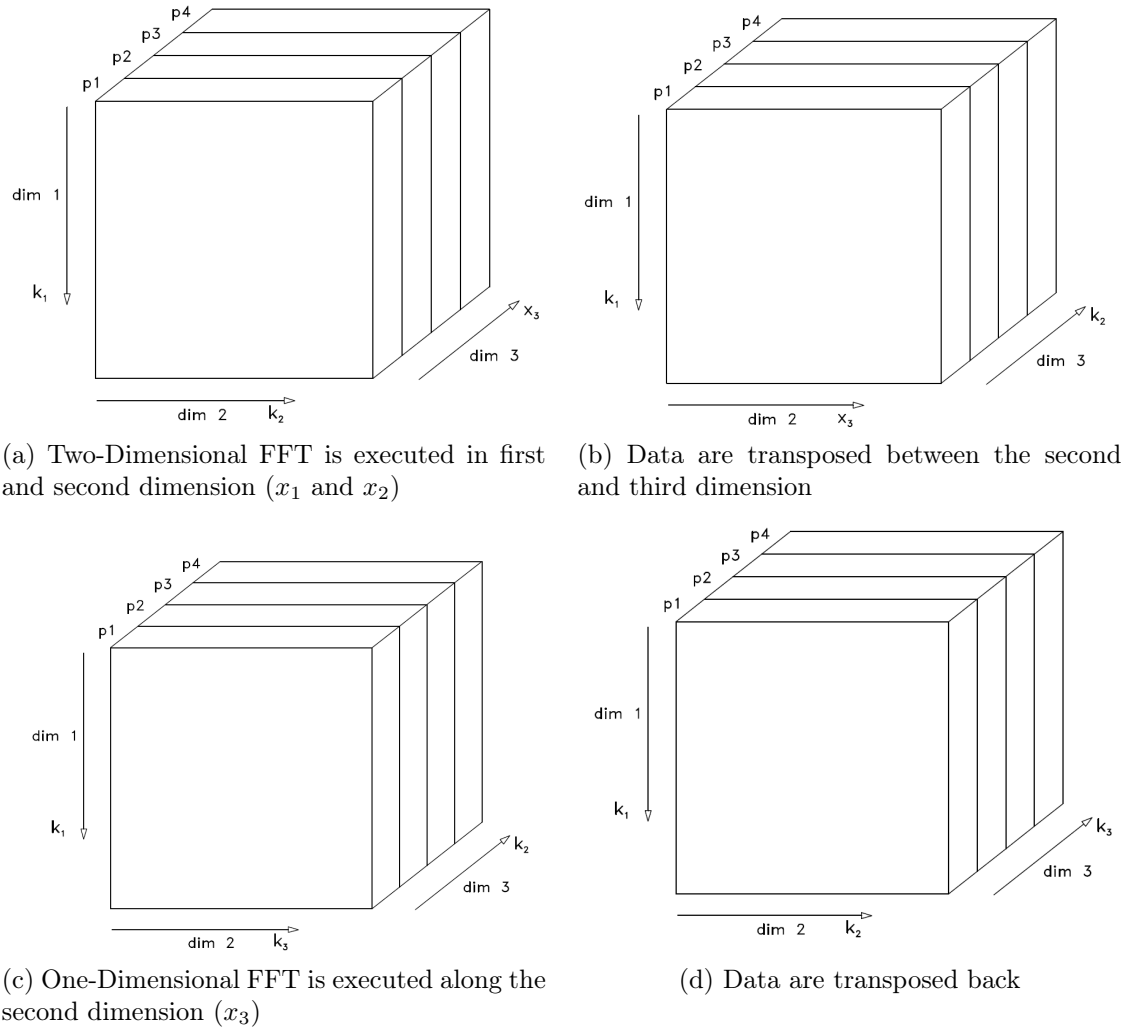
```

308     write(*,*) 'End of cicle ',int+1,'/',iext
309     end do
310     !.....End of inner loop (RK4)
311     call MPI_BARRIER(MPI_Comm_World,ierror)
312
313     !.....Data storage.....
314     call transforminv_notr(u0real,u0)
315
316     write(snapshot,'(i8)') (iext)
317     nomefile(1)='u_'//trim(adjustl(snapshot))//'.bin'
318     nomefile(2)='v_'//trim(adjustl(snapshot))//'.bin'
319     nomefile(3)='w_'//trim(adjustl(snapshot))//'.bin'
320
321     write(*,*) 'Saving results'
322     do jcomp=1,3
323         call saveres(u0real,jcomp,nomefile(jcomp))
324     end do
325
326     call MPI_Barrier(MPI_COMM_WORLD,ierror)
327     end do
328     !.....End of external loop
329
330 end if
331
332 deallocate(deal1,deal3loc)
333 deallocate(deal)
334 deallocate(HH1,HH2,HH3,HH4)
335 deallocate(u1)
336 deallocate(u0real,u0)
337 deallocate(nomefile)
338 deallocate(kk1,kk2,kk3loc,kk_quad)
339 deallocate(kk_quadnz)
340 deallocate(inds,inds3)
341
342 !.....Closing
343 print *, 'Stop!',nid
344 call MPI_Finalize(ierror)
345 stop
346
347 end program dns_hit_mpi

```

The main code reads line by line the following data from an input file called *in\_dns.txt*:

- the number of points  $n$  of the spatial discretization in  $x_1$  and  $x_2$  directions;
- the number of points  $n_3$  of the spatial discretization in  $x_3$ ;
- the time step  $\Delta t$  for the time advancement scheme;
- the total number of steps  $n_{\text{steps}}$ . Thus  $\Delta t \cdot n_{\text{steps}}$  gives the simulation time;
- the number of steps  $n_{\text{save}}$  after which saving the results;
- an integer which selects the fluid dynamic model: 1 for the Navier-Stokes equations and 2 for the Ladyzhenskaya model with  $r = 2$ ;
- the Reynolds number  $Re$ ;

Figure 6.4: Parallel three-dimensional FFT algorithm - subroutine *transform\_notr*

- the Ladyzhenskaya number  $La_2$  defined by (5.11).

Then it calculates the wavenumbers, initializes and saves the flow with the Taylor-Green field and transforms the fields to the wavenumbers' space (subroutine *transform\_notr*). The Fourier's coefficients of the velocity field are computed as discrete Fourier transform (DFT) using FFTW (version 3.3.9) libraries. The Fourier transform of data along  $x_3$ , which are spread among the different processes, is realized by transposing the second and the third direction of the three-dimensional array containing velocities, after DFTs in the first and the second direction have been calculated (Figure 6.4). In this point the main code is split by an *if-elseif* statement into two possible time advancements: one solves the Navier-Stokes equations and the other solves the Ladyzhenskaya equations with  $r = 2$ . The selection is realized using the sixth line of the input file. Both the advancements employ the fourth-order Runge-Kutta scheme which requires four evaluations of the space operator. The space operator is evaluated through the subroutine *space\_op* for the Navier-Stokes equations and the subroutine *space\_op\_lad* for the Ladyzhenskaya equations. These subroutines implement the Fourier-Galerkin method previously presented. In particular *space\_op\_lad* proceeds as follows

- it calculates *pseudo-spectrally* the symmetric convective stress tensor  $u_i u_j$  using the subroutine *ConvectiveStress*;

- calculates *pseudo-spectrally* the symmetric non-linear Ladyzhenskaya stress tensor

$$\frac{\tau_{ij}^{\text{Lad}}}{\text{La}_2} = \frac{1}{\text{La}_2} \cdot \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \quad (6.100)$$

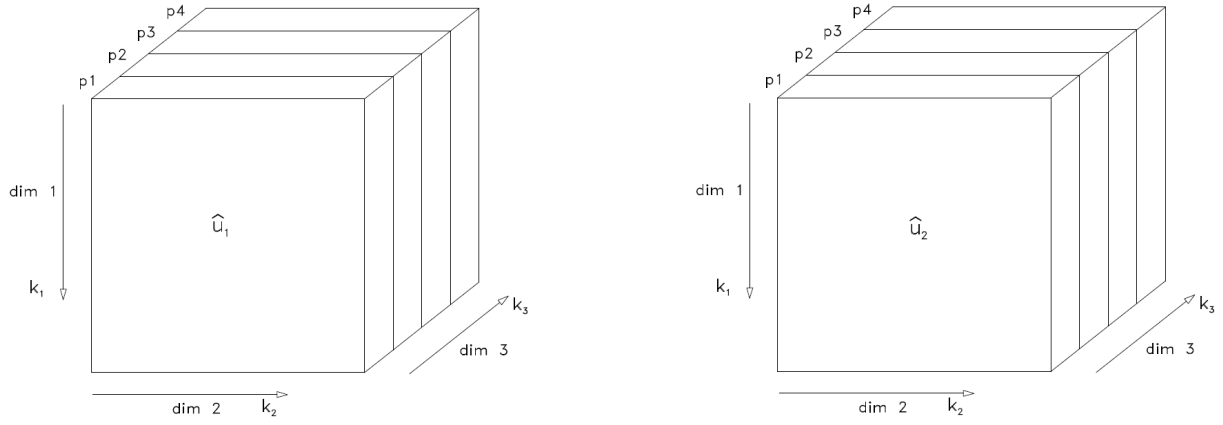
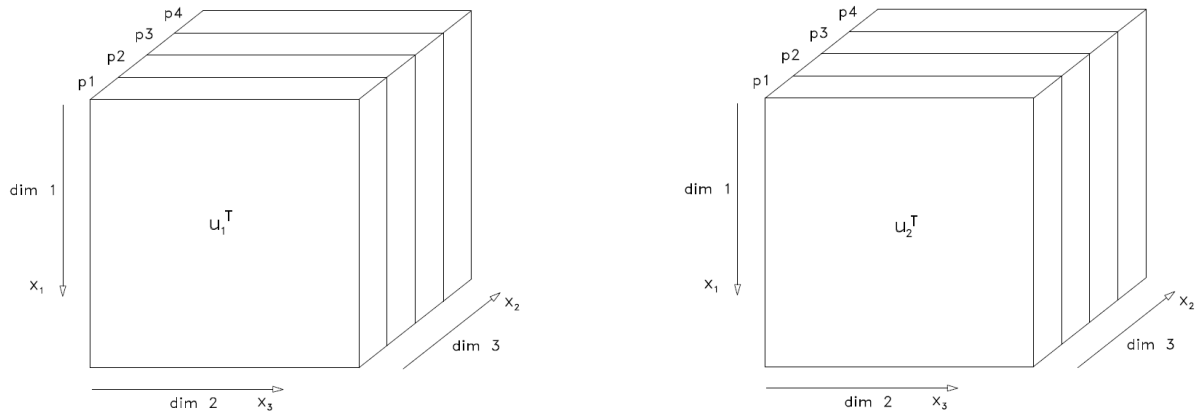
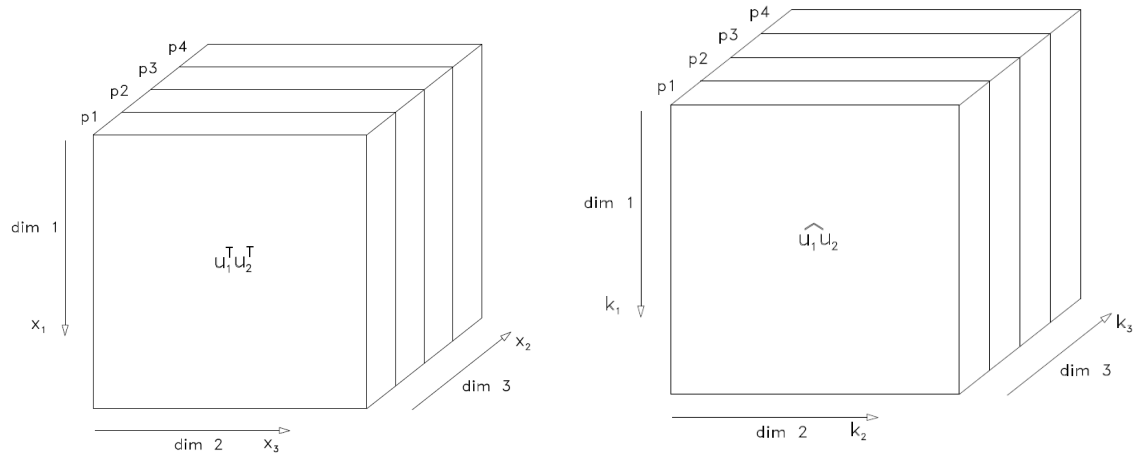
using the subroutine *LadyzhenskayaStress*;

- adds  $\tau_{ij}^{\text{Lad}}/\text{La}_2$  to  $-u_i u_j$ ;
- *de-aliases* the resulting array by setting to zero the aliased modes ( $n/3$  central modes), implementing the 2/3-rule;
- calculates the divergence of the resulting four-dimensional array which contains the convective and the non-linear viscous stresses de-aliased;
- adds the linear viscous terms.

After an intermediate velocity field is obtained in the Runge-Kutta substep, it is projected onto a solenoidal field solving the Poisson equation (6.89) for the pressure correction (subroutine *projection*), as previously explained. The subroutine *space\_op* follows the same procedure, obviously avoiding to calculate the Ladyzhenskaya viscous stress tensor.

The pseudospectral evaluations of non-linear terms in subroutines *ConvectiveStress* and *LadyzhenskayaStress* represent the heart of the program; they are shown in Appendix D. The main idea in pseudo-spectral methods is to evaluate the derivatives in the transform space, because is much easier, and the products in the real space. For this parallel program, however, transforming variables back and forth would implicate several data transpositions (MPI communications among the processes), like in the subroutine *transform\_notr*; one way to avoid too many communications in pseudo-spectral evaluations is to transform variables back to the real space, do not transpose back the third and the second direction, calculate the products with data still transposed, and then transpose back direction two and three while results are transformed to Fourier's space. These antitransform and transform are realized through the subroutines *transform\_tr* and *transforminv\_tr*. The outline of the pseudospectral evaluation of  $u_1 u_2$  is represented in Figure 6.5. Transpositions are realized using the subroutines *trasponi\_dir* and *trasponi\_inv* which belong to the program *DNS-TurIsMi* (version 1.4).

Finally, every  $n_{\text{save}}$  time steps the components of the resulting velocities are saved in binary files.


 (a) Data are originally given in Fourier's space:  $\hat{u}_1$  and  $\hat{u}_2$ 

 (b)  $\hat{u}_1$  and  $\hat{u}_2$  are transformed to real space using *transforminv\_tr*: 2D antitransform is executed in dimensions 1 and 2, data are transposed between directions 2 and 3, and 1D antitransform is executed in dimension 2. Data are not transposed back.

 (c) Product  $u_1 u_2$  is calculated

 (d)  $u_1 u_2$  is transformed to Fourier's space using *transform\_tr*: transform is executed in dimensions 1 and 2, data are transposed back between directions 2 and 3, and 1D transform is executed in dimension 2.

 Figure 6.5: Pseudospectral evaluation of  $u_1 u_2$

# Chapter 7

## Simulations and results

The program *dns\_hit\_mpi* has been run on *CASPER* High Performance Computer, one of the three InfiniBand clusters at the Politecnico di Torino whose characteristics are shown in Table 7.1; computational resources were indeed provided by *HPC@POLITO*, a project of Academic Computing within the Department of Control and Computer Engineering at the Politecnico di Torino.

|                       |  |
|-----------------------|--|
| Architecture          | Linux Infiniband-DDR MIMD Distributed Shared-Memory Cluster              |
| Node Interconnect     | Infiniband DDR 20 Gb/s   |
| Service Network       | Gigabit Ethernet 1 Gb/s  |
| CPU Model             | 2x AMD Opteron 6276/6376 (Bulldozer)<br>2.3 GHz (turbo 3.0 GHz) 16 cores |
| Sustained performance | 4.360 TFLOPS   |
| Peak performance      | 5.658 TFLOPS   |
| Green500 Index        | 422.31 MFLOPS/W  |
| Power Consumption     | 3.6 kW   |
| Computing Cores       | 512  |
| Number of Nodes       | 16   |
| Total RAM Memory      | 2 TB DDR3 REGISTERED ECC   |
| OS                    | Centos 7.6 - OpenHPC 1.3.8.1   |
| Scheduler             | SLURM 18.08.8  |

Table 7.1: CASPER cluster characteristics

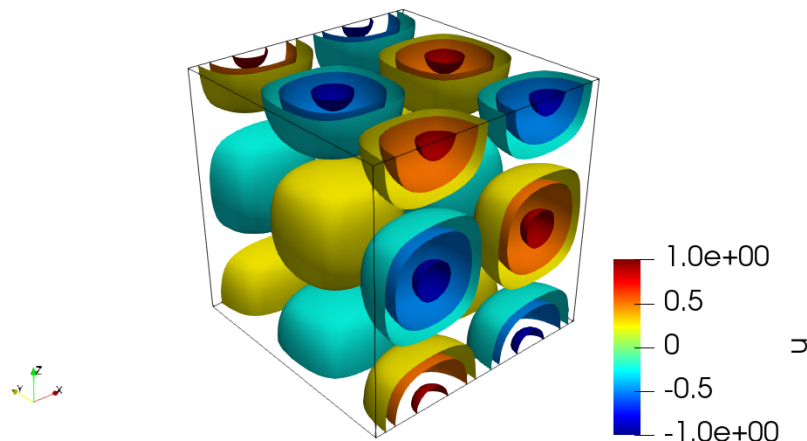
Four simulations have been realized on a grid formed by 128 points in each direction: the first (*Sim1*) solves Navier-Stokes equations, whereas the second (*Sim2*), the third (*Sim3*) and the fourth (*Sim4*) solve Ladyzhenskaya equations. Simulations' parameters in non-dimensional form are shown in Table 7.2. Assuming the largest scale to be on the order of  $L = \pi$  and the Reynolds number to be  $\text{Re} = 450$ , the dissipative scale would be approximatively

$$\eta \approx \frac{L}{\text{Re}^{3/4}} = 0.03215 \quad (7.1)$$

Thus, using the  $k_{\max}\eta \geq 1.5$  criterion, the minimum number of modes which allows to catch the dissipative scales would be  $N = 1.5/\eta \simeq 47$  which corresponds to 94 points in each direction. Using  $128^3$  points, simulations would solve the dissipative scales even if  $N/3$  modes are used for de-aliasing.

|                    | <b>Sim1</b>   | <b>Sim2</b>   | <b>Sim3</b>   | <b>Sim4</b>   |
|--------------------|---------------|---------------|---------------|---------------|
| $n$                | 128           | 128           | 128           | 128           |
| $n_3$              | 128           | 128           | 128           | 128           |
| Model              | Navier-Stokes | Ladyzhenskaya | Ladyzhenskaya | Ladyzhenskaya |
| Re                 | 450           | 450           | 450           | 450           |
| $La_2$             | -             | 12000         | 8000          | 6000          |
| $\Delta \tilde{t}$ | $10^{-3}$     | $10^{-3}$     | $10^{-3}$     | $10^{-3}$     |
| $n_{\text{steps}}$ | 20000         | 20000         | 20000         | 20000         |
| Time               | 20            | 20            | 20            | 20            |
| N. of processors   | 16            | 16            | 16            | 16            |
| Run Time (h:m:s)   | 14:56:09      | 48:01:00      | 41:07:05      | 40:59:43      |

Table 7.2: Simulations' parameters

Figure 7.1: Isosurfaces of  $x$ -component of  $\mathbf{u}^o$  (TGV) -  $u^o = \{\pm 0.25, \pm 0.5, \pm 0.9\}$ 

The Taylor-Green Vortex (5.17) is used as initial condition for all the simulations. The isosurfaces of the  $x$  and  $y$  components of the initial velocity field are represented in Figures 7.1 and 7.2; the isosurfaces of the resulting  $z$ -component of vorticity  $\omega_z$  are shown in Figure 7.3.

## 7.1 Results

Isosurfaces for the  $x$  and  $y$  components of the velocity and the  $z$ -component of the vorticity fields are shown for the simulations from Figure 7.4 to Figure 7.15. From these Figures it can be noted qualitatively that, similarly to Navier-Stokes equations, Ladyzhenskaya equations include vortices' breakup into smaller structures: initial energy, which is contained by the largest structures, is transferred to smaller ones as time passes. In fact Figure 7.16, which shows energy spectra, reveals that even for Ladyzhenskaya equations the cascade process takes place: for  $\tilde{t} \simeq 9$  spectra are approximately continuous and for  $k \leq 10$  there is a very small inertial range, for which  $E(k, t)$  is close to the expected Kolmogorov  $k^{-5/3}$  law. As the Reynolds and the Ladyzhenskaya numbers increase this range should become wider.



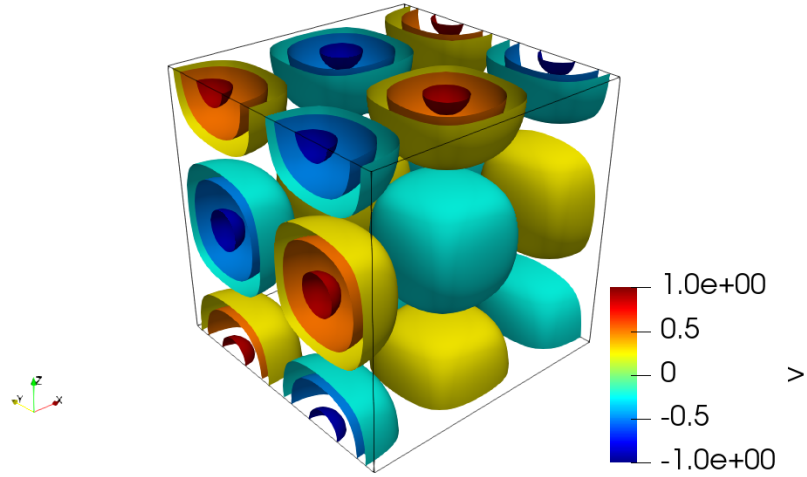


Figure 7.2: Isosurfaces of  $y$ -component of  $\mathbf{u}^\circ$  (TGV) -  $v^\circ = \{\pm 0.25, \pm 0.5, \pm 0.9\}$

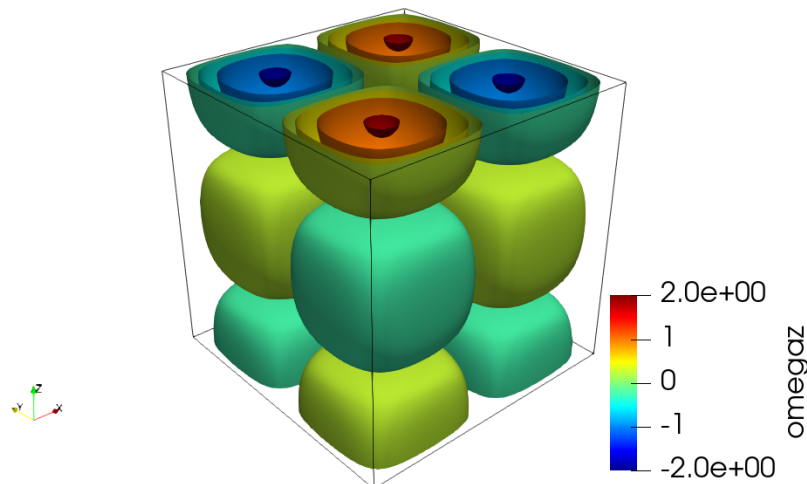


Figure 7.3: Isosurfaces of  $z$ -component of vorticity  $\omega^\circ$  (TGV) -  $\omega_z^\circ = \{\pm 0.25, \pm 0.5, \pm 1.0, \pm 1.9\}$

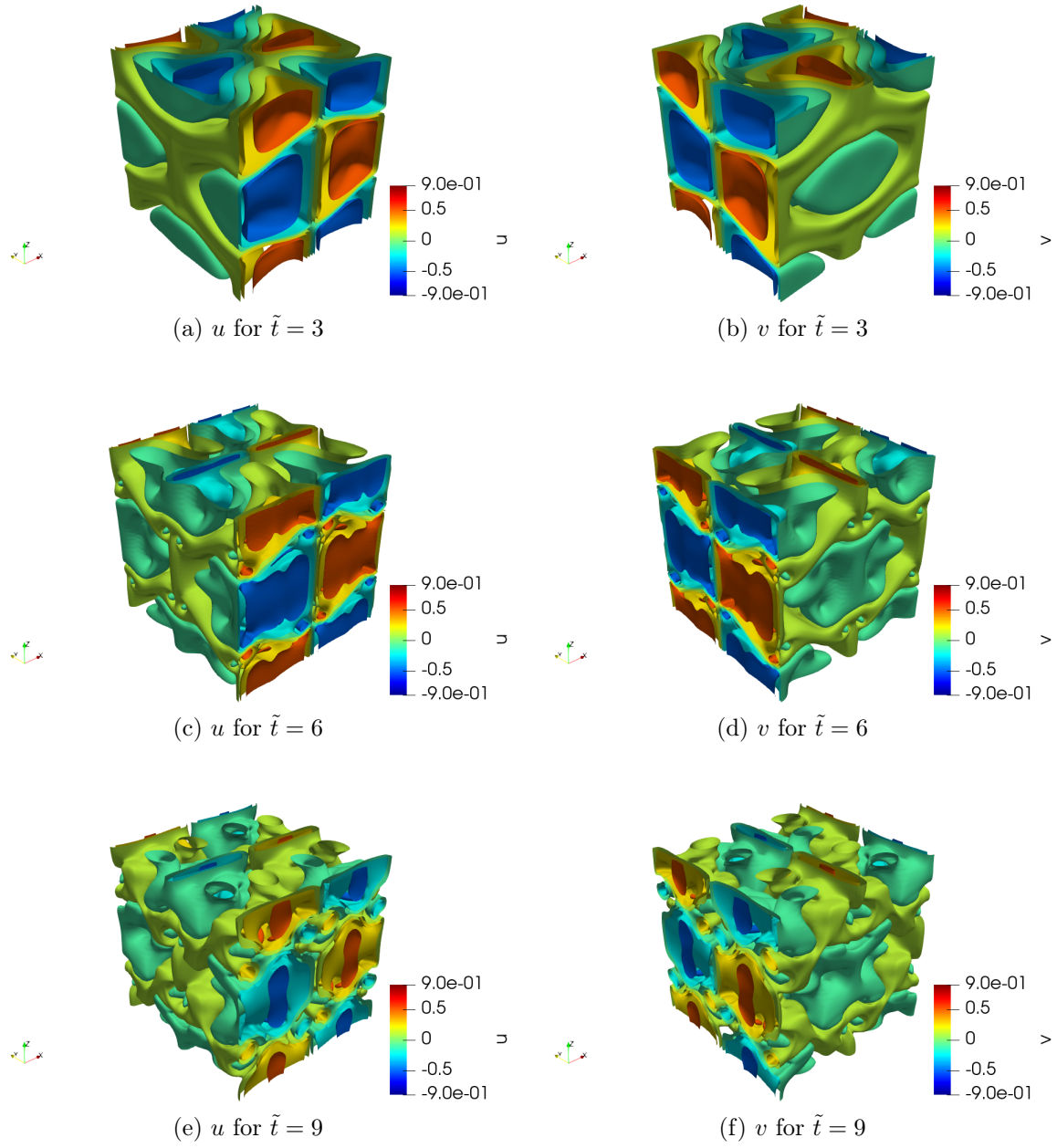


Figure 7.4: *Sim1* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{3, 6, 9\}$

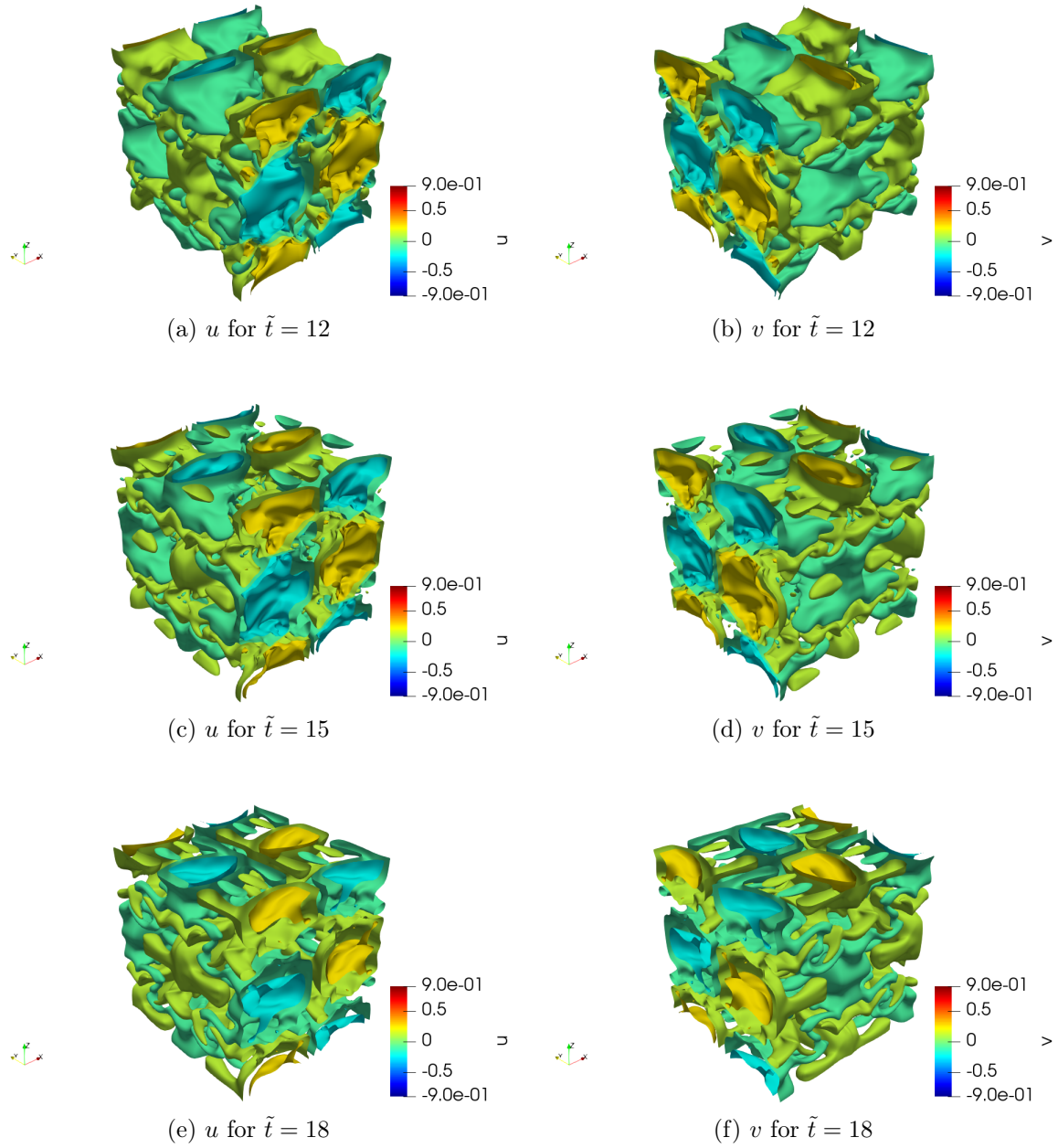


Figure 7.5: *Sim1* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{12, 15, 18\}$

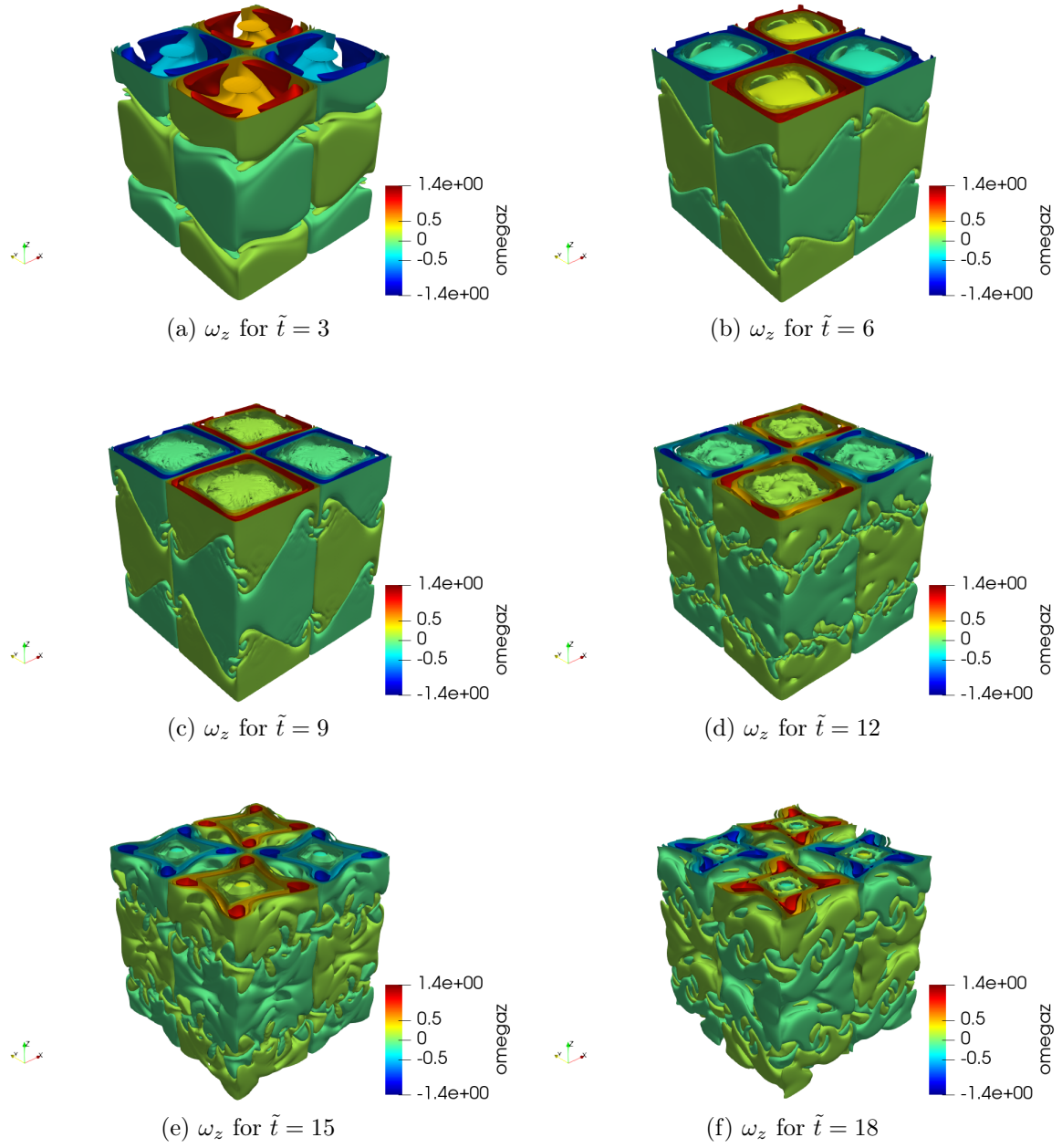


Figure 7.6: *Sim1* - Isosurfaces of  $z$ -component of  $\boldsymbol{\omega}^\circ$ :  $\omega_z = \{\pm 0.1, \pm 0.25, \pm 0.5 \pm 1\}$  for  $\tilde{t} = \{3, 6, 9, 12, 15, 18\}$

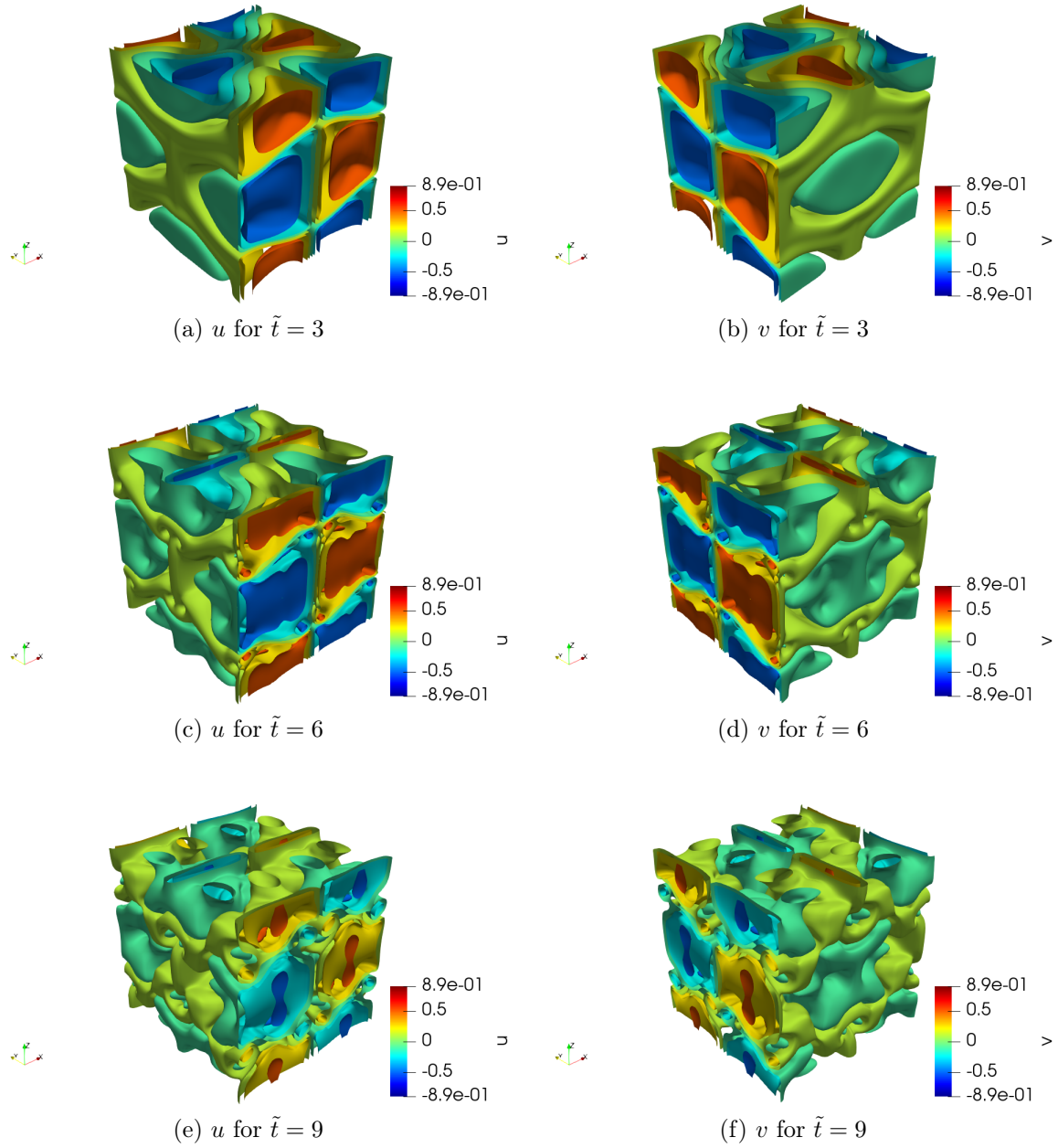


Figure 7.7: *Sim2* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{3, 6, 9\}$

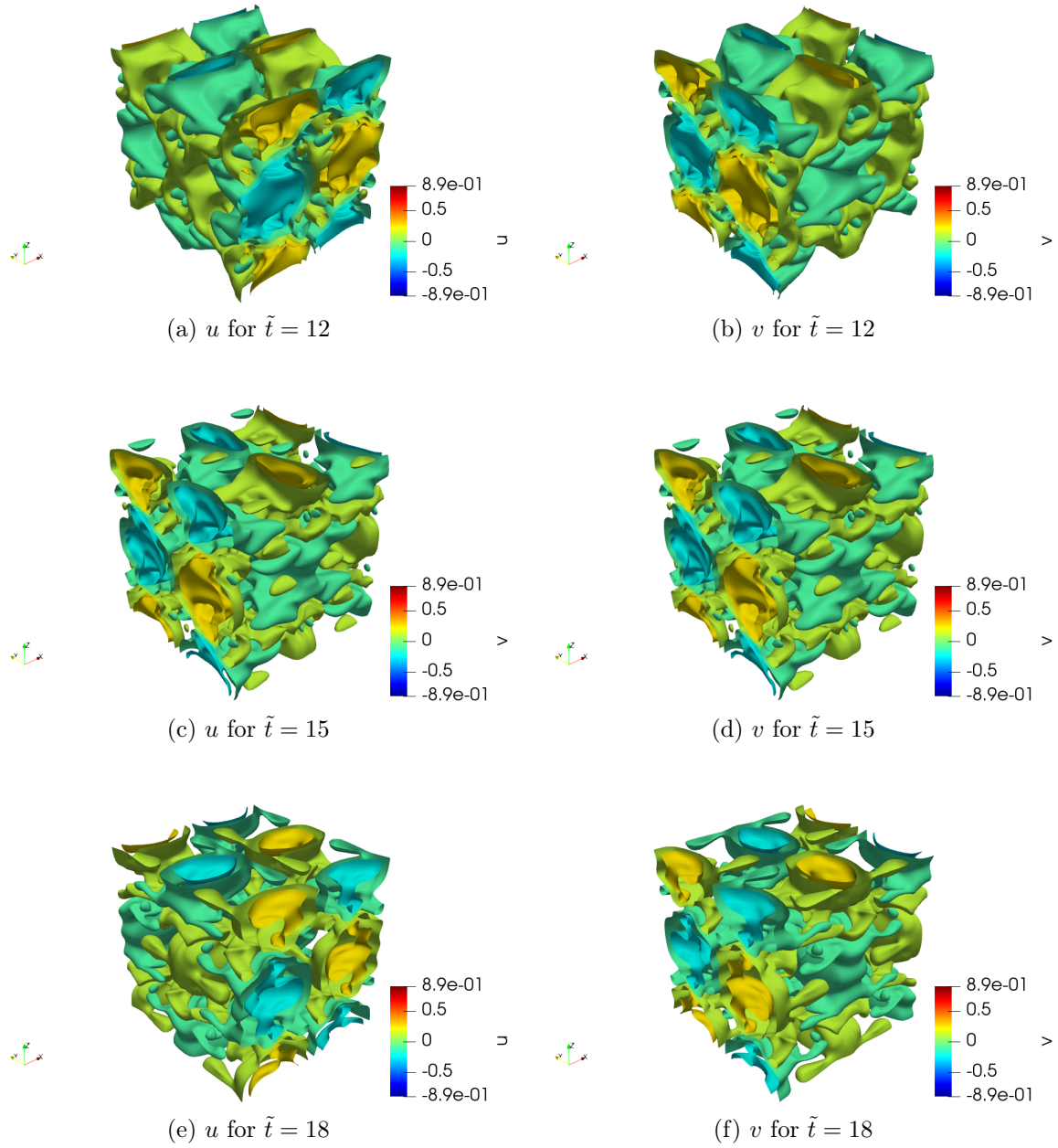


Figure 7.8: *Sim2* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{12, 15, 18\}$



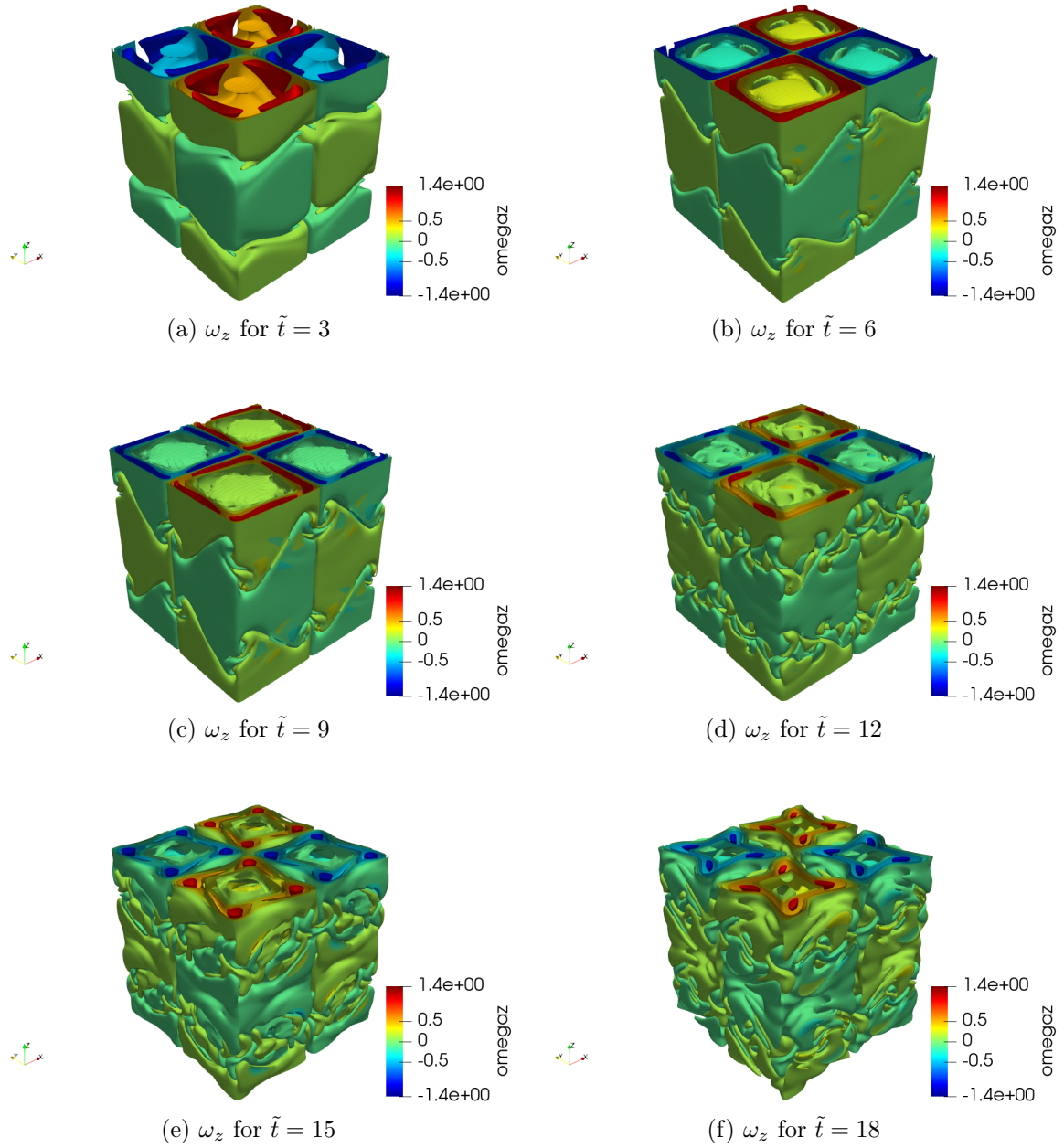


Figure 7.9: *Sim2* - Isosurfaces of  $z$ -component of  $\omega^\circ$ :  $\omega_z = \{\pm 0.1, \pm 0.25, \pm 0.5 \pm 1\}$  for  $\tilde{t} = \{3, 6, 9, 12, 15, 18\}$

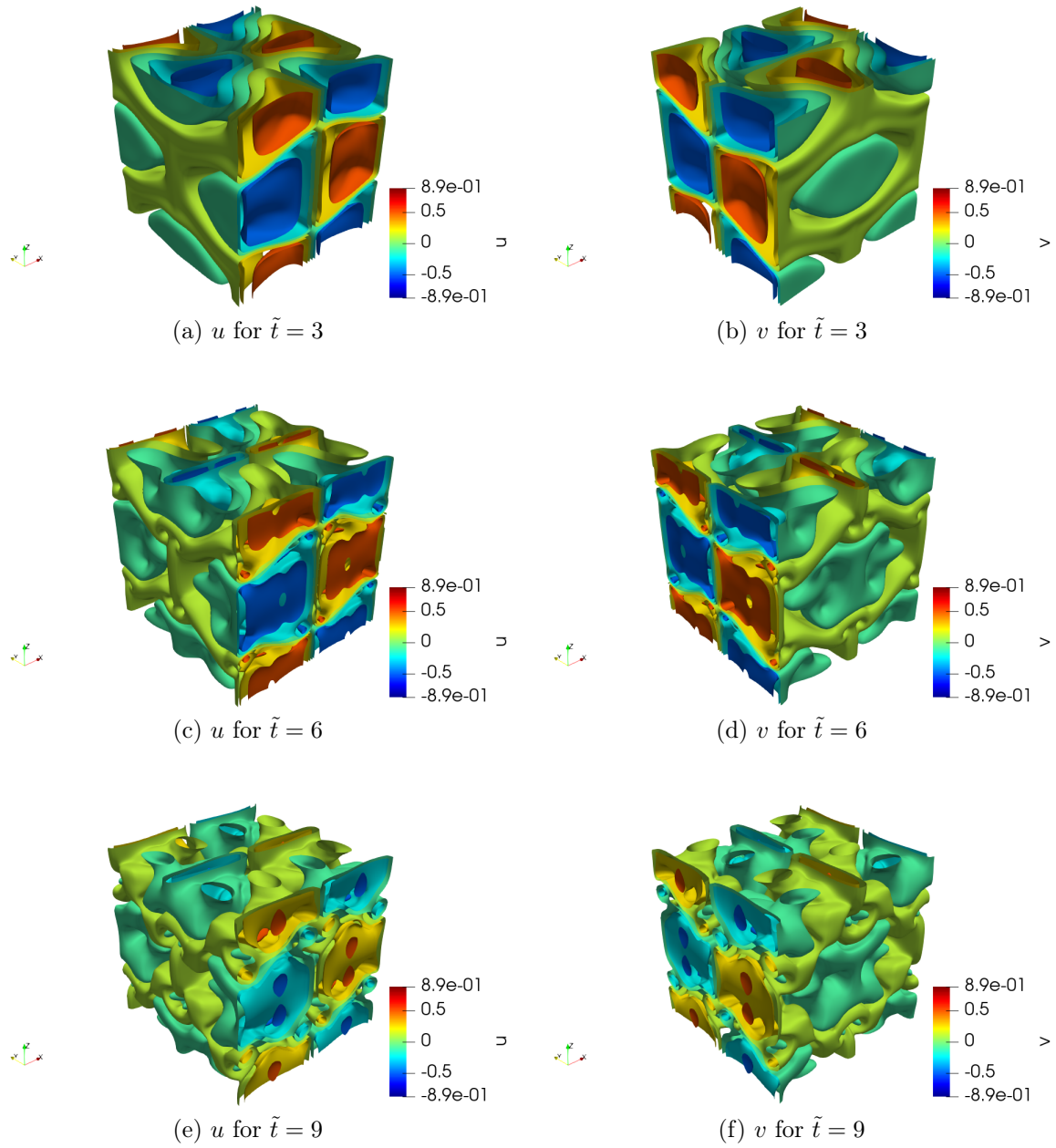


Figure 7.10: *Sim3* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{3, 6, 9\}$



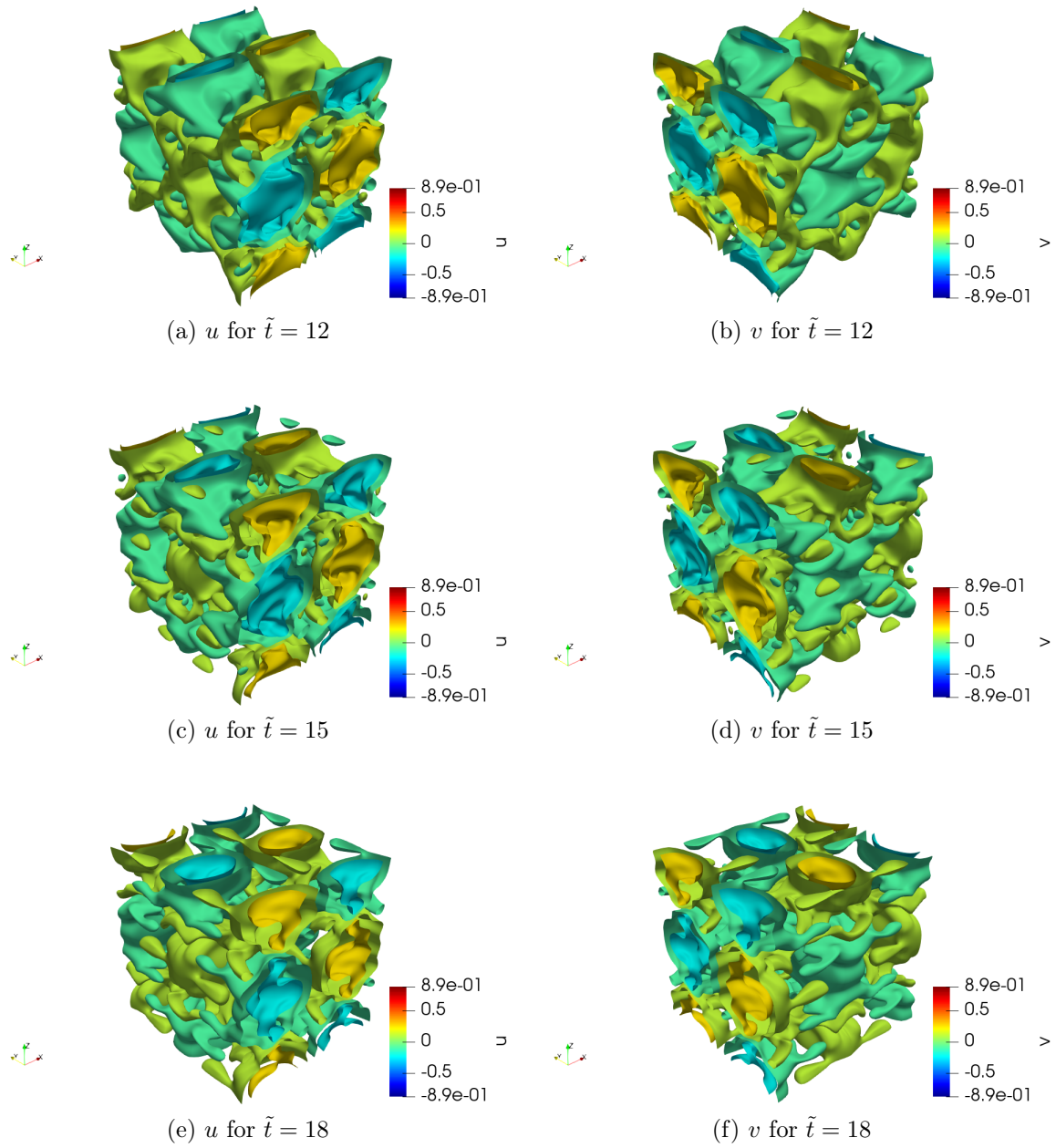


Figure 7.11: *Sim3* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{12, 15, 18\}$

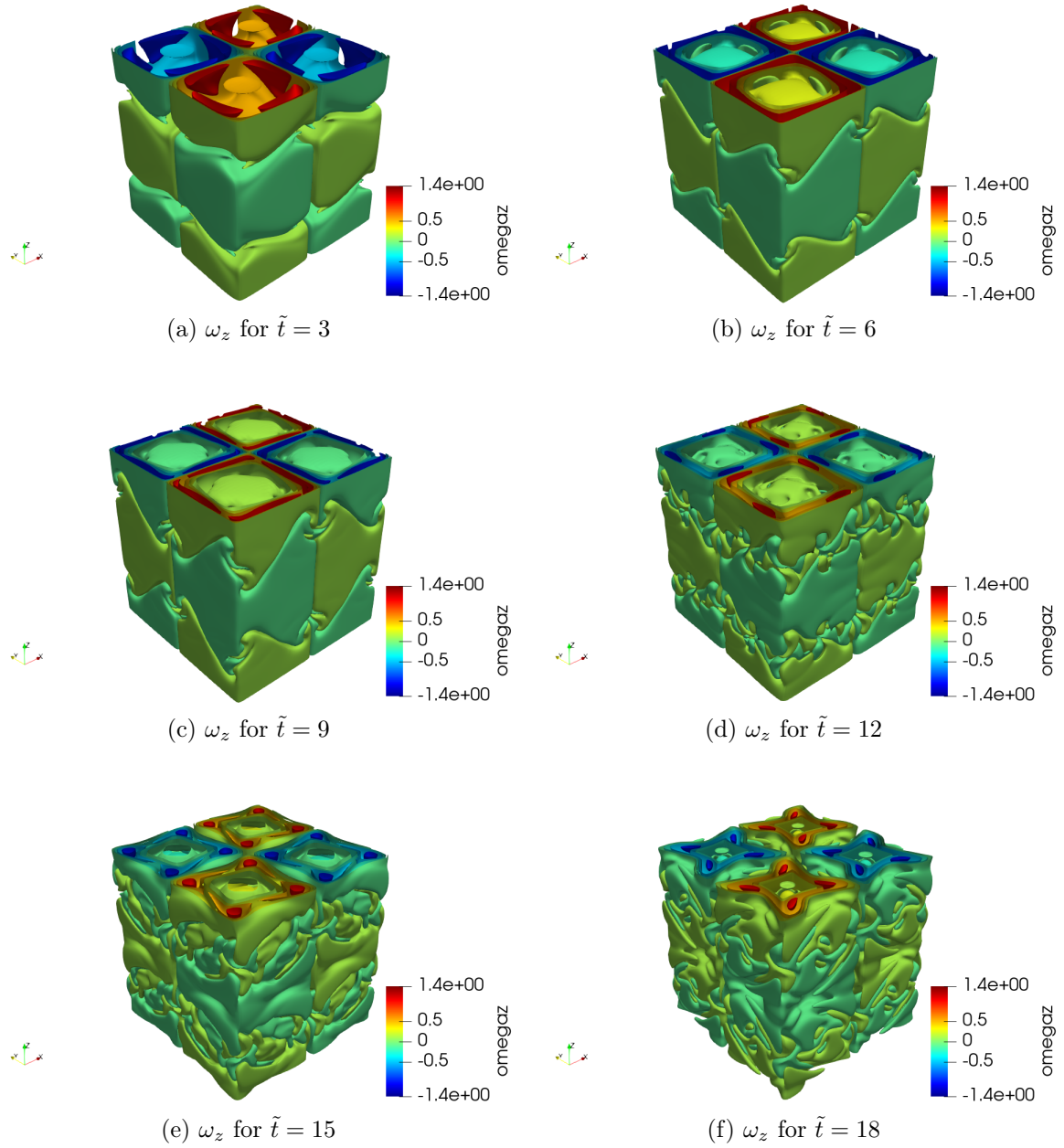


Figure 7.12: *Sim3* - Isosurfaces of  $z$ -component of  $\omega^\circ$ :  $\omega_z = \{\pm 0.1, \pm 0.25, \pm 0.5 \pm 1\}$  for  $\tilde{t} = \{3, 6, 9, 12, 15, 18\}$

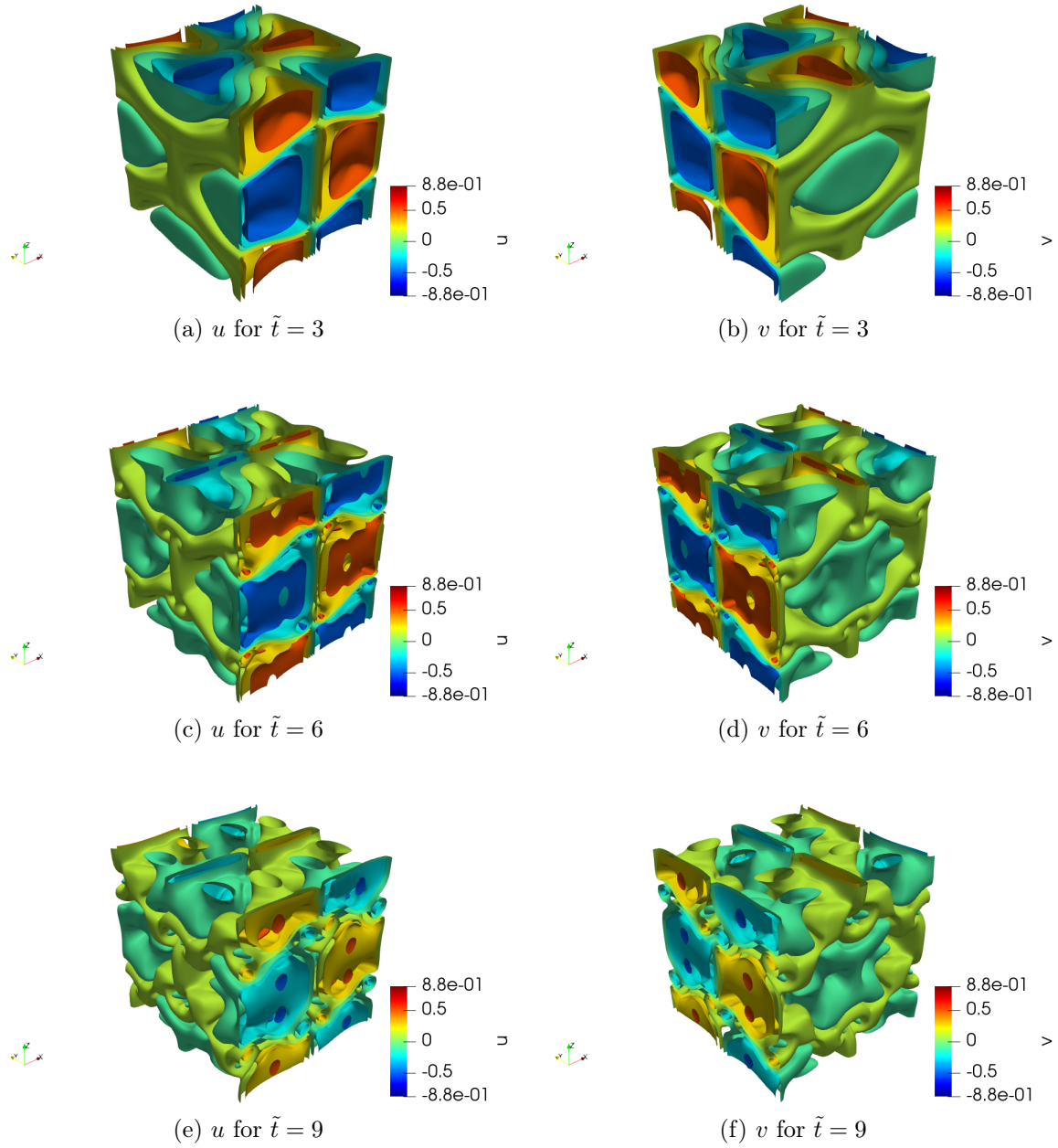


Figure 7.13: *Sim4* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{3, 6, 9\}$

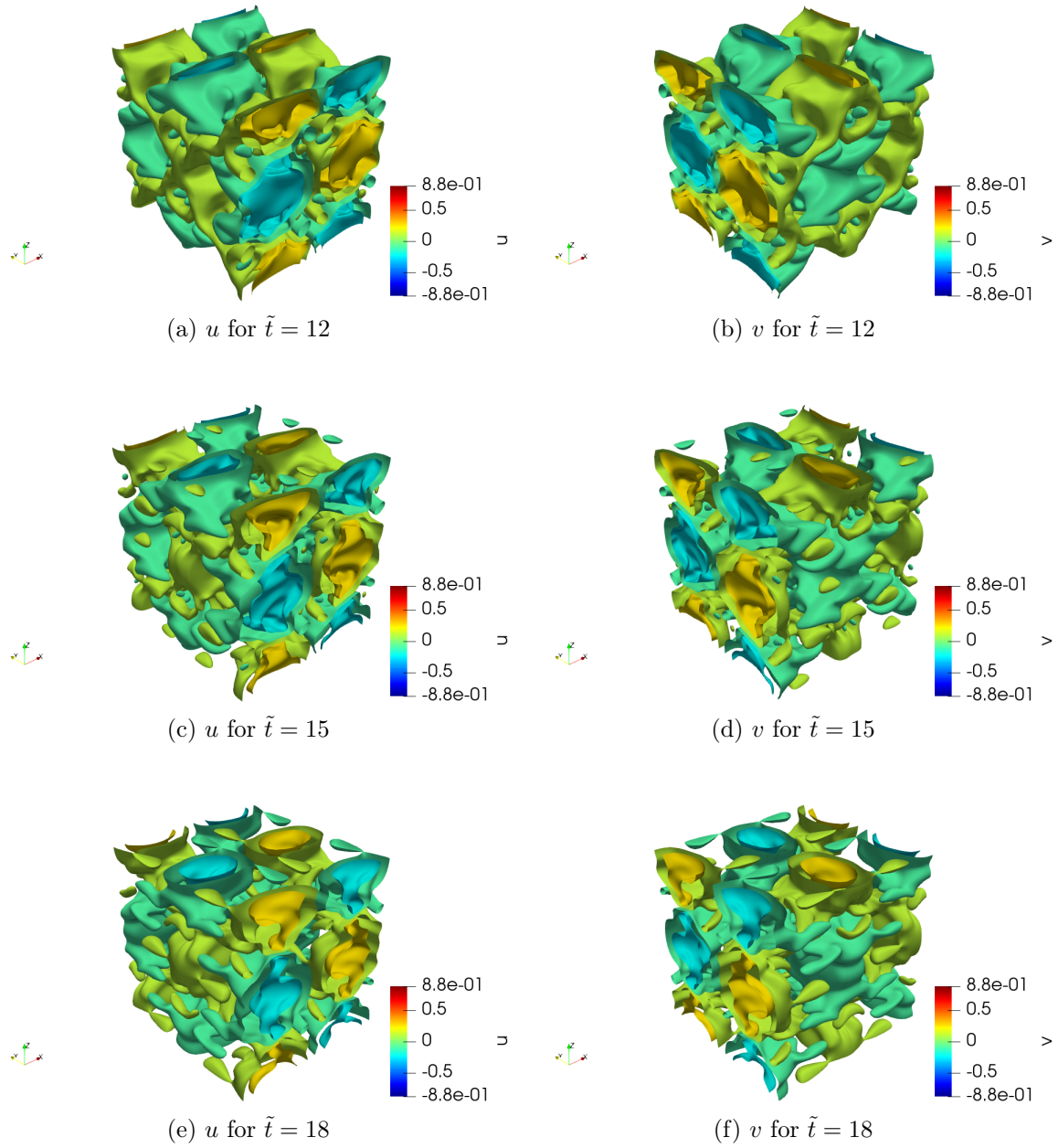


Figure 7.14: *Sim4* - Isosurfaces of  $x$  and  $y$  components of  $\mathbf{u}$ :  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  and  $v = \{\pm 0.1, \pm 0.25, \pm 0.5\}$  for  $\tilde{t} = \{12, 15, 18\}$

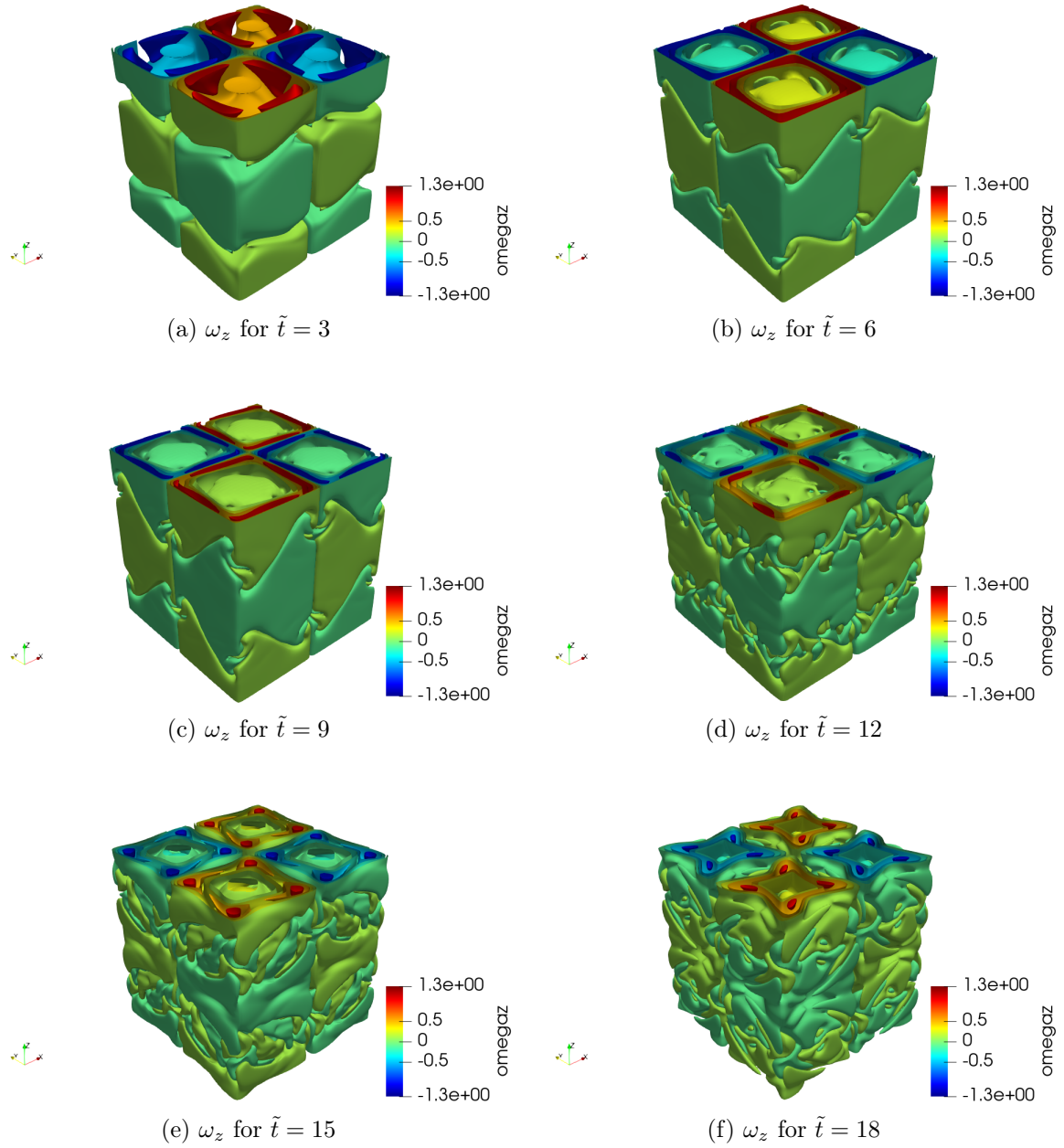


Figure 7.15: *Sim4* - Isosurfaces of  $z$ -component of  $\boldsymbol{\omega}^\circ$ :  $\omega_z = \{\pm 0.1, \pm 0.25, \pm 0.5 \pm 1\}$  for  $\tilde{t} = \{3, 6, 9, 12, 15, 18\}$



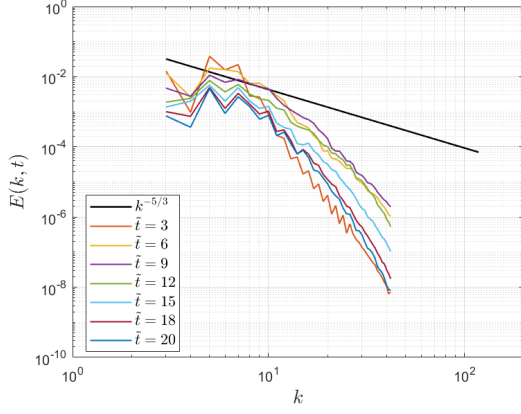
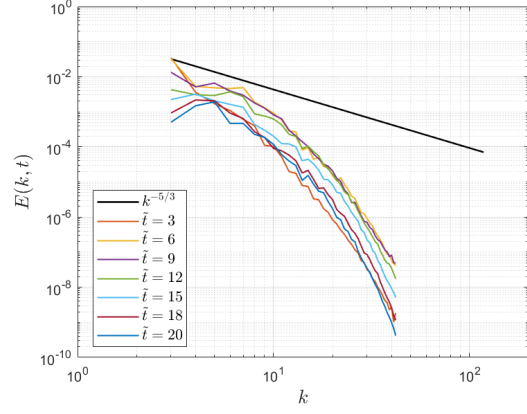
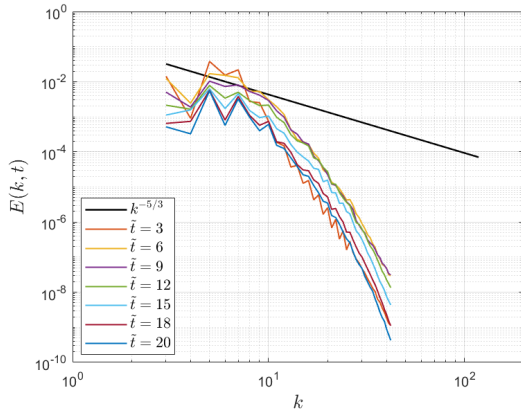
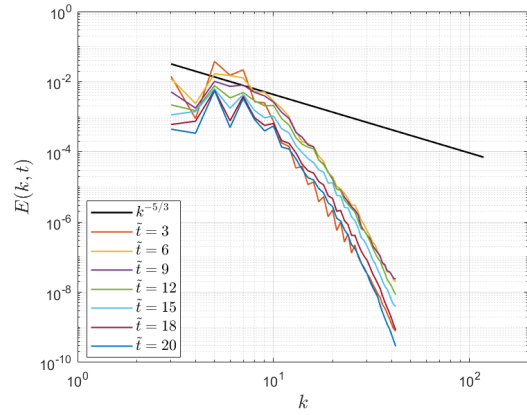
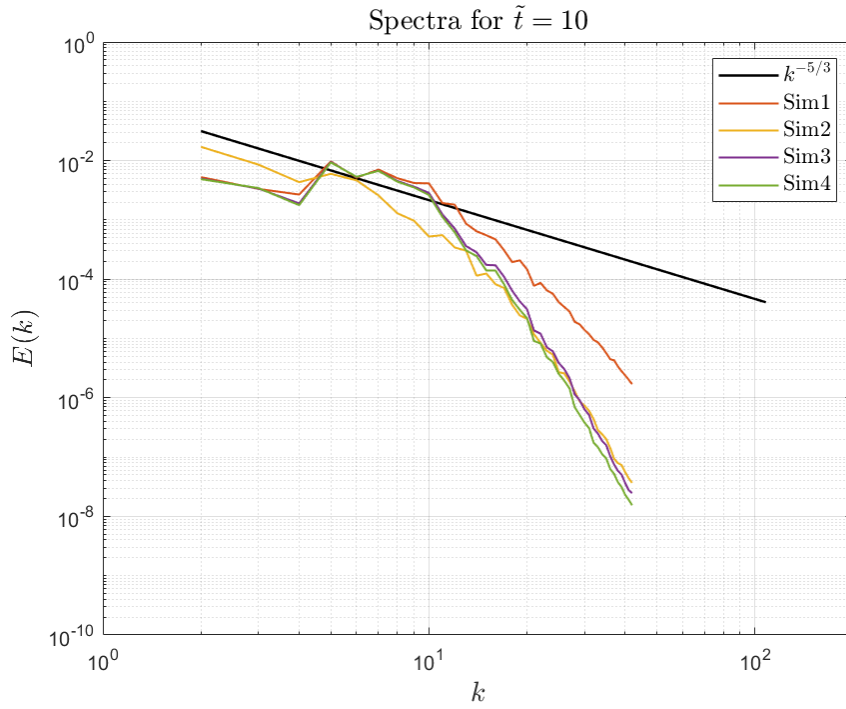

 (a) *Sim1*:  $\text{Re} = 450$ 

 (b) *Sim2*:  $\text{Re} = 450$  and  $\text{La}_2 = 12000$ 

 (c) *Sim3*:  $\text{Re} = 450$  and  $\text{La}_2 = 8000$ 

 (d) *Sim4*:  $\text{Re} = 450$  and  $\text{La}_2 = 6000$ 

 Figure 7.16: Energy Spectra for  $\tilde{t} = \{3, 6, 9, 12, 15, 18, 20\}$ .

As expected, even if structures are similar, the solutions of Ladyzhenskaya equations appear more damped; for  $\tilde{t} = 9$ , for example, velocity isosurfaces corresponding to the values  $u = \pm 0.5$  and  $v = \pm 0.5$  seem smaller as Ladyzhenskaya number decreases, i. e. strengthening the nonlinear viscous term. No external force is applied, then kinetic energy correctly decays (Figure 7.18). Moreover, even if for all the times energy is smaller as Ladyzhenskaya number decreases, because of enhanced diffusivity, the rates at which energy decays in Figure 7.19 have particular trends: energy decays faster for lower  $\text{La}_2$  until  $\tilde{t} \simeq 7$ , whereas for later times this trend is reversed and Navier-Stokes equations show higher dissipation. The dissipation depends on the components of the velocity gradient which decay faster for lower Ladyzhenskaya number because increased diffusivity tries to smooth out inhomogeneities in the velocity field, thus for certain times the velocity gradient is higher for higher Ladyzhenskaya number and the resulting dissipation is greater. For  $\tilde{t} \simeq 20$ , however, all the solutions give approximatively the same value of energy.

Figures 7.20 and 7.21 show the contribution of the Newtonian and the Ladyzhenskaya non-linear viscous terms to the total dissipation. These two contributions are calculated in physical space respectively as

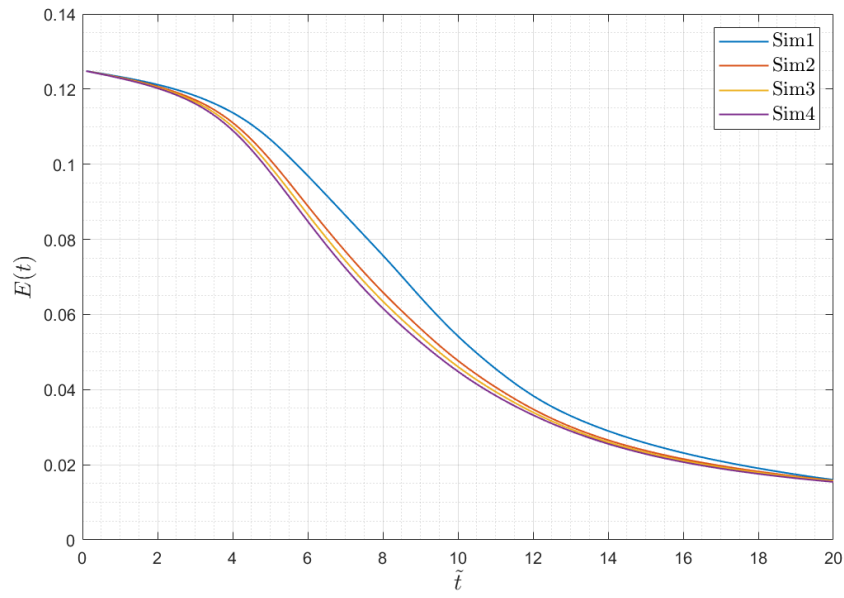
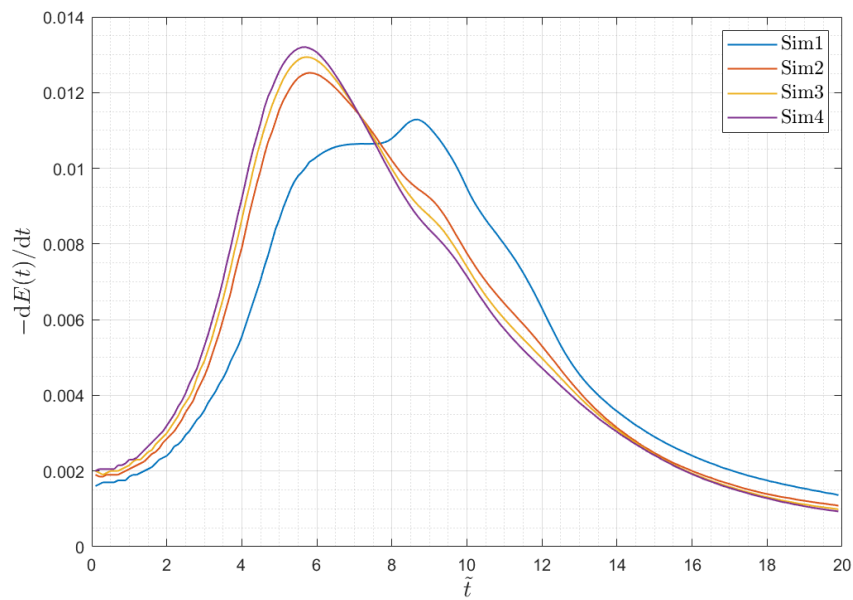
$$\varepsilon = \nu \sum_{i,j=1}^3 \left\langle \left( \frac{\partial u_i}{\partial x_j} \right)^2 \right\rangle \quad (7.2)$$


 Figure 7.17: Spectra comparison for  $\tilde{t} = 10$ .

and

$$\varepsilon^{\text{lad}} = \nu_1 \sum_{i,j=1}^3 \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \right\rangle \quad (7.3)$$

Newtonian dissipation is higher for higher Ladyzhenskaya number because, as previously explained, Ladyzhenskaya's terms affects the velocity gradient reducing it. Ladyzhenskaya viscous dissipation instead is higher for lower Ladyzhenskaya number for all the times. Total dissipation (Figure 7.22) and rate of decay of energy (Figure 7.19) are identical; this can be considered as proof that incompressibility condition and homogeneity are satisfied in all the simulations.

Figure 7.18: Energy Decay  $E(t)$ Figure 7.19: Rate at which energy decays:  $-dE/dt$



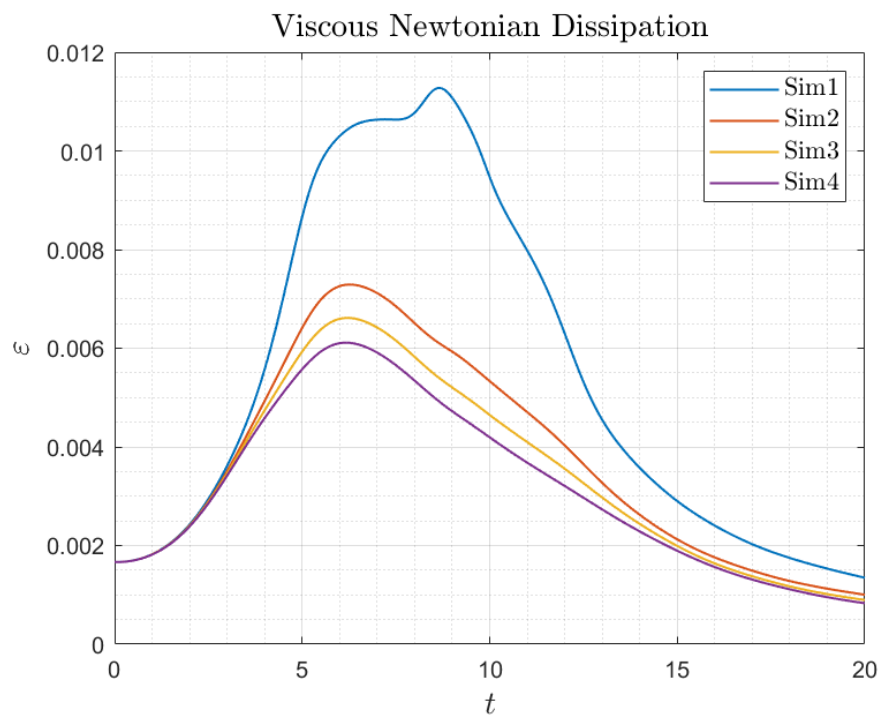


Figure 7.20: Viscous Newtonian Dissipation

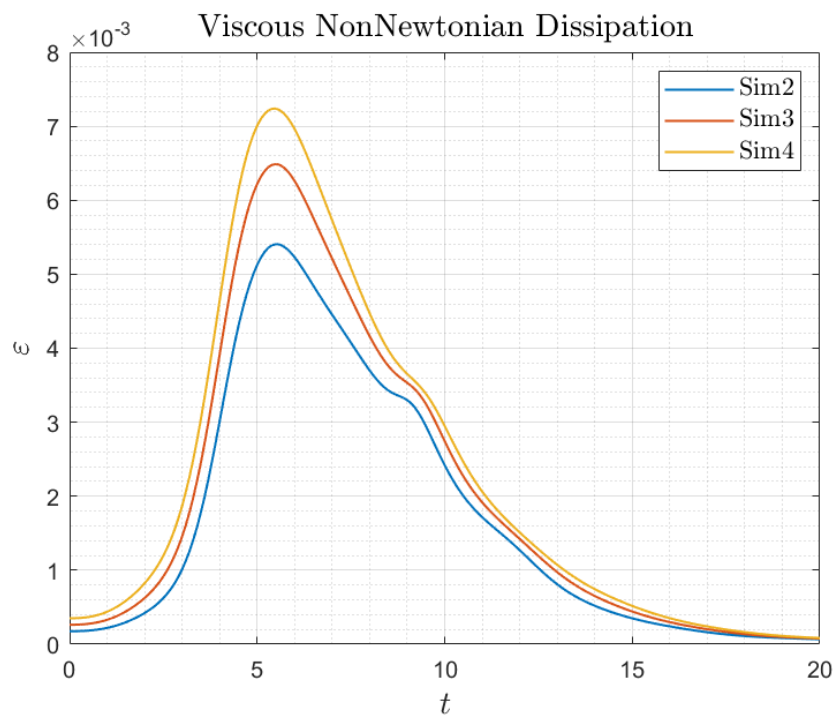


Figure 7.21: Viscous Non-Newtonian Dissipation

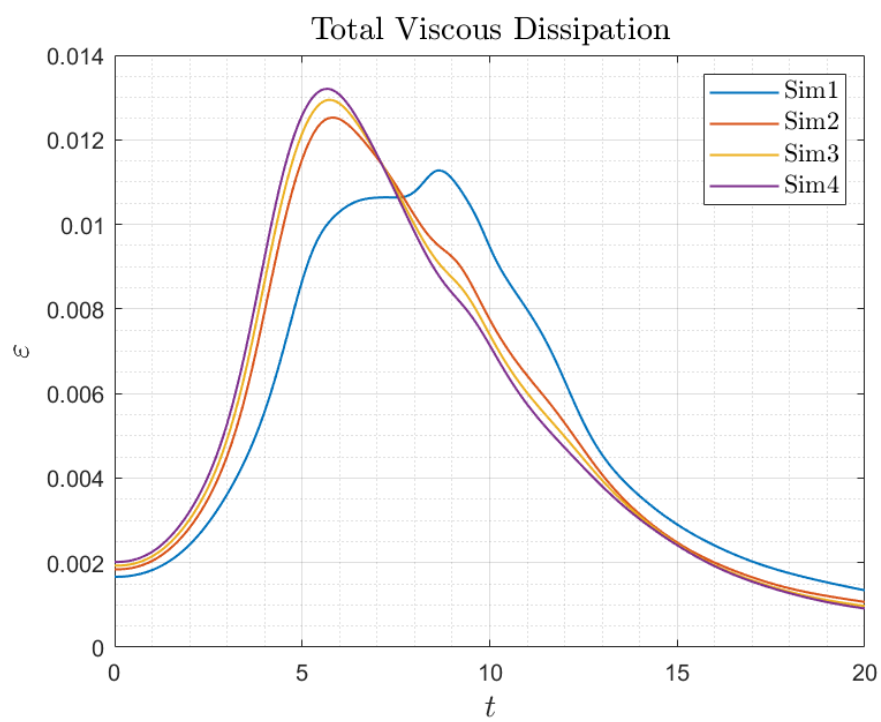


Figure 7.22: Total Dissipation

# Conclusions

Incompressible Navier-Stokes and Ladyzhenskaya equations have been obtained and discussed. For Ladyzhenskaya models weak solutions to the initial value problem are globally unique in time for any Reynolds and  $r \geq 1/5$ ; the analogous result for the Navier-Stokes equations has not been proved and is not believed to be true. This result, along with the less restrictive hypothesis on the velocity gradient, represents a motivation to investigate Ladyzhenskaya models. From a numerical point of view, codes which compute approximate solutions of the Navier-Stokes equations may be easily modified to handle the Ladyzhenskaya equations as well. Thus, the Fourier-Galerkin method coupled with the fourth-order Runge-Kutta time advancement has been implemented in a parallel Fortran program in order to simulate the free-decay of the Taylor-Green Vortex according to Navier-Stokes and Ladyzhenskaya equations assuming Turbulence to be homogeneous and isotropic. The additional non-linearity contained in Ladyzhenskaya equations does not generate any numerical instability for the cases which have been simulated. Solutions have been correctly obtained and commented. Similarly to Navier-Stokes', Ladyzhenskaya equations show turbulent behavior consisting in continuous spectra, vortices' breakup and energy cascade towards smaller scales: an inertial subrange is present in all the solutions. Because of the low Reynolds numbers this subrange is very small and most of the energy spectra are not actually close to Kolmogorov's  $5/3$  law. Moreover, Ladyzhenskaya's solutions are clearly more damped because of the additional diffusive term and kinetic energy is smaller strengthening this additional term. Newtonian and non-Newtonian contributions to the total energy dissipation have been calculated showing the effect of the non-linear viscous term in the early stages of vortex decay. In order to catch characteristic features of fully developed turbulence further studies should be conducted on Ladyzhenskaya equations for higher Reynolds number (for example  $Re \geq 3000$ ).

# Appendix A

## Leray Projection

The Leray Projection is a linear operator  $\mathbb{P}(\cdot)$  that can be seen as the projection onto the divergence-free vector fields. The Leray (or Helmholtz-Leray) operator can be defined recalling the Helmholtz-Leary decomposition.

**Helmholtz-Leary decomposition.** A given vector field  $\mathbf{u}$  can be decomposed as

$$\mathbf{u} = \nabla q + \mathbf{v} \quad (\text{A.1})$$

with  $\nabla \cdot \mathbf{v} = 0$ . This decomposition of  $\mathbf{u}$  is unique, up to an additive constant for  $q$ . Then the Leray operator applied to  $\mathbf{u}$  can be defined as

$$\mathbb{P}(\mathbf{u}) = \mathbf{v} \quad (\text{A.2})$$

Applying the Leray projection operator to the incompressible Navier-Stokes equations

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \rho \mathbf{f} - \nabla p + \mu \nabla^2 \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0$$

and using the properties of the operator leads to

$$\rho \frac{\partial \mathbf{u}}{\partial t} - \mu \mathbb{P}(\nabla^2 \mathbf{u}) + \rho \mathbb{P}[(\mathbf{u} \cdot \nabla) \mathbf{u}] = \mathbb{P}(\mathbf{f}) \quad (\text{A.3})$$

since, because of the divergence-free condition on  $\mathbf{u}$ ,

$$\mathbb{P}(\mathbf{u}) = \mathbf{u}$$

$$\mathbb{P}\left(\frac{\partial \mathbf{u}}{\partial t}\right) = \frac{\partial \mathbf{u}}{\partial t}$$

$$\mathbb{P}(\nabla p) = 0$$

The equation can be rewritten also as follows:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \mu \mathbb{S}(\mathbf{u}) + \rho \mathbb{B}(\mathbf{u}, \mathbf{u}) = \mathbb{P}(\mathbf{f}) \quad (\text{A.4})$$

where

$$\mathbb{S}(\mathbf{u}) = -\mathbb{P}(\nabla^2 \mathbf{u}) \quad (\text{A.5})$$

is the *Stokes operator* and  $\mathbb{B}(\cdot, \cdot)$  is the bilinear operator defined by

$$\mathbb{B}(\mathbf{u}, \mathbf{v}) = \mathbb{P}[(\mathbf{u} \cdot \nabla) \mathbf{v}] \quad (\text{A.6})$$

For boundary problems on unbounded domains in which space-periodic boundary condition are imposed, the Stokes operator simply reduces to the Laplacian:

$$\mathbb{S}(\mathbf{u}) = -\mathbb{P}(\nabla^2 \mathbf{u}) = -\nabla^2 \mathbf{u}$$

Moreover,  $\mathbf{f}$  is often assumed to be divergence-free so that  $\mathbb{P}(\mathbf{f}) = \mathbf{f}$ . Introducing these two assumptions the Navier-Stokes equation reduces to the *heat equation* with some additional nonlinear terms and a forcing term

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \mu \nabla^2 \mathbf{u} - \rho \mathbb{B}(\mathbf{u}, \mathbf{u}) + \mathbf{f} \quad (\text{A.7})$$

## Appendix B

# Reynolds-averaged Ladyzhenskaya equations

The Reynolds-averaged Ladyzhenskaya equations (shortened, *RAL*) can be derived from the Ladyzhenskaya equations by introducing Reynolds' decomposition of the velocity and pressure fields and averaging the resulting equations:

$$\begin{cases} \rho \frac{\partial \langle u_i \rangle}{\partial t} + \rho \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = \frac{\partial \langle p \rangle}{\partial x_i} + \mu_0 \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \rho \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} + \mu_1 \frac{\partial}{\partial x_j} \langle 2\hat{d}^2 D_{ij} \rangle \\ \frac{\partial \langle u_j \rangle}{\partial x_j} = 0 \end{cases} \quad (\text{B.1})$$

The term which makes these equations different from RANS is

$$\mu_1 \frac{\partial}{\partial x_j} \langle 2\hat{d}^2 D_{ij} \rangle = \mu_1 \frac{\partial}{\partial x_j} \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right\rangle$$

which can be decomposed as follows:

$$\begin{aligned} \mu_1 \frac{\partial}{\partial x_j} \langle 2\hat{d}^2 D_{ij} \rangle &= \mu_1 \frac{\partial}{\partial x_j} \left\langle \hat{d}^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) + \hat{d}^2 \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle = \\ &= \mu_1 \frac{\partial}{\partial x_j} \underbrace{\left\langle \hat{d}^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \right\rangle}_{S_{ij}} + \mu_1 \frac{\partial}{\partial x_j} \underbrace{\left\langle \hat{d}^2 \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle}_{T_{ij}} \end{aligned} \quad (\text{B.2})$$

In this equation the term  $S_{ij}$  can be rewritten as follows

$$S_{ij} = \left\langle \hat{d}^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \right\rangle = \langle \hat{d}^2 \rangle \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right)$$

since the average is basically an integration in time and  $(\partial \langle u_i \rangle / \partial x_j + \partial \langle u_j \rangle / \partial x_i)$  does not depend on time. The average of the quantity  $\hat{d}^2$  is

$$\langle \hat{d}^2 \rangle = \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \right\rangle = \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u_k}{\partial x_l} \right)^2 \right\rangle + \left\langle \left( \frac{\partial u_l}{\partial x_k} \right)^2 \right\rangle + 2 \left\langle \frac{\partial u_k}{\partial x_l} \frac{\partial u_l}{\partial x_k} \right\rangle$$

and introducing the Reynolds decomposition it becomes

$$\begin{aligned} \langle \widehat{d^2} \rangle = & \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \right)^2 + \left( \frac{\partial u'_k}{\partial x_l} \right)^2 + 2 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial u'_k}{\partial x_l} \right) \right\rangle + \\ & + \left\langle \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 + \left( \frac{\partial u'_l}{\partial x_k} \right)^2 + 2 \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \frac{\partial u'_l}{\partial x_k} \right) \right\rangle + \\ & + 2 \left\langle \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial \langle u_l \rangle}{\partial x_k} + \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial u'_l}{\partial x_k} + \frac{\partial u'_k}{\partial x_l} \frac{\partial \langle u_l \rangle}{\partial x_k} + \frac{\partial u'_k}{\partial x_l} \frac{\partial u'_l}{\partial x_k} \right\rangle \end{aligned}$$

Since the quantities  $\partial \langle u_i \rangle / \partial x_j$  do not depend on time and the time averages of the fluctuating fields are zero ( $\langle u'_i \rangle = 0$ ),  $\langle \widehat{d^2} \rangle$  reduces to

$$\begin{aligned} \langle \widehat{d^2} \rangle = & \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \right)^2 \right\rangle + \left\langle \left( \frac{\partial u'_k}{\partial x_l} \right)^2 \right\rangle + \left\langle \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 \right\rangle + \left\langle \left( \frac{\partial u'_l}{\partial x_k} \right)^2 \right\rangle + \\ & + 2 \left\langle \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial \langle u_l \rangle}{\partial x_k} \right\rangle + 2 \left\langle \frac{\partial u'_k}{\partial x_l} \frac{\partial u'_l}{\partial x_k} \right\rangle \\ \langle \widehat{d^2} \rangle = & \sum_{k,l=1}^3 \left[ \left( \frac{\partial \langle u_k \rangle}{\partial x_l} + \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 + \left\langle \left( \frac{\partial u'_k}{\partial x_l} + \frac{\partial u'_l}{\partial x_k} \right)^2 \right\rangle \right] \end{aligned} \quad (\text{B.3})$$

In conclusion, the term  $S_{ij}$  can be rewritten as follows

$$S_{ij} = \sum_{k,l=1}^3 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} + \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) + \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_k}{\partial x_l} + \frac{\partial u'_l}{\partial x_k} \right)^2 \right\rangle \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \quad (\text{B.4})$$

The term denoted by  $T_{ij}$  in equation (B.2) is instead

$$T_{ij} = \left\langle \widehat{d^2} \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle = \left\langle \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle$$

Introducing Reynolds' decomposition and denoting  $(\partial u'_i / \partial x_j + \partial u'_j / \partial x_i)$  with  $d'_{ij}$ , it becomes

$$\begin{aligned} T_{ij} = & \left\langle \left[ \sum_{k,l=1}^3 \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right)^2 \right] d'_{ij} \right\rangle = \left\langle \left[ \sum_{k,l=1}^3 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \right)^2 + \left( \frac{\partial u'_k}{\partial x_l} \right)^2 + 2 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial u'_k}{\partial x_l} \right) + \right. \right. \\ & \left. \left. + \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 + \left( \frac{\partial u'_l}{\partial x_k} \right)^2 + 2 \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \frac{\partial u'_l}{\partial x_k} \right) \right] d'_{ij} \right\rangle \end{aligned}$$

Solving for the products and commuting the average and the sum:

$$\begin{aligned} T_{ij} = & \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \right)^2 d'_{ij} \right\rangle + \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_k}{\partial x_l} \right)^2 d'_{ij} \right\rangle + 2 \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial u'_k}{\partial x_l} \right) d'_{ij} \right\rangle + \\ & + \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 d'_{ij} \right\rangle + \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_l}{\partial x_k} \right)^2 d'_{ij} \right\rangle + 2 \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \frac{\partial u'_l}{\partial x_k} \right) d'_{ij} \right\rangle \end{aligned}$$

Noting that  $(\partial \langle u_k \rangle / \partial x_l)^2$  and  $(\partial \langle u_l \rangle / \partial x_k)^2$  do not depend on the time and that

$$\langle d'_{ij} \rangle = \left\langle \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle = \left( \frac{\partial \langle u'_i \rangle}{\partial x_j} + \frac{\partial \langle u'_j \rangle}{\partial x_i} \right) = 0$$

the first and the fourth term in the previous equation drop out leading to

$$\begin{aligned} T_{ij} &= \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_k}{\partial x_l} \right)^2 d'_{ij} \right\rangle + 2 \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_k \rangle}{\partial x_l} \frac{\partial u'_k}{\partial x_l} \right) d'_{ij} \right\rangle + \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_l}{\partial x_k} \right)^2 d'_{ij} \right\rangle + \\ &\quad + 2 \sum_{k,l=1}^3 \left\langle \left( \frac{\partial \langle u_l \rangle}{\partial x_k} \frac{\partial u'_l}{\partial x_k} \right) d'_{ij} \right\rangle \\ T_{ij} &= \sum_{k,l=1}^3 \left\langle \left[ \left( \frac{\partial u'_k}{\partial x_l} \right)^2 + \left( \frac{\partial u'_l}{\partial x_k} \right)^2 \right] d'_{ij} \right\rangle + 2 \sum_{k,l=1}^3 \left[ \frac{\partial \langle u_k \rangle}{\partial x_l} \left\langle \frac{\partial u'_k}{\partial x_l} d'_{ij} \right\rangle + \frac{\partial \langle u_l \rangle}{\partial x_k} \left\langle \frac{\partial u'_l}{\partial x_k} d'_{ij} \right\rangle \right] \end{aligned} \quad (\text{B.5})$$

Using the partially simplified expressions of  $S_{ij}$  (B.4) and  $T_{ij}$  (B.5), the equation (B.1) can then be rewritten as follows:

$$\begin{cases} \rho \frac{\partial \langle u_i \rangle}{\partial t} + \rho \langle u_j \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} = \frac{\partial \langle p \rangle}{\partial x_i} + \mu_0 \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \rho \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} + \\ + \mu_1 \frac{\partial}{\partial x_j} \left[ \sum_{k,l=1}^3 \left( \frac{\partial \langle u_k \rangle}{\partial x_l} + \frac{\partial \langle u_l \rangle}{\partial x_k} \right)^2 \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) \right] + \mu_1 \frac{\partial Z_{ij}}{\partial x_j} \\ \frac{\partial \langle u_j \rangle}{\partial x_j} = 0 \end{cases} \quad (\text{B.6})$$

where

$$\begin{aligned} Z_{ij} &= \sum_{k,l=1}^3 \left\langle \left( \frac{\partial u'_k}{\partial x_l} + \frac{\partial u'_l}{\partial x_k} \right)^2 \right\rangle \left( \frac{\partial \langle u_i \rangle}{\partial x_j} + \frac{\partial \langle u_j \rangle}{\partial x_i} \right) + \sum_{k,l=1}^3 \left\langle \left[ \left( \frac{\partial u'_k}{\partial x_l} \right)^2 + \left( \frac{\partial u'_l}{\partial x_k} \right)^2 \right] d'_{ij} \right\rangle + \\ &\quad + 2 \sum_{k,l=1}^3 \left[ \frac{\partial \langle u_k \rangle}{\partial x_l} \left\langle \frac{\partial u'_k}{\partial x_l} d'_{ij} \right\rangle + \frac{\partial \langle u_l \rangle}{\partial x_k} \left\langle \frac{\partial u'_l}{\partial x_k} d'_{ij} \right\rangle \right] \end{aligned} \quad (\text{B.7})$$

and

$$d'_{ij} = \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}$$

Further simplifications are difficult to obtain; it is clear that the Reynolds-averaged Ladyzhenskaya equations are formally different from the RANS for which one can isolate a term, namely  $R_{ij} = -\rho \langle u'_i u'_j \rangle$ , depending on the fluctuating field only, and maintain the original structure for the mean field. In fact, even if in the RAL (B.6) the original structure of the Ladyzhenskaya equations could be recognized for the mean flow, the remaining term  $\partial Z_{ij} / \partial x_j$  depends on both the mean field and the fluctuating field.



# Appendix C

## Spectral approximation of smooth nonperiodic functions

Spectral approximation of an infinitely smooth nonperiodic function can be regarded as a finite expansion of eigenfunctions of a suitable Sturm-Liouville problem, i. e. a boundary eigenvalue problem for the Sturm-Liouville equation

$$-\frac{d}{dx} \left[ p(x) \frac{dy}{dx} \right] + q(x)y = \lambda r(x)y \quad x \in (a, b), \lambda \in \mathbb{C} \quad (\text{C.1})$$

The Sturm-Liouville equation is a real second-order linear ordinary differential equation for which the coefficients  $p(x)$ ,  $q(x)$  and  $r(x)$  are three given, real-valued functions such that:

- $p(x)$  is continuously differentiable, strictly positive in  $(a, b)$  and continuous at  $x = a$  and  $x = b$ ;
- $q(x)$  is continuous, non-negative and bounded in  $(a, b)$ ;
- $r(x)$  called the *weight* or *density* function is continuous, non-negative and integrable over  $(a, b)$ .

The problem includes also boundary conditions for  $y$  in  $x = a$  and  $x = b$ . Finding the  $\lambda$  for which there exists a non-trivial solution is part of the given Sturm-Liouville problem (eigenvalue problem). The corresponding non-trivial solutions are the eigenfunctions associated to each  $\lambda$ . If the function  $p(x)$  vanishes at the boundaries, the problem is said to be *singular* and the resulting eigenfunctions form an expansion basis which guarantees spectral accuracy.

If one assumes

$$\begin{aligned} p(x) &= (1-x)^{\alpha+1} (1+x)^{\beta+1} \\ q(x) &= 0 \\ r(x) &= (1-x)^{\alpha+1} (1+x)^{\beta+1} \end{aligned}$$

the Sturm-Liouville problem defined on  $[-1, 1]$  has eigenfunctions which are the Jacobi polynomials: polynomials that are orthogonal with respect to the weight  $(1-x)^{\alpha+1} (1+x)^{\beta+1}$  on the interval  $[-1, 1]$ . Legendre polynomials and Chebyshev polynomials of the second kind are special cases of the Jacobi polynomials. For  $\alpha = \beta = 0$  one obtains Legendre polynomials  $\{L_k(x), k = 0, 1, \dots, \}$ , whereas choosing  $\alpha = \beta = -1/2$  one obtains

Chebyshev polynomials of second kind  $\{T_k(x), k = 0, 1, \dots, \}$  which can be defined by the recurrence relation

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= 2x \\ T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \end{aligned} \tag{C.2}$$

# Appendix D

## Code Subroutines

```
1 subroutine space_op_lad(a,u,kk1,kk2,kk3loc,kk_quad,Re,La,deal)
2 ! Ladyzhenskaya equations (r=2) space operator: F(u)
3 ! du/dt=F(u)
4 ! F(u)=div(-uu+tau_lad/La)+(1/Re)*Laplacian(u)
5
6 include 'mpif.h'
7 common nid,noprocs,n1,nloc,n3,n3loc
8 double complex:: a(0:n1-1,0:n1-1,0:n3loc-1,1:3)
9 double complex:: u(0:n1-1,0:n1-1,0:n3loc-1,1:3)
10 double precision:: kk1(0:n1-1,0:n1-1,0:n3loc-1),kk2(0:n1-1,0:n1...
    -1,0:n3loc-1)
11 double precision:: kk3loc(0:n1-1,0:n1-1,0:n3loc-1),kk_quad(0:n1...
    -1,0:n1-1,0:n3loc-1)
12 double precision:: Re,invRe,La,invLa
13 double precision:: deal(0:n1-1,0:n1-1,0:n3loc-1)
14 double complex:: imu
15 double complex,allocatable,dimension(:,:,:)::prods,divprods,...
    ladyz
16 double complex,allocatable,dimension(:,:,:)::pterm
17
18 invRe=1.0d0/Re
19 invLa=1.0d0/La
20 imu=DCMPLX(0.0d0,1.0d0)
21
22 ! convective stress ui*uj
23 allocate(prods(0:n1-1,0:n1-1,0:n3loc-1,1:6))
24
25 ! Ladyzhenskaya viscous stress d^2*D_{ij}=sum(D_{kl}^2)*D_{ij}
26 ! with D_{ij} rate-of-strain tensor
27 allocate(ladyz(0:n1-1,0:n1-1,0:n3loc-1,1:6))
28
29 ! divergence of -ui*uj+(1/La)*d^2*D_{ij}
30 allocate(divprods(0:n1-1,0:n1-1,0:n3loc-1,1:3))
31
32
33 call ConvectiveStress(prods,u)
34 !prods(:,:,: ,1) is uu
35 !prods(:,:,: ,2) is vv
36 !prods(:,:,: ,3) is ww
37 !prods(:,:,: ,4) is uv
38 !prods(:,:,: ,5) is uw
```

```

39      !prods(:,:,:,6) is vw
40      call LadyzhenskayaStress(ladyz,u,kk1,kk2,kk3loc)
41      !ladyz(:,:,:,1) is d^2*D_{11}
42      !ladyz(:,:,:,2) is d^2*D_{22}
43      !ladyz(:,:,:,3) is d^2*D_{33}
44      !ladyz(:,:,:,4) is d^2*D_{12}
45      !ladyz(:,:,:,5) is d^2*D_{13}
46      !ladyz(:,:,:,6) is d^2*D_{23}
47
48      prods=-prods+invLa*ladyz ! -u_i*u_j+(1/La)*d^2*D_{ij}
49
50      !dealiasing
51      do jcomp=1,6
52      do ll=0,n3loc-1
53      do jj=0,n1-1
54      do ii=0,n1-1
55          prods(ii,jj,ll,jcomp)=prods(ii,jj,ll,jcomp)*deal(ii,jj,ll)
56      end do
57      end do
58      end do
59      end do
60
61      call divergence(divprods,prods,kk1,kk2,kk3loc)
62
63      a(:,:,:,1)=divprods(:,:,:,1)-invRe*kk_quad(:,:,:) *u(:,:,:,1)
64      a(:,:,:,2)=divprods(:,:,:,2)-invRe*kk_quad(:,:,:) *u(:,:,:,2)
65      a(:,:,:,3)=divprods(:,:,:,3)-invRe*kk_quad(:,:,:) *u(:,:,:,3)
66
67
68      deallocate(prods,ladyz,divprods)
69
70      return
71 end subroutine

```

```

1  subroutine ConvectiveStress(prods,u)
2      include 'mpif.h'
3      common nid,noprocs,n1,nloc,n3,n3loc
4      double complex:: prods(0:n1-1,0:n1-1,0:n3loc-1,1:6)
5      double complex:: u(0:n1-1,0:n1-1,0:n3loc-1,1:3)
6      double precision, allocatable:: u_real(:,:,:)
7      double precision, allocatable:: prod_real(:,:,:)
8
9      allocate(u_real(0:n1-1,0:n3-1,0:nloc-1,1:3))
10     allocate(prod_real(0:n1-1,0:n3-1,0:nloc-1))
11
12     !prods(:,:,:,1) is uu
13     !prods(:,:,:,2) is vv
14     !prods(:,:,:,3) is ww
15     !prods(:,:,:,4) is uv
16     !prods(:,:,:,5) is uw
17     !prods(:,:,:,6) is vw
18
19
20     !Using transform subroutine
21     !transforminv_tr(uT,uhat) --> transposition forward (complex-...
        straight to real-transposed)
22     !transform_tr(uhat,uT) --> transposition backward (real-...

```

```

    transposed to complex-straight)
23
24 call transforminv_tr(u_real(:,:,:1),u(:,:,:1))
25 call transforminv_tr(u_real(:,:,:2),u(:,:,:2))
26 call transforminv_tr(u_real(:,:,:3),u(:,:,:3))
27
28 prod_real(:,:,:)=u_real(:,:,:1)*u_real(:,:,:1) !uu
29 call transform_tr(prods(:,:,:1),prod_real(:,:,:))
30
31 prod_real(:,:,:)=u_real(:,:,:2)*u_real(:,:,:2) !vv
32 call transform_tr(prods(:,:,:2),prod_real(:,:,:))
33
34 prod_real(:,:,:)=u_real(:,:,:3)*u_real(:,:,:3) !ww
35 call transform_tr(prods(:,:,:3),prod_real(:,:,:))
36
37 prod_real(:,:,:)=u_real(:,:,:1)*u_real(:,:,:2) !uv
38 call transform_tr(prods(:,:,:4),prod_real(:,:,:))
39
40 prod_real(:,:,:)=u_real(:,:,:1)*u_real(:,:,:3) !uw
41 call transform_tr(prods(:,:,:5),prod_real(:,:,:))
42
43 prod_real(:,:,:)=u_real(:,:,:2)*u_real(:,:,:3) !vw
44 call transform_tr(prods(:,:,:6),prod_real(:,:,:))
45
46
47
48 deallocate(u_real)
49 deallocate(prod_real)
50
51 return
52 end subroutine

```

```

1 subroutine LadyzhenskayaStress(ladyz,u,kk1,kk2,kk3loc)
2 ! This subroutine calculates Ladyzhenskaya's non-linear
3 ! symmetric viscous stress tensor:
4 ! tau_lad_ik=sum_{j,l=1}^3(duj/dxl+dul/dxj)^2 (dui/dxk+duk/dxi)=
5 ! =2*II_{2D}*D
6 ! where D is the rate of strain tensor and II_{2D} its
7 ! second invariant
8
9 include 'mpif.h'
10 common nid,noprocs,n1,nloc,n3,n3loc
11 double complex:: ladyz(0:n1-1,0:n1-1,0:n3loc-1,1:6)
12 double complex:: u(0:n1-1,0:n1-1,0:n3loc-1,1:3)
13 double precision:: kk1(0:n1-1,0:n1-1,0:n3loc-1),kk2(0:n1-1,0:n1-1,...
    -1,0:n3loc-1),kk3loc(0:n1-1,0:n1-1,0:n3loc-1)
14 double complex,allocatable,dimension(:,:,:):RoS
15 double complex:: imu
16 double precision,allocatable:: d_hat_quad(:,:,:),lad_real(:,:,:,:)
17 double precision,allocatable:: Ros_real(:,:,:,:)
18 imu=dcmplx(0.0d0,1.0d0)
19
20 allocate(RoS(0:n1-1,0:n1-1,0:n3loc-1,1:6)) !Rate-of-Strain in ...
    Fourier Space
21 allocate(RoS_real(0:n1-1,0:n3-1,0:nloc-1,1:6)) !Rate-of Strain in...
    physical Space
22 allocate(d_hat_quad(0:n1-1,0:n3-1,0:nloc-1))

```

```

23  allocate(lad_real(0:n1-1,0:n3-1,0:nloc-1))
24
25  Ros(:,:,:,1)=imu*kk1(:,:,:) *u(:,:,:,1)  !du/dx
26  Ros(:,:,:,2)=imu*kk2(:,:,:) *u(:,:,:,2)  !dv/dy
27  Ros(:,:,:,3)=imu*kk3loc(:,:,:) *u(:,:,:,3)  !dw/dz
28  Ros(:,:,:,4)=imu*kk2(:,:,:) *u(:,:,:,1)+imu*kk1(:,:,:) *u(:,:,:,2)...
      !du/dy+dv/dx
29  Ros(:,:,:,5)=imu*kk3loc(:,:,:) *u(:,:,:,1)+imu*kk1(:,:,:) *u...
      (:,:,:,3)  !du/dz+dw/dx
30  Ros(:,:,:,6)=imu*kk3loc(:,:,:) *u(:,:,:,2)+imu*kk2(:,:,:) *u...
      (:,:,:,3)  !dv/dz+dw/dy
31
32
33  call MPI_Barrier(MPI_COMM_WORLD,ierror)
34
35
36  do jcomp=1,6
37      call transforminv_tr(RoS_real(:,:,:,jcomp),Ros(:,:,:,jcomp))
38  end do
39
40  d_hat_quad(:,:,:) = 4.0e0*(RoS_real(:,:,:,1)*RoS_real(:,:,:,1)+...
      RoS_real(:,:,:,2)*RoS_real(:,:,:,2)&
41  &+RoS_real(:,:,:,3)*RoS_real(:,:,:,3))+2.0e0*(RoS_real(:,:,:,4)*...
      RoS_real(:,:,:,4)&
42  &+RoS_real(:,:,:,5)*RoS_real(:,:,:,5)+RoS_real(:,:,:,6)*RoS_real...
      (:,:,:,6))
43
44
45  lad_real(:,:,:) = 2.0e0*d_hat_quad(:,:,:) *RoS_real(:,:,:,1)
46  CALL transform_tr(ladyz(:,:,:,1),lad_real)
47
48  lad_real(:,:,:) = 2.0e0*d_hat_quad(:,:,:) *RoS_real(:,:,:,2)
49  CALL transform_tr(ladyz(:,:,:,2),lad_real)
50
51  lad_real(:,:,:) = 2.0e0*d_hat_quad(:,:,:) *RoS_real(:,:,:,3)
52  CALL transform_tr(ladyz(:,:,:,3),lad_real)
53
54  lad_real(:,:,:) = d_hat_quad(:,:,:) *RoS_real(:,:,:,4)
55  CALL transform_tr(ladyz(:,:,:,4),lad_real)
56
57  lad_real(:,:,:) = d_hat_quad(:,:,:) *RoS_real(:,:,:,5)
58  CALL transform_tr(ladyz(:,:,:,5),lad_real)
59
60  lad_real(:,:,:) = d_hat_quad(:,:,:) *RoS_real(:,:,:,6)
61  CALL transform_tr(ladyz(:,:,:,6),lad_real)
62
63  deallocate(RoS,RoS_real,d_hat_quad,lad_real)
64
65  return
66 end subroutine

```

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