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MASTER'S THESIS IN

INDUSTRIAL MATHEMATICS

Large Eddy simulation of homogeneous isotropic turbulence

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Contents

1 Abstract

This master thesis will concentrate on the subject of Large Eddy Simulation of homogeneous, isotropic turbulence in a three dimensional domain with periodic boundary conditions, using an initial energy spectrum equivalent to the Comte-Bellot and Corrsin turbulence spectrum from 1971 [4]. The purpose of the simulation is to investigate the behaviour of the solution with focus on energy decay. A reference solution will be compared to the simulation data, but we shall find that the data sets are quite un-similar. The mechanisms potentially causing this discrepancy will be discussed. The many approaches to turbulence simulation will be discussed in the theory section, and recommendations for further investigations of the FFI spectral element software will be suggested.

2 Acknowledgements

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3 Introduction

The simulation of fluid mechanical problems is far from trivial. The governing laws of fluid motion, the Navier-Stokes equations (see section 5.1), are non-linear, and no general solutions valid for all boundary problems and initial conditions have been found to date. The theme for this thesis will be numerical solutions of the Navier-Stokes equations using a Spectral Element method and Large Eddy simulation with a Variational Multiscale turbulence model. The effects of the model will be evaluated and compared with a reference solution obtained using a high-resolution Fourier spectral method with de-aliasing. What do I mean by "a solution" in this context? In the data analysis, I look only at scalar valued quantities. Mostly the kinetic energy, which is an integrated squared norm of the velocity vector field on the whole domain. The ability of the program to make those scalar quantities behave in a matter that is similar and numerically close to the reference solution, will be the test of the quality of the tested solution procedure.

3.1 Testing the modeled behaviour of turbulent energy

Our task when working with fluid mechanics may be to determine the motion of the fluid at each point in a limited space for a limited time. If the velocity and / or pressure fields are turbulent, the fluid motion is no longer completely deterministic. Therefore, we change our job description to determining averaged and integrated quantities like the total turbulent kinetic energy, the total enstrophy (se equation 119 for a definition of the enstrophy), the averaged velocity or quantities more related to the turbulent eddies, like length scale, velocity scale and specific Reynolds number. By using averaging procedures and high / low-pass filters, we might actually succeed, and obtain solutions satisfying some demands on error and accuracy. In order for the calculations to have commercial use, we need to have strong evidence that what we are doing makes sense, hence the need for field-tested and "flight-proven" [17] theories. The Kolmogorov theory of turbulence from 1941 [15], often called the K-41 theory, contains the majority of the tools needed to investigate turbulence. For instance, the Kolmogorov -5/3 spectral energy density decay rule for the cascade of turbulent energy is widely used as a benchmark test for turbulence simulation. The ideas of an energy cascade from large to smaller eddies originated by Richardson (1922) [20] and later Kolmogorov 1941. In the resulting theory there is a statement that the amount of turbulent kinetic energy at any time corresponding to the normed frequency vector k, should be proportional to the wave number k raised to the power of -5/3 times the current energy dissipation raised to the power of 2/3. Stated formally, we have the following proportionality relation:

$$E(k,t) \propto \epsilon^{2/3} k^{-5/3} \tag{1}$$

By using an algorithm for solving the Navier-Stokes equations that incorporates a spectral element method and a variational multiscale method for the Large-Eddy simulation, we wish to investigate the energy decay and compare to a reference solution. The importance of showing that the solution behaves satisfactory, even for somewhat coarse grids, is the fact that the tested turbulence model is verified as appropriate for similar cases, and may be utilized in future works. Being able to use a turbulence model that produces good results is crucial for the solving of complex problems on limited computer resources and time.

3.2 The market for CFD

When dealing with non-linear equations like the Navier-Stokes equations in general geometries, we need to prove that our solution has converged, and that the error is controlled by some numerical error bounds, since the general, analytic solution does not exist. On the other hand, since the problems to solve are highly complex, they call for the help of experts, which creates a need for applied mathematicians. This is how we can make money. One of the large actors in the field of CFD (computational fluid dynamics), ANSYS who has the ownership of the software program FLUENT, had a total revenue of $ 385.3M in 2007. The market for CFD is large and interesting to try and enter for new actors and CFD entrepreneurs who desire a piece of the cake, whether the desired piece is large or small. The probability of being acquired by a large actor is quite high.

3.3 The continuum hypothesis

Obtaining high-quality results in the field of fluid dynamics requires the need for good models. The standard physical approximation is the continuum hypothesis: We regard the fluid as a mathematical continuum. The opposite of this assumption, is to regard the fluid as an ensemble of molecules connected through inter-molecular bindings that may be either polar, as in water and many other fluids, or of the Van der Waals type as in many gases. The quantum mechanics regime, where these forces dominate, calls for exact calculations of energies and the solving coupled Schrödinger equations for the system of interactions. In the fluid dynamics regime, which is macroscopic, we may apply the continuum hypothesis without much fear of great error introduced by it. The number of molecules that makes up most of the computational domains we are dealing with, is often several orders of magnitude larger than the Avogadro number, which is $N_a \simeq 6.022 \times 10^{23}$. To solve the Schrödinger equation for a system of that many particles would require huge

amounts of computer memory, which we do not have at hand. The continuum approximation has been proven very successful indeed, therefore we stick to it. The need for modeling using quantum particle behaviour may be needed for some problems [21], but they will not be considered in this thesis. The continuum hypothesis is necessary, and the only sane choice for most industrial problems. A just question is when the continuum approximation breaks down. The answer is that it rarely breaks down in most applications. If the number of molecules involved in the computational domain is very small, the continuum may be broken or that reason. However, the continuum may be subject to very high velocities and pressure fluctuations, calling for other models to describe supersonic of even relativistic effects. In extremely turbulent liquids, the dimension of the smallest revolving eddies will be very small, and might force our models to incorporate quantum effects. But even then, good approximation models for energy dissipation will probably be preferred rather than going to the extreme effort of modeling the whole system down to the smallest part, which is not feasible in the next few decades at least.

4 Problem

The job description is to validate and further develop the spectral element Navier-Stokes solver with the variational multiscale approach to large eddy simulation. The software is developed at FFI. Hereafter, the preferred way of addressing the Large-Eddy Simulation technique is by calling it the LES. The variational multi-scale method will be named VMS, and the Spectral Element Method will be called SEM.

4.1 VMS-LES

The Variational Multiscale Large - Eddy Simulation (VMS-LES) method was introduced by Hughes et al. [11]. The approach of variational scale projection down to an orthogonal basis represented something new to large eddy simulation. Traditionally, the large eddies (and by large, I mean those eddies having typical length of circulation larger than some cutoff wavelength), were resolved using spatial filtering. Typical filter would be a Gaussian or a sharp cutoff filter. Because of the finite and constant filter width, the spatial filtering method had some consistency issues when dealing with closed domains. What happens to the filtering / integration at the boundary? The best results were achieved when using periodic boundary conditions. The variational multiscale approach is not like spatial filtering. It is a mathematical tool for advanced analysis that assumes an inner product space with a hierarchical basis. From the hierarchical basis, the desired small and large scales are collected in distinct sets named small and large subsets. Then we project the test-solution down to either of these sub-spaces, using the inner product. This is called variational projection. The subspaces to project the solution onto, are assumed finite dimensional. The full space may be infinite dimensional. We keep the large eddy philosophy in mind, the idea of resolving the large scales and modeling the small. We choose to resolve the large scales, and model the small scales. This is a natural choice, since the dimension of the small scale space may be infinite, hence impossible to fully resolve numerically. In filter-based LES, the modeling was of the subgrid-scale stresses. In VMS-LES, the modeling is of the large-scale projection of the small-scale stresses. Those two have different consequences. This method of scale separation may be seen as a more physically appealing technique, and a closer connection with the multiscale behaviour of turbulence than the spatial filter.

4.2 SEM

The Spectral Element Method (SEM) with the special non-uniform discretization of the domain provides an optimum distribution of integration points for Gauss-Lobatto Legendre numerical integration. The discretiza-

tion, together with the choice of basis functions, the Legendre polynomials, provides a high-order method on each element. The order of the method is nearly two times the polynomial degree N one each element. The SEM is a very useful tool for calculating higher-order statistics of the fluid motion. However, it seems that the industry is still using finite element methods (FEM) to a larger scale. At one hand, the industry and scientific community is rapidly adapting to (and inventing) new technology. Still, a great number of software solutions used by the groups mentioned, are still reliant on Fortran 77, C and C++ as the main development programming languages, even though they should be considered "old" in a sense. However, if it is not broke, do not fix it. Fortran has survived many decades because it is doing the job. For FFI, the goal is not to develop a SEM solver and commercialise it. They basically need a higher order method with the all the positive characteristics of the FEM in general geometric situations, multi-grid environments, to have a means of testing other (not-so high order) software against the higher order. As in other industries, the military industry relies on technology to do the job. FFI wants to double check in some situations.

4.3 Decay of Homogeneous Isotropic Turbulence

A turbulent flow with no volume forces and applied external pressure in an infinite domain or finite with periodic boundary conditions, will eventually loose part of the kinetic energy because of energy dissipation of the smallest eddies. The kinetic energy lost by the dissipation is gained as internal energy. If there were boundaries or physical walls like in a channel, the dissipation could result in deformation of the wall-structures or surface. In a channel with an average velocity above some lower limit, there will always be wall-turbulence, and perhaps turbulence in the central part of the channel. If there is a constant or non-constant average velocity of pressure field not equal to zero, the flow non-isotropic. On the other hand, if the flow is isotropic or have no mean velocity, all fluctuations will eventually die out completely, and all kinetic energy will dissipate. Since there are no boundaries by assumption, the large wavelength movements will eventually also loose all their energy, or at least in theory, if the fluid has zero average velocity. In practice, there may be some persistent structures in the fluid. That is part of the reason why we have statistical formulations of the laws regarding fluid dynamics. A law would state that the ensemble average of any quantity should behave in accordance with the law. For any isolated case, the behaviour would be according to a stochastic process, and the measured statistics would be considered estimates.

The theoretic evolution of kinetic energy is derived using the Fourier transform of the velocity field, and statistical tools like two-point correlation functions and similarity. The Similarity hypothesis is the assumption that

velocity fluctuations on scale $\updownarrow$ within the inertial range of velocity scales (the range of fluctuations frequencies in between the smallest and the largest) are self-similar. The description of the energy decay is found in the Kolmogorov -5/3 power law for the energy spectrum [18], given a spherical shell in the wave-vector space (axes k_1, k_2, k_3) of Fourier modes having wave number of frequency vector norm equal to k. The wedges are denoting the statistical average of the quantity, not the momentary value of the quantity itself:

$$E(k) = 2\pi k < |\hat{u}(k)|^2 >= C\epsilon^{2/3}k^{-5/3} \tag{2}$$

Also, from the website [18], the direct enstrophy cascade asserts that the energy should behave like this, when the enstrophy flux is denoted ϵ_ω and the C' is a constant:

$$E(k) = C'\epsilon_\omega^{2/3}k^{-3} \tag{3}$$

4.4 Modeling

Working with the Navier-Stokes equations (section 5.1), there are two main paths one could take.

- Solve the exact equations using a fine grid and probably a Fourier spectral method if the domain is regular enough. The number of grid points will be high.
- Solve some other set of derived equations, for example the RANS (section 5.4) or LES (section 5.5) equations. Those equations are exact also, but approximations must be made for some quantities, in order to achieve a simpler set of equations than the Navier-Stokes.

Strategy number two gives rise to the closure problem. If we list the Navier-Stokes equations and the RANS, we see two major differences. For the following I use tensor notation for the subscripts. Repeated or equal indices between terms imply summation, and subscripted indices after a comma indicates partial differentiation with respect to that variable or variable number:

$$u_{i,t} + (u_j u_i)_{,j} + p_{,i} - \nu u_{i,ii} = f, \quad u_{j,j} = 0 \tag{4}$$

$$\bar{u}_{i,t} + (\bar{u}_i \bar{u}_j)_{,j} + \bar{p}_{,i} - \nu \bar{u}_{i,ii} + \overline{u_i' u_j'} = \bar{f}, \quad \bar{u}_{j,j} = 0 \tag{5}$$

The second (RANS) equation incorporates two things:

- Splitting of the velocity and pressure field into mean and fluctuating part (Reynolds Aaveraging), such that $u = \bar{u} + u', \quad p = \bar{p} + p'$

- Ensemble averaging of the Navier-Stokes equations

The main difference between the two equations is that the second is the expression for the ensemble average of the velocity and pressure field, and it involves a term $\overline{u_i' u_j'}$, which we do not want to solve explicitly, so we approximate its behaviour by a model. We have four fields to solve, and four equations. The term we are modeling does not include any of the fields we are solving explicitly (u_1, u_2, u_3, p).

Approximating the subgrid-scale stresses (which will take more complicated forms in the LES and VMS-LES in sections 5.5, vms) by a model is the ever-lasting issue that is still subject to research. The models of today are often based on the Smagorinsky model, originally developed by Smagorinsky in 1963 [22] to improve the calculations in a meteorology setting. The model has later seen improvements like dynamic estimation / calculation of a parameter known as the Smagorinsky parameter, or further addition of terms to the model. We will discuss more of that in section 5.8, this discussion was mainly to introduce the subject of modeling, since it is an important part of the thesis.

5 Theory

The theory needed to get a certain basic knowledge about the mathematical field of numerics, and of the physics behind the turbulence that we are trying to approximate or solve mathematically will be provided for the reader. The strategy is to present the Navier-Stokes equations that we are working to solve, followed by numerical techniques for approximation and simplification of these equations, followed by some turbulence theory. It is important to discuss many of these fields, to better be able to discuss the results and the simulations, and to see a bigger picture. In the end, the big picture will look very small indeed. The theory provided will only dig slightly beneath the surface of the majority of the many subjects, but will hopefully help the reader acquire some understanding and feel about the general ideas and assumptions we make.

5.1 Navier-Stokes Equations

In any discussion about fluid dynamics, the governing equations of motion need to be listed. The Navier-Stokes equations are the governing equations of fluid dynamics. They were, along with the theory of elasticity, derived during the 19th century. The Navier-Stokes equations were published i 1822 [19]. Quite late, given the fact that Newton's Laws of motion had been well known for many years, since their publication in Newton's book Philosophiæ Naturalis Principia Mathematica in 1687. The Euler equations or an ideal fluid were derived by Euler in 1755 [6], those are the equations of a non-viscid fluid. In the beginning, Navier did not fully understand the concept of viscosity, which Stokes later clarified in 1845 [23], and gave their final form, which is used today. Before we present the equations, let us do some initial work to establish an understanding of fluids or liquids and physical laws in those materials.

The continuity equation of a fluid is the following, in integral (*weak*) form, stating that the flux of mass through a closed surface equals the instant decay of material in the enclosed volume. This equation expresses a law governing the fluid transportation, for a liquid:

$$\int_{\partial\Omega} \rho\mathbf{u}\cdot\mathbf{n}dS = -\frac{\partial}{\partial t}\int_{\Omega}\rho dV \Rightarrow \tag{6}$$

$$\int_{\Omega}(\nabla\cdot(\rho\mathbf{u}) + \partial_t\rho)dV = 0 \Rightarrow \tag{7}$$

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = \partial_t\rho + (\mathbf{u}\cdot\nabla)\rho + \rho\nabla\cdot\mathbf{v} = 0 \tag{8}$$

We introduce a new operator called the material derivative or convective derivative:

$$\frac{D}{Dt} = \partial_t + \mathbf{v} \cdot \nabla$$

The expression now takes the following form:

$$\begin{aligned} &\partial_t \rho + v \cdot \nabla \rho + \rho \nabla \cdot v = 0 \Rightarrow \\ &\frac{D\rho}{Dt} = -\rho(\nabla \cdot \mathbf{v}) \end{aligned} \tag{9}$$

Where ρ is the scalar density of the fluid and $\mathbf{v}$ is the three dimensional velocity vector. All these variables depend on all the coordinates and the time.

The equations regarding conservation of momentum /Newton's second law for materials, is the following in fluid mechanics:

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \tfrac{1}{\rho}\nabla \cdot \sigma + \mathbf{f} \tag{10}$$

$$\partial_t \rho + \nabla \cdot (\rho u) = 0 \tag{11}$$

$\mathbf{u} =$ velocity, $\quad p =$ pressure, $\quad \rho =$ fluid density, $\sigma =$ Stress tensor

The operator ∇ is the *del* operator, which is the sum of partial derivatives along the coordinate axes.

$$\nabla := \sum_j e_j \frac{\partial}{\partial x_j}$$

The Navier-Stokes equations of a Newtonian fluid are the following [16], on a domain $\Omega \subset \mathbb{R}^d$, where the d denotes the dimension of the problem are the main governing equations for a fluid mechanical problem. Flow variable dependence on space coordinates and time is suppressed for simplicity of notation

$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{\nabla p}{\rho} + \frac{(\kappa + \mu/3)}{\rho}\nabla(\nabla \cdot \mathbf{v}) + \frac{\mu \nabla^2 \mathbf{v}}{\rho} + \mathbf{f} \tag{12}$$

$$\begin{aligned} &\mathbf{v}, \mathbf{f} \in \mathbb{R}^d \\ &p, \rho \in \mathbb{R} \\ &\mathbf{x} \in \mathbb{R}^d, t \in \mathbb{R} \\ &\mu, \kappa \in \mathbb{R} \end{aligned}$$

Boundary and initial conditions for this non-linear, partial differential equation may also be defined, to achieve closedness, which may cause a unique solution. As we shall see, the uniqueness of solutions to some problems may be challenged by turbulence, a phenomenon scientists all over the world try to understand completely, but there is not one, but many ways to model

turbulence. It is tempting to mention the equations governing an *incompressible* Newtonian fluid, where *incompressible* means that ρ is constant or invariant in each point in the domain, or that the convective derivative of ρ is zero. Using the continuity equation 9, we get the result (if $\rho \neq 0$)

$$\frac{D\rho}{Dt} = 0 \Rightarrow \nabla \cdot \mathbf{v} = 0 \tag{13}$$

The equation for this incompressible fluid is now simpler:

$$(\partial_t + \mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2 \mathbf{v} + \mathbf{f} \tag{14}$$

The term $\mu/\rho := \nu$ is usually named the kinematic viscosity.

We obtain other forms of the equation by taking vector operations. The vorticity equation is derived taking the curl of the Navier-Stokes equations, which yields the following:

$$\partial_t \omega + u \cdot \nabla\omega - \omega \cdot \nabla u = \nu\nabla^2\omega, \quad \omega \equiv \nabla \times u \tag{15}$$

For further readings on the Navier Stokes equations and development of Fluid Mechanics, see the excellent (but somewhat high-level) book of Landau and Lifshitz [16], and to learn how to solve them, see a book about advanced numerical methods. To earn money on discoveries that will give a breakthrough in the questions about uniqueness and smooth- ness of solutions to these equations, you should consider solving one of the Millennium Problems. Find the problem description in [7]. Win 1M dollars.

5.2 Spectral Element Method

The spectral element method, hereafter denoted the SEM, is a discretization process together with a proper choice of basis, test and trial functions for solving differential equations. Valuable features are the spectral accuracy, the versatility in being able to adapt to complicated geometries and meshes. The generalization to higher dimensions using tensor-product discretization of the space. The order of accuracy is spectral, meaning that the error decreases exponentially with the increased number of basis functions used to represent the trial solution, a feature found in spectral methods and eigenfunction expansions. The discretization in SEM results in a partition of the axes in K elements, K does not have to be the same in all directions. Inside each element, there are N non-uniformly spaced grid points, not including the two elemental boundary points. We have a description of the discretization using the grid-parameter $h = (K, N)$. The grid inside each element is not uniform, but still structured. The non-uniformness arises from the fact that the points are optimum with respect to Gauss-Lobatto quadrature (integration) with respect to an orthogonal basis. In most spectral element

methods, the choice of basis functions on each element, is the Jacobi orthogonal polynomials. They are members of the family of Jacobi polynomials, which are the only polynomial eigenfunctions to a singular Sturm-Liouville (SSL) problem. The reason why Legendre is the chosen one, is because they are orthogonal in the unweighted function space $L^2(-1,1)$.

The combination of optimization of points with respect to integration, and the optimization of polynomial basis with respect to convergence of solution, leads to the SEM algorithm. Now that the basis functions are chosen, and the domain is discretized, now is the time to solve problems. To solve a general problem, pick a differential equation. Let us choose a second order, two dimensional stationary problem, the Helmholtz equation. The objective is to solve the scalar potential function u, given the values at the boundary of finding a scalar quantity

$$\begin{aligned} \mathcal{P}(u) \equiv -\partial_{xx}u(x,y) - \partial_{yy}u(x,y) + \lambda^2 u(x,y) \qquad &= f(x,y) \qquad (16) \\ u(\partial\Omega) = 0 \qquad &(17) \\ \Omega = [-1,1] \times [-1,1] \qquad & \end{aligned}$$

To begin with, we seek a weak solution to the variational formulation. Pick a solution space, which we shall soon derive. Given a test function $v_h \in V$ and a trial function $u_h \in U$, solve the variational problem in such a way that the residual function $u_{res} = u - u_h$ is orthogonal to the test function space V. Namely, solve the variational problem

$$< \mathcal{P}(u - u_h), v_h >= 0, \quad \forall v_h \in V \qquad (18)$$

We provide the variational form of this equation:

$$\int_{-1}^{1}\int_{-1}^{1} -u_{h,xx}v_h - u_{h,yy}v_h + \lambda^2 u_h v_h dxdy = \int_{-1}^{1}\int_{-1}^{1} f(x,y)v_h(x,y)dxdy \qquad (19)$$

Then we use integration by parts to end up with a first order integral-differential equation.

$$\int_{-1}^{1}\int_{-1}^{1} u_{h,x}v_{h,x} + u_{h,y}v_{h,y} + \lambda^2 u_h v_h dxdy = \int_{-1}^{1}\int_{-1}^{1} f(x,y)v_h(x,y)dxdy \qquad (20)$$

This is a first order system. In the strong formulation and before the integrations by parts, it looked like we should seek solutions from $C^2(\Omega)$. Now, we look for solutions in the larger space $H^1(\Omega)$, which is the Sobolev space of functions whose derivatives as well as the functions themselves belong to $L^2(\Omega)$. Restricting a little, we recognise that we should look for solutions in the space $H_0^1(\Omega)$, chich contain equivalence classes of functions in $H^1(\Omega)$ that satisfy the homogeneous boundary conditions 17.

5.2.1 Integration of the variational equation

The numerical integration has not been fully discussed yet. I mentioned that the discretization was due to the Gauss-Lobatto-Legendre quadrature, which chooses the optimum conbination of integration points $\{\xi_j\}_{j=0}^N$ and integration weights $\{\rho_j\}_{j=0}^N$, given an orthogonal basis. The points are chosen as the extremal points of the highest degree polynomial in the basis, in addition to the end points of the domain. The extremal points must in general be found numerically. When theses points are found, there is a theorem saying that the integral of any polynomial of degree less than or equal to 2N-1 on the interval (-1,1) will be represented exactly by the weighted sum

$$\int_{-1}^{1} p_m(x)dx \equiv \sum_{j=0}^{N} p_m(\xi_j)\rho_j \tag{21}$$

The exactness only holds for polynomials of degree less than or equal to 2N-1. Error estimates and theorems about Gauss quadratures are found in books about numerical techniques, I used a book by Kincaid and Cheney [14].

Moving on, we see that the variational form of the equation now will be represented as a weighted sum (still using the tensor product form for dimensions higher than one). If we can manage to have many cancellations in the sum because of either othogonality or other features, we will be happy. Unfortunately, the Legendre basis does not give too many advantages and cancellations of coefficients in the weighted sum. The orthogonality holds only for the inner products between basis functions. And given the weights and sum instead of integral, the orthogonality is lost. This is where we change our test and trial function representations. From working with a modal basis like the Legendre polynomials, which provides orhogonality but does not provide much cancellations in the weighted sum of integrals, we change to a nodal basis like the Lagrange interpolating polynomials. Given a set of points $\{xi_j\}_j = 0^N$, the Lagrange interpolating polynomial number k is the one being zero on all nods except node number k. I.e. if the Lagrange interpolant number k is denoted by h_k,

$$h_k(x) = \prod_{j=0, j\neq k}^{N} (x - x_j)/(x_k - x_j) \tag{22}$$

In the weighted sum, the terms involving u_h ad v_h products will naturally cancel out everywhere except a few points, since we now represent the functions as tensor products of series of Lagrange interpolants, i.e.,

$$u_h = \sum_{i=0}^{N}\sum_{j=0}^{N} c_{ij}h_i(x)h_j(y) \tag{23}$$

The product of any two Lagrange interpolants at unequal points will necessarily be zero:

$$h_i(x)h_j(x)|_{x=\xi_j} = \delta_{ij} \tag{24}$$

So now we sum up the terms, we have this representation, the k denotes the element number in the 2D domain, we assume summation over all indices. We assume symmetrical domain with respect to length and polynomial degree, such that integration points and weights are equal in x- and y- dimensions, to simplify notation and maximize readability, notising that having unequal characteristic points and weights in each direction still preserves the cancellation effect because of the tensor product form of the test and trial functions. The h subscript is dropped from now on, to further increase readability. The function u_h, now only called u, should still not be interpreted as the real solution, but as the chosen approximation based on the order of polynomials and the nature of the "real" solution.

$$\begin{aligned} &u_x^k(\xi_i,\xi_j)v_x^k(\xi_i,\xi_j)\rho_i\rho_j + u_y^k(\xi_i,\xi_j)v_y^k(\xi_i,\xi_j)\rho_i\rho_j + \\ &\lambda^2 u^k(\xi_i,\xi_j)v^k(\xi_i,\xi_j)\rho_i\rho_j = f(\xi_i,\xi_j)v^k(\xi_i,\xi_j)\rho_i\rho_j \end{aligned} \tag{25}$$

The subscripted x and y variables indicate partially differentiated functions. Represented as series of Lagrange interpolants, the equation becomes the following, we use the following u and v, summation signs dropped but still implicitly there (this helps increase the readability)

$$u^k = c_{ij}h_i^k(\xi_i)h_j^k(\xi_j), \quad v^k = h_i^k(\xi_i)h_j^k(\xi_j) \tag{26}$$

The full equation becomes, implied direct stiffness summation where the repeated element boundary points are not accounted for twice. The summation is carried out over all the elements, and boundary conditions are imposed.

$$\begin{aligned} &c_{ij}^k h_{i,x}^k(\xi_i)h_j^k(\xi_j)h_{m,x}^k(\xi_m)h_n^k(\xi_n)\rho_i\rho_j + c_{ij}^k h_i^k(\xi_i)h_{j,y}^k(\xi_j)h_m^k(\xi_m)h_{n,y}^k(\xi_n)\rho_i\rho_j + \\ &\lambda^2 c_{ij}^k h_i^k(\xi_i)h_j^k(\xi_j)h_m^k(\xi_m)h_n^k(\xi_n)\rho_i\rho_j = f^k(\xi_i,\xi_j)h_i^k(\xi_i)h_j^k(\xi_j)\rho_i\rho_j \end{aligned} \tag{27}$$

5.3 Spectral Methods - DNS

A spectral method is a way of solving a system of multi-dimensional partial differential equations using Fourier transformation. Any function in the Hilbert space $L^2(\Omega)$, may be closely approximated by its discrete fourier transform. If the function is not continuous, the approximation will not be very good at the discontinuities. Gibbs phenomenon may occur. However,

if the function is C or even C^1, the approximation is usually very good, and the error decreases exponentially with the number of modes in the finite approximation to the infinite series.

5.3.1 Differential Equations

The derivative of a one-parameter (x) dependent function f with respect to the parameter x is the following, denoted $f'(x)$:

$$f'(x) = \frac{d}{dx} f(x), \quad x \in \Omega = (-\infty, \infty) \tag{28}$$

If we take the fourier transform of the function $f(x)$, we get a different function called $\hat{f}(k)$, dependent on a different parameter k:

$$\hat{f}(k) = \int_{\Omega} f(x) e^{-ikx} dx \tag{29}$$

If we transform not the function itself, but its derivative, we get the following algebraic relation between the transform of $f'(x)$, denoted $\hat{f}'(k)$ and the transformed function $\hat{f}(k)$

$$\hat{f}'(k) = \int_{\Omega} f'(x) e^{-ikx} dx = f(x) e^{-ikx}|_{-\infty}^{\infty} - ik\hat{f}(k) = -ik\hat{f}(k) \tag{30}$$

To achieve the formula, we must assume that the function decays properly in $\pm\infty$, or simply that the function is zero at the boundaries of the domain. he point is, we have now a beautiful, algebraic relation between the derivative of the function and the transform of the function itself. Applying this technique to the Navier-Stokes equations, and treating the time as a free parameter (we transform the spatial velocity and pressure fields at a frozen time-instant), we get the following equations, called the Fourier-Galerkin approximation to the Navier-Stokes equations:

$$\mathcal{F}(u_i)(\mathbf{x}, t) = \hat{u}_i(\mathbf{k}, t), \quad \mathcal{F}(p)(\mathbf{x}, t) = \hat{p}(\mathbf{k}, t) \Rightarrow \tag{31}$$

$$\hat{u}_{i,t} + \widehat{(u_i u_j)}_{,j} - \iota k_i \hat{p} + \nu k_i^2 \hat{u}_i = \hat{f} \tag{32}$$

$$-\iota k_j \hat{u}_j = 0 \tag{33}$$

Given initial conditions, this system may be solved fast by a numerical software for Fast Fourier Transforms. The accuracy of the method is spectral. Hence, the method is often used to obtain a Direct Numerical Simulation (DNS) reference solutions for relatively simple test-problems like homogeneous, isotropic turbulence. FFT is an optimized algorithmic implementation of the discrete fourier transform as defined here:

Definition 5.1 *The Discrete Fourier Transform of an N-dimensional vector* $\mathbf{v}$ *is a bijection from the space of complex N-dimensional vectors to itself. This is the rule:*

$$\begin{aligned} &DFT : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathcal{F}(\mathbf{v}) = \hat{\mathbf{v}} \\ &\mathbf{v} = (v_0, v_1, \cdots, v_{N-1}), \quad \hat{\mathbf{v}} = (\hat{v}_0, \hat{v}_1, \cdots, \hat{v}_{N-1}) \\ &\hat{v}_m = \frac{1}{N} \sum_{n=0}^{N-1} v_n e^{-2\pi i n m/N} \end{aligned} \tag{34}$$

Because the DFT is a bijection, the inverse function exists and takes on a quite simple form. Let us take a look:

$$\begin{aligned} &DFT^{-1} : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathcal{F}^{-1}(\hat{\mathbf{v}}) = \mathbf{v} \\ &v_m = \sum_{n=0}^{N-1} \hat{v}_n e^{2\pi i n m/N} \end{aligned} \tag{35}$$

5.4 RANS - Reynolds Averaged Navier Stokes

There are ways of averaging the flow, that may help the user extract some data and information regarding different average measurements of the flow. For instance, a time average of a flow may smooth out a flow, to help the user see essential characteristics, for instance if the flow is quasi-stationary. A time average is the following:

$$\overline{U}(x) \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T U(x,t)\ dt \tag{36}$$

A space, or volume average may be used on a stationary flow to smooth out and see less fluctuations. In the extreme smoothing, the user would only ask the question if there is a net transport of fluid in one direction, and a space average may answer that question. A space average is the following, it does not have to be three dimensional but may be either one or two dimensional:

$$\overline{U}(t) \equiv \lim_{V \to \infty} \frac{1}{V} \int_\Omega U(x,t)\ d\Omega, \quad V \equiv \int_\Omega d\Omega \tag{37}$$

An ensemble average is the average of many trials, the limiting sum of all trials divided by number of trials, as the following formula suggests:

$$\overline{U}(x,t) \equiv \lim_{N \to \infty} \sum_{n=1}^{N} U_n(x,t) \tag{38}$$

Given such an average, we have the decomposition of the velocity vector u in a mean and a fluctuating part:

$$u = \bar{u} + u'$$

We do the same decomposing in to mean and fluctuating part for the scalar valued pressure p,

$$p = \bar{p} + p'$$

Then, we insert the decomposed form of the velocity and pressure in to the Navier-Stokes equation, and take the average of the system. We get the following system, known as the Reynolds Averaged Navier-Stokes equations:

$$\bar{u}_{i,t} + (\bar{u}_i\bar{u}_j)_{,j} + \bar{p}_{,i} + \nu\bar{u}_{i,jj} - (\bar{R}_{ij}(u'))_{,j} = 0 \tag{39}$$

$$\bar{u}_{j,j} = 0 \tag{40}$$

The sum $\bar{R}_{ij}(u')$, called the mean fluctuating Reynolds stress [3], is defined by the following expression:

$$\bar{R}_{ij}(u') = -\overline{u_i'u_j'}$$

Without the bar over the R, the sum is called the fluctuating Reynolds stress. Remembering the Navier-Stokes equations on the tensor notation form, and observing that the following form of the non-linear term is equivalent to the previously used form under the incompressibility assumption

$$(u_iu_j)_{,j} = u_{i,j}u_j + u_iu_{j,j} = u_ju_{i,j} \iff u_{j,j} = 0$$

The equations are represented in different ways in different papers, however when we talk about RANS and LES and soon VMS-LES, the tensor product form is more useful. The RANS equation has its form because we make a number of assumptions, known as the Reynolds conditions [24], listed here.

Definition 5.2 *For any flow variables ψ and ϕ, the following hold by assumption:*

$$\overline{\psi + \phi} = \bar{\psi} + \bar{\phi} \tag{41}$$

$$\overline{a\psi} = a\bar{\psi} \text{ for anu constant } a. \tag{42}$$

$$\bar{a} = a \text{ for any constant } a \tag{43}$$

$$\overline{\frac{\partial\psi}{\partial x}} = \frac{\partial\bar{\psi}}{\partial x} \quad \forall x \in \{\mathbf{x}, t\} \tag{44}$$

$$\overline{\bar{\psi}\phi} = \bar{\psi}\bar{\phi} \tag{45}$$

We note that the average of any fluctuation from the mean must be identically zero, otherwise the mean itself is not the mean. The following simple remark will support that logic:

$$\overline{u'} = \overline{u - \bar{u}} = \bar{u} - \bar{u} \equiv 0$$

So, for the busy reader, the "problematic" term becomes, when averaging:

$$(\overline{\bar{u}_i\bar{u}_j + \bar{u}_i u'_j + u_i\bar{u}_j + u'_i u'_j})_{,j} = (\bar{u}_i\bar{u}_j + \overline{u'_i u'_j})_{,j}$$

It may be useful to follow S. Scott Collis [3] when he is reluctant to cancel out the cross-stress terms, denoted by

$$C_{ij}(\bar{u}, u') = -(\bar{u}_i u'_j + u'_i\bar{u}_j)$$

The term cancels out when averaged, but it could still be kept if we are using a different approach, and different regime. In numerics, anything can happen, so we might as well keep it. The reason Collis [3] keeps it in his theory, is that he discusses a lot of methods and decompositions, and to compare it is necessary to keep this term. The RANS equations may be solved by modeling the Reynolds

5.5 LES (Large Eddy Simulation)

Form Ferzigers page 60 [8], I find the following definition of LES:

> LES is a method in which the larger scales of motion of the turbulence are simulated while the smaller ones are approximated or modeled.

The definition given by Ferziger is short, general and consise, which all definitions should be, by definition (see Wikipedia for the definition of a definition [26]). In other words, LES is a way of doing numerical analysis of certain special mathematical equations like Navier-Stokes or other non-linear PDFs (Partial Differential Equations). We are brought to the subject of identifying what is meant by an eddy (for the non-English reader). From an electronic dictionary we find the following explanation. An eddy is:

> "A current of air or water running back, or in a direction contrary to the main current." (Red Hat KDE Dictionary [5])

Let us stick to that definition. Contrary to the main current, meaning that an eddy is a separate structure in the field, with movements seemingly independent of the averaged flow. As scientists, we may also define an eddy the following way, involving only frequency terms:

Definition 5.3 *Given a Fourier-transformation of the velocity field in any substance, each Fourier component corresponds to a circulation pattern, superimposed on the field itself. Specifically, the Fourier series of the field component v_j is the following:*

$$v_j = \sum\sum \sum_{\mathbf{n}=-\infty}^{\infty} c_{\mathbf{n}} e^{\iota \mathbf{k}_{\mathbf{n}}\mathbf{x}} \tag{46}$$

5.5.1 LES Hypotheses

LES incorporates some important hypotheses about turbulence that may originate from the Kolmogorov theory. Firstly, the approximation that the large-scale dynamics of turbulent flow are determined by the large-scale eddies. This leads to the idea of resolving the large scales and modeling the small scales, since the main dynamics will be intact even if the small scales are not resolved. The second hypothesis is that the small-scale eddies in any turbulent field (perhaps with the exception of channel flow) are almost isotropic. An isotropic tensor is very simple, and easier to approximate than an anisotropic one. This assumption makes good sense by intuition. We have seen turbulent fields like a waterfall, and the smaller whirls and bubbles seem to whirl in no preferred direction. If we model only the very smallest scales (determined by a parameter specifying the ration of resolved to unresolved scales) in turbulent flow, and resolve say 99% of the large scales, we have almost DNS. If we only resolve a small fraction of the large scales, we have almost RANS.

To derive the LES equations, we proceed in a way similar to the RANS method. We apply something similar to a Reynolds decomposition of the field, but now an eddy size-decomposition, leaving the velocity and pressure in two assumingly distinct departments, the large-eddy group and the small-eddy group:

$$\mathbf{u} = \bar{\mathbf{u}}_{Large} + \hat{\mathbf{u}}_{Small} \tag{47}$$

$$p = \bar{p}_{Large} + \hat{p}_{Small} \tag{48}$$

The separation of the fields in to the two groups is non-trivial. We shall see two methods, one almost similar to the space-averaged RANS (the spatial filtering), and the other more similar to the Fourier-Galerkin method (variational projection), but with any choice of basis functions.

5.5.2 Spatial Filtering

The large and small eddies may be separated using a spatial filter. The LES equations with the spatial are derived using the integration of the velocity or pressure field with the filter kernel over a field which may be space (up to three dimensions) or time. The most common is to filter on the grid. The filtering is the following procedure, for a filter kernel G and the function u

$$\bar{u}(x) = \int_{\Omega} G(x, x')u(x')dx \tag{49}$$

For a homogeneous filter kernel, the filter argument depends on the distance between points, and is widely used. Many filters are homogeneous (depending on the relative distance between), like the Gaussian smoothing

filter. One advantage of a homogeneous filter is the commutativity between filtering and differentiation [3],[11]. In the following equation, $\bar{G}$ is the filter kernel:

$$\bar{u} = \int_{\Omega'} \bar{G}(\mathbf{x} - \mathbf{x}')u(\mathbf{x}')d\Omega' \tag{50}$$

Many different filters have been used in LES of (homogeneous turbulence) throughout the years. Ferziger [8] lists three filters, the *Gaussian*, the *Box* and the *cutoff* filters. Filtering of a function may be used to isolate characteristics, like long-time behaviour or averages in space. A smoothing procedure is an example of a filtering process. A filter operation is often a convolution or the inner product with a distribution. Filtering is linear, i.e. for any filter kernel g, the following holds (bar above symbol denotes filtered quantity)

$$\overline{\phi + \psi} = \bar{\phi} + \bar{\psi} \tag{51}$$

$$\overline{a\phi} = a\bar{\phi} \tag{52}$$

$$\tag{53}$$

We can not make as many valid assumptions as we did for the averaging filter, since when dealing with general filters, many non-linear effects may occur. For instance, two rules that can not be generally true for filtering, are the following:

$$\overline{\bar{\phi}\bar{\psi}} = \bar{\phi}\bar{\psi} \quad \text{NOT TRUE!!} \tag{54}$$

$$\overline{\bar{\phi}\psi} = \bar{\phi}\bar{\psi} \quad \text{NOT TRUE!!} \tag{55}$$

A turbulent field contains a lot of *random* fluctuations, and by *random* I mean that nature itself is close to deterministic, but as the observer we can only deal with a finite amount of information. We can not differentiate between individual particles by a quantum-mechanical hypothesis, neither can we assign artificial mindsets to lifeless particles of matter, hence they obey the physical laws that science is uncovering with footsteps of random size. I use the term random frequently hereafter.

The space-filtered-NSE are the following, obtained by filtering the equations themselves and representing the fields in their eddy-size decomposition form (we only apply the large-eddy filter):

$$\bar{u}_{i,t} + (\bar{u}_i\bar{u}_j)_{,j} + \bar{p}_{,i} + \nu\bar{u}_{i,jj} - (\bar{R}_{ij}(\hat{u}) + \bar{C}_{ij}(\bar{u}, \hat{u})_{,j} = 0 \tag{56}$$

$$\bar{u}_{j,j} = 0 \tag{57}$$

Where the C and R again have the same meaning as before, namely

$$R_{ij}(\hat{u}) = -\hat{u}_i\hat{u}_j \tag{58}$$
$$C_{ij}(\bar{u},\hat{u}) = -(\bar{u_i}\hat{u}_j + \hat{u}_i\bar{u_j}) \tag{59}$$

The bar over the Reynolds and Cross stress term denotes filtering of the whole expression. As with RANS, the procedure denotes with the bar on top was averaging, and a lot of terms cancelled. Here, with filtering, we can not make the same assumptions as we did before with the Reynolds conditions, but the following is assumed to hold for any filtering operation,

5.5.3 Variational Projection

Filtering in space led to the fact that more relevance was given to nearby points (close to the filter center (pivot point)) than to distant ones. A different type of filtering is obtained when the kernel is member of an orthogonal basis in a Hilbert space. An inner product in a Hilbert space is associated with a projection of a function down to the subspace defined as the linear span of a basis element. By taking the inner products with basis elements, we extract components and may represent the function as a linear combination of basis elements in the space. This is true, since the function is assumed to be in that space. To prove it, theorems from mathematical analysis are needed. I suggest reading the book by Hunter and Nachtergaele [12].

In order to decompose a turbulent field completely as an expansion in an orthogonal basis, we need to find a representative basis for turbulent fields. The Fourier basis is versatile, and it should be no surpise that even turbulence may be adequately represented as a Fourier series. This is usually dedicated to a small chapter of its own in papers on he subject, called Prope Orthogonal Decomposition (POD), resulting in he conclusion that the Fourier basis is the POD of the turbulent field. The analysis is not straightforward, but I choose to redirect the reader to other sources for this analysis, since I choose to concentrate on other subjects. I found the master thesis by Christian Wollblad [27] to explain this adequately. Assuming periodic turbulent fields on the domain $\Omega = (0, L)^3$, Ω being the smallest domain encompassing all the eddies of the flow. Then the field (u,p) is a linear combination of fourier modes, i.e.

$$u_j(\mathbf{x}, t_0) = \sum_{n_1,n_2,n_3=-\infty}^{\infty} \alpha^j_{n_1,n_2,n_3} e^{\iota\mathbf{k}\cdot\mathbf{x}}, \quad \mathbf{k}_r = \frac{2\pi n_r}{L},\ j, r \in \{1, 2, 3\} \tag{60}$$

The Fourier basis is dense in The Hilbert space L^2. L^2 is separable. A separable vector space is one that has a countable basis. I refer again to

[12]. A basis being countable means that the basis is possible to systemize and list in an enumerable sequence. For instance, the Fourier basis is the sum of all modes, which are systemized using the positive and negative integers, which is a countable set. In one dimension, mode number n is given by

$$e_n(x) = \exp(inx) \tag{61}$$

A countable set may be separated in distinct sets, given a separation rule. The basis may also be hierarchical, meaning that the numbering of an element in the set of basis elements corresponds to the "scale" of the element. For example, the $L^2([-1,1])$-orthogonal polynomial set called the Legendre polynomials, discussed in the Spectral Element section 5.2, given by the following formula, represent a hierarchical set, or basis if they are used as a basis.

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \tag{62}$$

The following recursive relation may be useful for numeric work and computer software implementation, so I include it

$$L_0(x) = 1, \quad L_1(x) = x, \quad L_{k+1}(x) = \frac{2k+1}{k+1}xL_x(x) - \frac{k}{k+1}L_{k-1}(x), \quad k \geq 2 \tag{63}$$

The Legendre polynomial of order n has n roots, and behaves quite nicely. An illustration of the first six Legendre polynomials on the interval [-1,1], including number 20 can be seen in figure 5.5.3.

Let us partition the solution space $\mathcal{V}$ in two distinct linear spaces, one "Large scale" subspace $\bar{\mathcal{V}}$ and the "Small scale" subspace $\hat{\mathcal{V}}$. If the full space is the orthogonal sum of the large scale and the small scale space, then we write

$$\mathcal{V} = \bar{\mathcal{V}} \oplus \hat{\mathcal{V}} \tag{64}$$

Let us choose an orthonormal, hierarchical basis of the full space, denoted by the greek letter Φ. The basis is hierarchical, so we may split the basis in two distinct sets, for each of the Large scale and the Small scale space, denoted by bar and hat to illustrate the different belongings of the basis elements.

$$\Phi = \sum_j \bar{\Phi}_j + \sum_j \hat{\Phi}_j \tag{65}$$

Let us write down the un-weighted inner product of two elements ϕ and ψ on the space $\mathcal{V}$ and its subspaces, which is the $L^2(\Omega)$ inner product

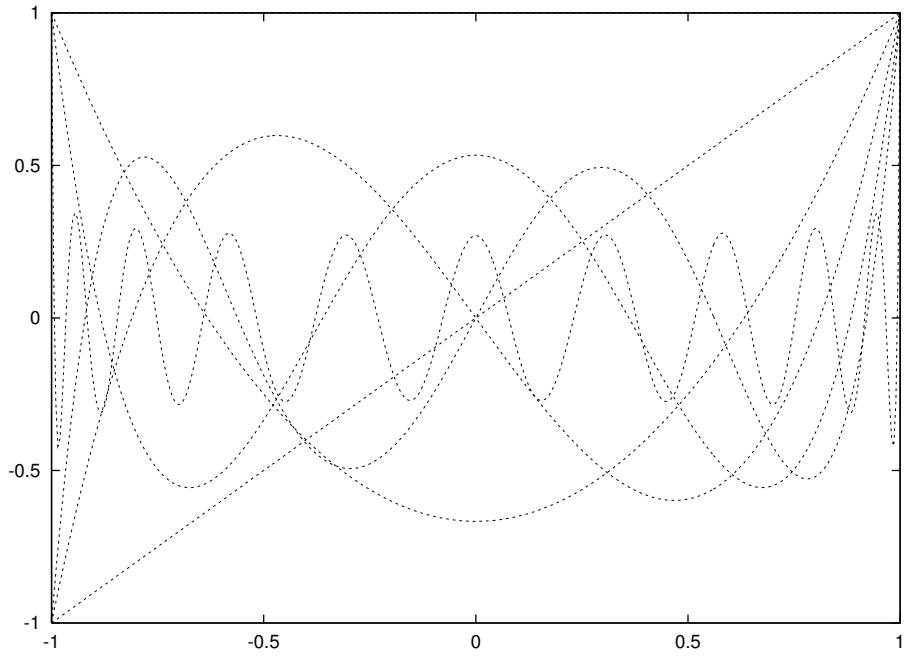

Figure 1: The first six Legendre polynomials on [-1,1] and L_20

$$(\phi, \psi) := \int_\Omega \phi(x)\psi^*(x)dx, \quad * \text{ denotes complex conjugation and transpose} \tag{66}$$

The variational projection of a state variable u down to a subspace $\bar{\mathcal{V}} \subset \mathcal{V}$, is an inner product of u with the set of basis functions for the particular subspace. The inner product becomes a little simpler if we enforce the space to have an orthonormal set of basis elements, since the L^2 norm of the inner product between two elements basis elements is unity if the functions are equal, zero otherwise. I.e., for two basis elements Φ_j and Φ_k, the following holds

$$(\Phi_j, \Phi_k) = \delta_{jk} \tag{67}$$

A projection is a mathematical operation known from vector algebra, using the scalar product. The dot product between a and b is commutative, and returns how much of vector b is "seen" from vector a, multiplied by the length of a. The complex inner product uses complex conjugation to make sure the square inner product of a vector by itself is real-valued. The projection of a vector onto another vector is an operation returning a new vector, the operation may be schematically illustrated the following way,

$$\text{proj}: \ v \in V \rightarrow V \tag{68}$$
$$\text{proj}_w v = v \cdot w^* = ||v|| \ ||w|| cos\theta \tag{69}$$

For functions, the projection is defined by the integral inner product. We use the Fourier basis on the interval $[0, 1]$ now, and describe the projection of a function f down to the complex basis element e_n, being the function $\exp(2\pi\imath nx)$

$$(\text{proj}_{e_n} f)(x) = \left[\int_0^1 f(x) \exp(2\pi\imath nx) dx \right] e^{2\pi\imath nx} \tag{70}$$

As with vectors, where the projection yield another vector, the function-projection yields a function. Then the projection of u onto the large scale space $\bar{\mathcal{V}}$ is the following, called $\bar{u}$

$$\bar{u} = (u, \sum_j \bar{\Phi}_j) = \sum_j \int_\Omega u(x) \phi^*(x) dx \tag{71}$$

5.6 VMS (Variational Multi Scale)

The VMS method was introduced by Hughes et al. 2000 [11]. They used a two-level splitting called large and small scale splitting, together with a cutoff in the small scales. Their work and methods were later clarified by Collis [3] with regards to the effect of the unresolved scales on the resolved scales. One big advantage with the method is illustrated by Collis in his three-level partitioning of the scales, which he denotes the large, the small and the unresolved scales.

I will only consider the three-level splitting introduced by Collis 2002 [3], and implemented by my supervisors and colleagues in the spectral element software at FFI. The VMS equations come from splitting / decomposing the solution space in Large, Small and Unresolved scale spaces, denoted by bar, tilde and hat.

$$\text{Large-scale space } = \overline{\mathcal{V}} \tag{72}$$
$$\text{Small-scale space } = \widetilde{\mathcal{V}} \tag{73}$$
$$\text{Unresolved-scale space } = \widehat{\mathcal{V}} \tag{74}$$

The full space is the sum of these spaces, they are assumed disjoint and also orthogonal for most practical uses.

$$\mathcal{V} = \overline{\mathcal{V}} \oplus \widetilde{\mathcal{V}} \oplus \widehat{\mathcal{V}} \tag{75}$$

The trial solution is denoted u, and is a linear combination of the large, small and unresolved scale space basis functions.

$$u = \bar{u} + \tilde{u} + \hat{u} = \int_\Omega u\bar{\Phi}(x)dx + \int_\Omega u\tilde{\Phi}(x)dx + \int_\Omega u\hat{\Phi}(x)dx \tag{76}$$

They are inserted in to the weak / variational form of the Navier-Stokes equations, and the test functions are chosen from the distinct spaces one by one, giving us three equation systems. Before we list the equations, let us develop a notation that may be helpful for compactness. Denote by $\mathcal{N}$ the Navier-Stokes operator, namely

$$\mathcal{N}(U) = \mathcal{N}\left(\begin{array}{c} \mathbf{u} \\ p \end{array} \right) = \\ \left(\begin{array}{c} \partial_t \mathbf{u} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + 1/\rho \nabla p - \nu \triangle \mathbf{u} \\ \nabla \cdot \mathbf{u} \end{array} \right) = \left(\begin{array}{c} \mathbf{f} \\ 0 \end{array} \right) = F \tag{77}$$

Mind the implicit definition of the state vector U, containing the pressure and velocity stacked on top of each other in a vector for compactness of notation. In Fortran we use the implicit none declaration, I would like to have the opportunity to implicitly define certain things for compactness of notation. When doing a variational projection with a test function W = $(\mathbf{w}, q) \in \mathcal{V}$, we write

$$B(W,U) \equiv < W, \mathcal{N}(U) > \equiv \mathcal{L}(W,U) - \mathcal{R}(\mathbf{w},\mathbf{u}) = < W, F > \tag{78}$$

Fully written out, and integration by pars applied, following the following rules for transformation of vector operations involving the ∇ symbol, div, grad and Laplacian, when homogeneous boundary conditions are applied

$$< \mathbf{w}, \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) > = \int_\Omega \mathbf{w} \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) d\mathbf{x} = -\int_\Omega \nabla \mathbf{w} \cdot (\mathbf{u} \otimes \mathbf{u}) d\mathbf{x} \tag{79}$$

$$< \mathbf{w}, \nabla p > = \int_\Omega \mathbf{w} \nabla p d\mathbf{x} = -\int_\Omega p \nabla \cdot \mathbf{w} \mathbf{x} \tag{80}$$

$$< \mathbf{w}, \triangle \mathbf{u} > = \int_\Omega \mathbf{w} \triangle \mathbf{u} d\mathbf{x} = \int_\Omega \nabla^s \mathbf{w} \nabla^s \mathbf{u} d\mathbf{x} \tag{81}$$

The symmetric gradient operator is the following one,

$$(\nabla^s \mathbf{u})_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{82}$$

We get the following expressions, using the inner product notation.

$$B(W,U) = < \mathbf{w}, \partial_t \mathbf{u} > - < \nabla \mathbf{w}, \mathbf{u} \otimes \mathbf{u} > - < \nabla \cdot \mathbf{w}, p > \\ + < \nabla^s \mathbf{w}, 2\nu \nabla^s \mathbf{u} > + < q, \nabla \cdot \mathbf{u} > \tag{83}$$

The inner product is the following standard unweighted one, star denotes complex conjugation

$$< f_i, g_j >= \int_\Omega f_i g_j^* d\mathbf{x} \tag{84}$$

When we do the same procedure as with the RANS and the LES, projecting the state vector U onto the various sub-spaces, representing U as the sum of subspace-projected components as in equation 76, we get three equations, using the shortest and least confusing notation for the inner products / variational projections of the full solutions onto the various subspaces,

$$B(\overline{\mathbf{W}}, \overline{U} + \widetilde{U} + \widehat{U}) =< \overline{\mathbf{W}}, F > \tag{85}$$

$$B(\widetilde{\mathbf{W}}, \overline{U} + \widetilde{U} + \widehat{U}) =< \widetilde{\mathbf{W}}, F > \tag{86}$$

$$B(\widehat{\mathbf{W}}, \overline{U} + \widetilde{U} + \widehat{U}) =< \widehat{\mathbf{W}}, F > \tag{87}$$

We shall see that there is a need for modeling the unresolved Reynolds and cross stress terms, following the procedure of Collis and also Wasberg et al. [25]. If we make the necessary calculations, we see the full system and many terms of variational projection of some functions in one subspace to a different subspace. If the subspaces are orthogonal, the variational projection of functions from different subspaces vanish. We can not assume total orthogonality in a turbulent field. Instead we write the equations out as a whole

$$\begin{aligned}&\mathcal{L}(\overline{W}, \overline{U}) + \mathcal{L}(\overline{W}, \widetilde{U}) - \mathcal{R}(\overline{\mathbf{w}}, \overline{\mathbf{u}}) - < \overline{W}, F > -\mathcal{R}(\overline{\mathbf{w}}, \widetilde{\mathbf{u}}) - \mathcal{C}(\overline{\mathbf{w}}, \overline{\mathbf{u}}, \widetilde{\mathbf{u}}) \\ &= -\mathcal{L}(\overline{W}, \widehat{U}) + \mathcal{R}(\overline{\mathbf{w}}, \widehat{\mathbf{u}}) + \mathcal{C}(\overline{\mathbf{w}}, \overline{\mathbf{u}}, \widehat{\mathbf{u}}) + \mathcal{C}(\overline{\mathbf{w}}, \widetilde{\mathbf{u}}, \widehat{\mathbf{u}})\end{aligned} \tag{88}$$

$$\begin{aligned}&\mathcal{L}(\widetilde{W}, \widetilde{U}) + \mathcal{L}(\widetilde{W}, \overline{U}) - \mathcal{R}(\widetilde{\mathbf{u}}, \widetilde{\mathbf{u}}) - < \widetilde{W}, F > -\mathcal{R}(\widetilde{\mathbf{u}}, \overline{\mathbf{u}}) - \mathcal{C}(\widetilde{\mathbf{u}}, \overline{\mathbf{u}}, \widetilde{\mathbf{u}}) = \\ &- \mathcal{L}(\widetilde{W}, \widehat{U}) + \mathcal{R}(\widetilde{\mathbf{w}}, \widetilde{\mathbf{u}}) + \mathcal{C}(\widetilde{\mathbf{u}}, \overline{\mathbf{u}}, \widehat{\mathbf{u}}) + \mathcal{C}(\widetilde{\mathbf{w}}, \widetilde{\mathbf{u}}, \widehat{\mathbf{u}})\end{aligned} \tag{89}$$

$$\begin{aligned}&\mathcal{L}(\widehat{W}, \widehat{U}) + \mathcal{L}(\widehat{W}, \overline{U}) + \mathcal{L}(\widehat{W}, \widetilde{U}) - \mathcal{R}(\widehat{\mathbf{w}}, \widehat{\mathbf{u}}) - \mathcal{C}(\widehat{\mathbf{w}}, \overline{\mathbf{u}}, \widehat{\mathbf{u}}) - \mathcal{C}(\widehat{\mathbf{w}}, \widetilde{\mathbf{u}}, \widehat{\mathbf{u}}) \\ &= \mathcal{R}(\widehat{\mathbf{w}}, \overline{\mathbf{u}}) + \mathcal{R}(\widehat{\mathbf{w}}, \widetilde{\mathbf{u}}) + \mathcal{C}(\widehat{\mathbf{w}}, \overline{\mathbf{u}}, \widetilde{\mathbf{u}}) + < \widehat{W}, F >\end{aligned} \tag{90}$$

The assumptions being made by Collis, Hughes et al. (implicitly, clarified by Collis) and Wasberg et al. are the following:

- The separation between large and unresolved scales is sufficiently large so that there is negligible direct dynamic influence from the unresolved scales on the large scales.

- The dynamic impact on the unresolved scales on the small scales are on the average dissipative in nature.

The consequences of modeling assumptions on the equations are essentially that all correlations between large and small scale are set to zero (all Reynolds and cross stresses involving large and unresolved components in the first equation are nulled out), and the terms involving unresolved-small scale correlations are replaced with a dissipative model term like the Smagorinsky model term. That means, no modeling other than assuming zero influence in the projected space is assumed, and the large-scale equation is solved by a solution method, described in the next paragraph.

5.6.1 Discrete scale partitioning

The basis of choice is the Legendre orthogonal polynomials. However, solving a matrix problem with the Legendre coefficients is not very efficient, and may be more optimized. One optimization is to transform from Legendre polynomial test-function to a Lagrange interpolating polynomial, having more appreciable features when doing the linear algebra. We say, we switch from o modal basis, being he Legendre polynomials, to a nodal basis, the Lagrange interpolating polynomials. A remarkable difference in character is also that the Legendre is a hierarchical basis, polynomial number N having order N. The Lagrange interpolating functions are all of the same polynomial degree, so any scale partitioning would be quite non-intuitive in that regime. However, there is an invertible, linear transformation between them, so we can easily switch between them, at a small additional cost of computing the transformations. For the VMS-LES, the hierarchical structure of the Legendre basis is heavily desired for the multiscale modeling approach. We also introduce scale partitioning operators that basically isolate large and small scales from the fully resolved system.

5.7 Smagorinsky Closure

The equations stemming from averaging, filtering or other procedures transforming the problem from finding the instant velocity and pressure field at all points to all times, to finding statistical quantities like the average or mean velocity during a short time interval at each point, or finding the smoothed out, spatial average velocity or pressure field at a region, all include some nonlinear part that is the reason we just can not solve the Navier-Stokes equations analytically for all boundary value problems, all geometries and all initial conditions. For the averaged equations, we have the Reynolds velocity cross tensor, with terms vanishing because the operation of filtering or orthogonal projection of a smallscale-component down to a large-scale component is zero. The distributive law for variational projection of a product

is assumed to be he following, as in equation 55.

$$\overline{(u \otimes u)} = \overline{(\bar{u} \otimes \bar{u})} + 2\overline{(\bar{u} \otimes \hat{u})} + \overline{(\hat{u} \otimes \hat{u})} \tag{91}$$

$$= (\bar{u} \otimes \bar{u}) + 0 + \overline{(\hat{u} \otimes \hat{u})} \tag{92}$$

The Smagorinsky model for the term called T, namely

$$T = (\bar{u} \otimes \bar{u}) - \overline{(u \otimes u)} \tag{93}$$

The T is called the subgrid-scale stress in Hughes et al 1999 **??**.

5.8 Subgrid-scale modeling

Approximating the subgrid-scale stress by a model is the ever-lasting issue that is still subject to research. The models of today are often based on the Smagorinsky model, originally developed by Smagorinsky in 1963 [22] to improve the calculations in a meteorology setting. The model has later seen improvements like dynamic estimation / claculation of a parameter known as the Smagorinsky parameter, or further addition of terms to the model. Other models for closure are the The majority of closure models have been based on the Smagorinsky model. The subgrid-scale stress is the difference between the tensor-product LES-filtering of the non-linear convection term and the tensor product of filtered quantities, i.e.

$$\mathbf{T} = \bar{u} \otimes \bar{u} - \overline{u \otimes u} \tag{94}$$

The Smagorinsky eddy viscosity model that provides a closure to the undetermined subgrid-scale stress is only modeling the deviatoric part of $\mathbf{T}$, namely

$$\text{dev } \mathbf{T} = \mathbf{T} - (\frac{1}{3}\text{tr } \mathbf{T})\mathbf{I} \tag{95}$$

The Smagorinsky closure is the following:

$$\mathbf{T}_S = 2\nu_T \nabla^s \bar{u} \tag{96}$$

The eddy viscosiy ν_T is given by the expression using the smagorinsky constant C_S, the filter width $\triangle$ and the symmetric gradient operator ∇^s operating on the filtered velocity field $\bar{u}$.

$$\nu_T = (C_S \triangle)^2 |\nabla^s \bar{u}| \tag{97}$$

The "symmetric gradient" operator ∇^s is the following construction,

$$\nabla^s \bar{u} = \frac{1}{2}(\nabla \bar{u} + (\nabla \bar{u})^T) \tag{98}$$

$$|\nabla^s \bar{u}| = (2\nabla \bar{u} \cdot \nabla \bar{u})^{1/2} \tag{99}$$

The values of the Smagorinsky constant has traditionally been chosen around 0.23 for homogeneous turbulence simulations, and around 0.1 for channel flows.

Hughes et al [11] make a list of shortcomings of the Smagorinsky model. Among the effects that should be adressed in new models, is that the Smagorinsky eddy viscosity tensor $\mathbf{T}_S$ does not replicate the asymptotic behaviour of the subgrid-scale stress $\mathbf{T}$ near walls. Further, the tensor precludes backscatter of energy from small to large scales.It will also produce excessive damping of the resolved structures in transistion. The dynamic Smagorinsky viscosity model is model taking those thoughts in to account, taking the Smagorinsky constant C_S not to be constant, but as a function of space and time. As Ferziger [8] remarks, the integral scale of turbulence L, is used in the derivation of the model equation, and it should therefore not be a surprise if the model parameter is not constant. The original work on this method was done by Germano et al. 1991 [9]. The calculation of C at any point is performed using a least squares minimization of error.

For general inhomogeneous flows, it is natural for the "constant" to be non-constant in time and space, being closer to 0.23 for almost homogeneous space-time slabs, and closer to 0.1 for slabs with more mean shear.

Kang et al. 2003 [13] say that the standard and dynamic Smagorinsky model lead to a small pile-up of energy spectra near the cutoff wavenumber in LES (Moin et al. 1991 and Meneveau et al. 1996).

5.9 Initial Velocity Field

The setup of the initial turbulent velocity field will now be discussed. The initial velocity field should be turbulent, isotropic, homogeneous and divergence free in order to be physically feasible for the simulation. In general, a turbulent field consists of many eddies of different scales, from the largest about the size of the domain, to the smallest whose size is closely related to the characteristics of the turbulent field. The more turbulent and higher Reynolds number, the smaller eddies will occur. In general, the field is a sum of sine and cosine functions, with a maximum frequency given by the turbulence scales calculation. I choose to look at the Comte-Bellot and Corrsin (CBC) **??**,**??** wind tunnel experiment from 1966 and 1971. These wind tunnel simulations are of the most used for initiating numerical methods in the simulation of homogeneous, isotropic turbulence. Numerous articles written by people using the CBC data as a benchmark for their numerical methods. Taylor microscale Reynolds number Re_λ for the CBC experiment was approximately 130, which is quite low compared to the newer tests that utilize active grids to generate more turbulence. A well documented article is Kang et al. 2003 [13]. I choose the CBC experiment for my initialization process. One reason is that Collis [3] and also my supervisors, who run the collis spectral method on a laptop computer, are using the CBC initial spectrum.

From the Collis code, I find a good approximation formula for the spectrum, which is only represented by 20 data points in the original CBC article from 1971. I have chosen to use the Collis analytical formula as the approximation to the CBC data, instead of implementing my own interpolation routine. It is a necessity to not deviate too much from the reference solution, since we shall compare results.

To implement the initial velocity field, we move to a Fourier representation of the velocity. In a homogeneous, isotropic turbulent field, there is no mean velocity, and the velocities show no preference of direction in space. In fact, the claims for the turbulence to be homogeneous and isotropic, are that the statistical moments of velocity correlation functions should be invariant of coordinate system translations and rotations. Moving back to the initial velocity, the only thing that is specified for a turbulent field is the kinetic energy corresponding to a given frequency vector norm. In three dimensions, the fourier modes are given by three integral multiples of the characteristic length in each direction, which is 2π / domain length in that direction. The energy spectrum specifies the total kinetic energy in all modes having frequency k. I represent each coefficient as a complex number:

$$c_{\mathbf{k}} = r_{\mathbf{k}} e^{\iota \phi_{\mathbf{k}}} \tag{100}$$

This complex number is initialized using a random function. This random number makes the initial phase be random, and will basically do the same job as the Alan Wray method used in **??**. After initialising all the coefficients for all velocity components (I do not initialize the pressure field), I use the Fourier interpolating polynomial to give a value to each point in my domain. The algorithm for this process is the following, written a s a pseudocde.

```
Algorithm #1 - Faster when M greater than KN
--------------------------------------------
# Find the X-velocity V at each point in the domain,
# using the DFT fourier interpolation on an irregular
# grid. The coefficients are called r_ijk, and the angle
# matrices are called phi_1, phi_2, phi_3

INT I # number of fourier modes in direction 1
INT J # number of fourier modes in direction 2
INT K # number of fourier modes in direction 2
INT X # number of evaluation points in direction 1
INT Y # number of evaluation points in direction 2
INT Z # number of evaluation points in direction 3

ARRAY b[I][J]
REAL tmp1, tmp2
ARRAY phi_1[I]
```

```
ARRAY phi_2[J]
ARRAY phi_3[K]
ARRAY coeff[I][J][K]
ARRAY f[X][Y][Z]
im   # imaginary number, square root of -1

for all z in Z   #Complexity/size = NK
    for all i in -N0:N0  #Complexity/size = M
        for all j in -N1:N1  #Complexity/size = M
            for all k in -N2:N2  #Complexity/size = M
               b[i][j] += exp(im*phi_3[k]*z)*coeff[i][j][k]
            end for (k)
        end for (j)
    end for (i)

    for all x in X   #Complexity/size = NK
        for all y in Y   #Complexity/size = NK
            for all i in -N0:N0   #Complexity/size = M

                for all j in -N1:N1   #Complexity/size = M
                    tmp2 += exp(im*phi_2[j]*y)*b[i][j]
                end for (j)

                tmp1 +=exp(im*phi_1[i]*x)*tmp2
            end for (i)
            f[x][y][z] = tmp1
        end for(y)
    end for (x)
end for (z)
#-------------------------------------
```

This algorithm has complexity $(NK)M^3 + (NK)^3M^2$. Dominating term is $(NK)^3M^2$, which depends more heavy on the number of evaluation points per direction. This is better when $NK < M$, which may often happen when parallellized. When parallel computation is utilized, the number of grid points per process goes down since the domain is decomposed in smaller subdomains, each process consisting of a number of elements K and a number of grid points N. The number of modes is fixed, does not benefit from parallelization.

$$E(k) = \sum_{|\mathbf{k}|=k} 2\pi k^2 \int\int\int |||hat\mathbf{u}||^2 d\mathbf{k} \tag{101}$$

Figure 2 shows the absolute value of the velocity field at time t=3.3, using the Voluviz software developed at FFI by Anders Helgeland and colleagues.

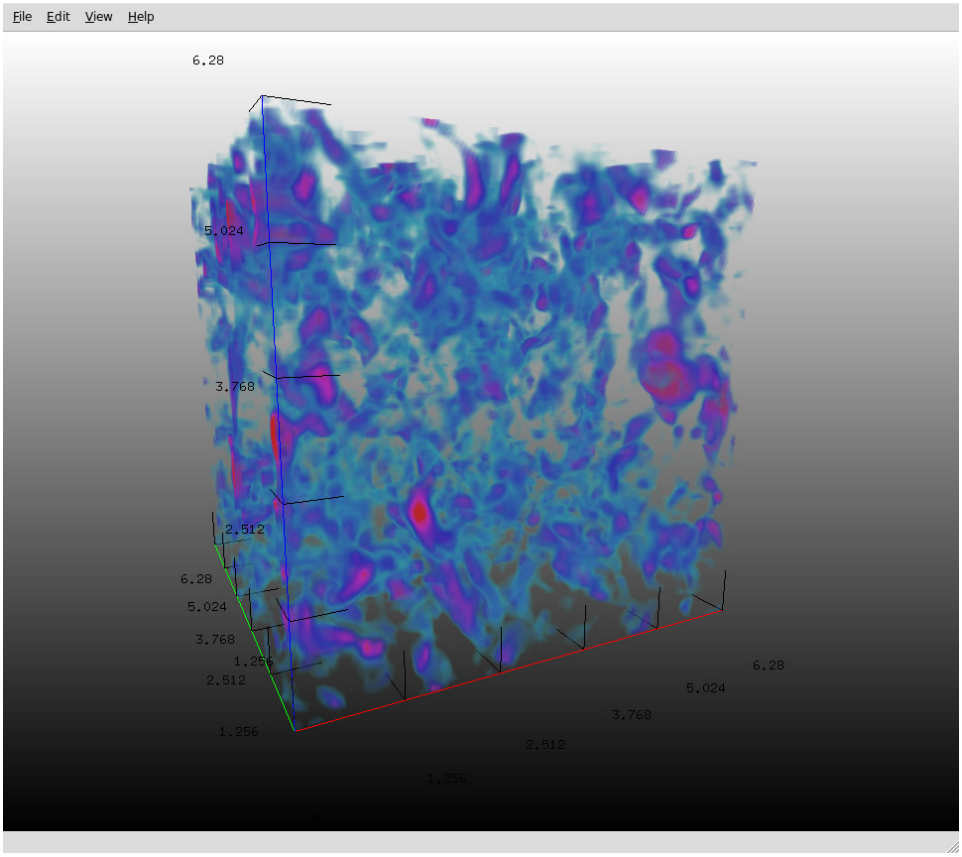

Figure 2: $|u(x,t)|$, t = 3.3. Colour table: Red marks the higher value.

5.10 Homogeneity

Following Dubois et al. [24], we shall now define homogeneity of a random field.

Definition 5.4 *A random field $u(x;\theta)$ is said to be spatially homogeneous when all its moments and joint moments are invariant under any space translation of the set of points $\{x_i\}_{i=1,\cdots,m}$ in $\mathbb{R}^n$, that is,*

$$m^{l_1\cdots l_m}_{j_1\cdots j_m}(x_1+r,\cdots,x_m+r) = m^{l_1\cdots l_m}_{j_1\cdots j_m}(x_1,\cdots,x_m) \tag{102}$$

for any separation vector $r \in \mathbb{R}^n$, $\quad 1 \le l_i \le n, i = 1,\cdots,m$

Meaning, any statistical moment, defined the following way:

Definition 5.5 *For a probability density or random function $y : \mathbb{R}^n \to \mathbb{R}$, a p'th order moment is:*

$$m_{j_1 \dots j_m}^{r_1 \dots r_m} = E\left(\prod_{i=1}^{n} X_{j_i}^{r_i}\right) = \int_{\Omega^n} \prod_{i=1}^{n} X_{j_i}^{r_i} y(x) d^n x \tag{103}$$

Where the indices r_i sum up to p, and the j_i-indices denote the moment contribution from variable number i.

$$\sum_{i=1}^{m} r_i = p, \quad \sum_{i=1}^{m} j_i = p$$

The zero'th first moment is equal to 1, the first (order) moment is the expected value, the second (order) moment is the variance, the third is known as skewness, the fourth is called kurtosis. A statistical moment of order m is a constructionHomogeneity of the turbulence means that the stochastic quantity called the two-point correlation tensor yields the same value whenever the arguments x and x' are separated by the same distance r. In other words, the field may not have regions of special behaviour, since any two regions separated by a distance vector r, must have the same statistical behaviour.

5.11 Isotropy

The homogeneity may allow a certain type of eddies like the long elliptic ones, and a stream with a distinct direction of the net flow may exhibit homogeneous behaviour. But if we change the coordinate system, we will see that the two-point correlation tensor changes. Isotropy is a condition on a system that the statistical quantities shall be invariant under any rotation and translation of the coordinate system. Other implications are that the average velocity can not differ from zero, see Dubois et al. [24].

5.12 The Scales of Turbulence, Reynolds numbers and useful quantities

Definition 5.6 *In a fluid enclosed in a geometric structure with characteristic length L, kinematic viscosity ν, and velocity v, the Reynolds number is the ratio*

$$R = vL/\nu$$

For high Reynolds numbers (R>X) [], the motion of the fluid will have turbulent character. Talking about scales, it is worth mentioning the concept of similarity also. According to Landau and Lifshitz [16], the movement of bodies of geometrically similar shape, or the flow in an enclosure with similar geometric shape, should have some similar characteristics, ans should in fact be similar if they scale the same way. It should be possible to project the flow of one geometric situation with a viscous fluid one-to-one to an up- or

downscaled verions of the same situation. The concept is explained better in Landau and Lifshitz, but it is very important. The law of similarity by O. Reynolds 1883 states that flows of the same type with the same Reynolds number are similar. This goes for turbulence as well as laminar fluid flow. See for instance Landau and Lifshitz [16] for a brief discussion about similarity.

Definition 5.7 *Turbulence is the notion of randomness in the fluid. A turbulent flow is a flow regime characterized by chaotic, stochastic property changes. This includes low momentum diffusion* $(\nabla \cdot (\rho v))$*, high momentum convection and rapid variation of pressure and velocity in space and time. Non-turbulent flows are called laminar.*

Definition 5.8 *The Reynolds number for a turbulent eddy of size* λ *is defined as [16]*

$$R_\lambda = v_\lambda \lambda / \nu$$

Where v_λ *is the velocity fluctuation of the eddy, and* ν *is the kinematic viscosity of the fluid and eddy. Since an eddy is a two-dimensional ellipse, the velocity fluctuation increases more than linearly with diameter,*

The Integral scale is the scale of the energy-containing eddies, the Taylor microscale is the scale for the inertial subrange eddies, the kolmogorov microscale is the scale for the dissipation range eddies. See http://amsglossary.allenpress.com [1]. The Kolmogorov length, η, and Kolmogorov velocity scale v, are ([10])

$$\lambda_{\text{kolm}} = (\text{usually } \eta) = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}, \quad v_{\text{kolm}} = (\text{usually } v) = (\nu\epsilon)^{1/4} \tag{104}$$

If we know the dissipation and the kinematic viscosity, we can easily calculate these numbers. The Taylor Microscale length λ_{tayl} is the following, defined in Dubois et al, [24] (among many)

$$\lambda_{tayl} = \left(-\frac{R_{LL}(0)}{\partial^2 R_{LL}/\partial r^2(0)}\right)^{1/2} \tag{105}$$

Also, the following formula may be used, relating the Taylor microscale to the kinetic energy and enstrophy (see Dubois page 38 [24])

$$\lambda_{tayl}^2 = 5\frac{\langle u(x)\rangle}{\langle \omega(x)\rangle} \tag{106}$$

Following other ways of calculation, among them formulas used by Christian Wollblad in his master thesis "DNS of Homogeneous Isotropic Turbulence and the Importance of Boundaries" [27], which originally were developed by (amogn others) Batchelor [2] and Hinze [10], turn out to be useful.

However, I choose to follow Dubois because I like the structure, and the easiness of following the sequence of arguments. We start by defining a characteristic velocity for the inertial range eddies, which may be fairly accurate approximated as the mean velocity of the whole domain, arguing that when squared, only the largest velocity contributions contribute in a large degree to this number, u_{rms}

$$u_{tayl} = 1/3\langle|u(x)|^2\rangle = \frac{2}{3}E$$

Using this characteristic velocity, we are about to define the characteristic length, which may be interpreted as the average length scale of the eddies in the inertial range.

$$\lambda_{tayl} = \left(-\frac{R_{LL}(0)}{R_{11}(0,0,0)}\right) \tag{107}$$

$$\lambda = \left(\frac{15\nu u_{1,rms}^2}{\epsilon}\right)^{1/2}$$

The Taylor microscale Reynolds number is given by th ratio of characteristic length and velocity to kinematic viscosity,

$$R_\lambda = \frac{v_\lambda \lambda}{\nu} = \frac{\sqrt{2/3E}\sqrt{10\nu E/\epsilon}}{\nu} = \sqrt{\frac{20/3}{\nu\epsilon}}E \tag{108}$$

5.12.1 Scales of Turbulence

Scale means rapidity of fluctuation, and the more violent fluctuations, the smaller is the length scale of a fluctuation. The scale is inversely proportional to n, the number of zeros in the polynomial. The scale concept is eminent in turbulence. What is turbulence? According to the discussion in Landau and Lifschitz, the turbulence is mainly small-scale eddies, dynamic systems of fluid circulating with radius of circulation being orders of magnitude smaller than the system dimensions. This movement may be seen as probabilistic or stochastic, given that a particle may stay in a cycle for long time, spin around some critical point and then leave, move on with the fluid or even get trapped. The Strange attractor and other structures may be seen. The scales of turbulence will be discussed further in this chapter, for now it is enough to note that there are large scales, eddies having rotation radius equal to almost half the domain length, called the integral scale eddies, intermediate size eddies around one third or one tenth of the large-scale radius, called the Taylor microscale eddies, and the tiniest eddies in the regime where fluctuating fluid calms down and transforms the kinetic energy to heat, dissipated in the system. This smallest scale is called the

Kolmogorov microscale, and the size of those eddies must be proportional to the following quantity, by dimensional analysis arguments

$$L_{Kolm} \equiv \eta \propto (\nu^3/\epsilon)^{1/4}$$

The integral scale is the length scale of the eddies containing most of the kinetic energy, i.e. the largest eddies, they often have the highest absolute velocity too. By intuition, we should expect the variation of the largest eddies to be almost the same size as the domain of calculation (which again may be chosen a priori to contain an integral number of eigen-periods of the largest eddies). We start by defining the characteristic velocity for the largest eddies, which may be fairly accurate approximated as the mean velocity of the whole domain, arguing that when squared, only the largest velocity contributions contribute in a large degree to this number, u_{rms}

$$u_{large} = u_{rms} = 1/\sqrt{3}\langle |u(x)|^2 \rangle^{1/2} \tag{109}$$

The integral the following, defined in (among others) Dubois et al. ([24])

$$L = \frac{\int_0^\infty R_{11}(r,0,0)dr}{R_{11}(0,0,0)} \tag{110}$$

How to compute all of these? The following "risky" fast formulas may be utilised **??**:

$$\frac{dE}{dt} = -\epsilon \tag{111}$$

$$\lambda_g^2 \simeq -\frac{15\nu u'^2}{dE/dt} \tag{112}$$

$$\epsilon/2\nu = \langle \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} \rangle \tag{113}$$

$$\frac{u'^3}{-\partial E/\partial t} \simeq L \tag{114}$$

The integral scale is found using the following formula,

$$L = \frac{\pi}{2u^2}\int_0^\infty \frac{E(k,t)}{k}dk \tag{115}$$

Or the more approximate, thumb-rule explicit formula,

$$L \simeq u'^3/\epsilon \tag{116}$$

We can use eihter of these. There is a little issue with Fourier transforms of functions defined on non-uniform grids. It is not straightforward, and still there is a lot of trouble getting the energy for velocity components on the sphere

$$S_k = \mathbf{k} : |k| = k$$

The energy dissipation is clearly defined as the rate of change in kinetic energy, namely

$$\epsilon = \frac{dE_{kin}}{dt} = \frac{d}{dt}\int_\Omega 0.5u^2 d\Omega \tag{117}$$

We may also utilize the fourier representation of the velocity, where the fourier transform of the velocity field is

$$\mathcal{F}(u) = \hat{u}, \quad \epsilon = \frac{dE_{kin}}{dt} = \frac{d}{dt}\int_{k^3} 0.5\hat{u}^2 dk^3 \tag{118}$$

All of these are naturally stochastic, time-averaged quantities, considered valid as ensemble averages.

The enstrophy is given by the integrated squared norm of the vorticity vector, which is equivalent to the integral of the Frobenius norm of the gradient of the velocity, i.e. (see Dubois et al. [24])

$$E(u) = \int_\Omega |\nabla u|^2 dx = \sum_{i,j=1}^{3} |\frac{\partial u_i}{\partial x_j}|^2 \tag{119}$$

The energy is denoted $e(u)$, and is given by the following relation,

$$e(u) = \frac{1}{2}\int_{\Omega\subseteq\mathbb{R}^3} |u(x)|^2 dx = \frac{1}{2}\int_\Omega u_i u_i dx \tag{120}$$

The enstrophy determines the rate of dissipation, which may be seen from the following argument, taking the dot product of u and the incompressible Navier-Stokes equations ($u_{j,j} = 0$), integrating over the whole domain Ω, assuming periodic boundary conditions for the pressure and velocity or if Ω is the whole of $\mathbb{R}^3$, vanishing velocity, velocity gradients and pressure at infinity, we get the following relation, still following Dubois et al. [24]

$$\int_\Omega (u_i u_{i,t} + u_i u_j u_{i,j} - \nu u_i u_{i,jj} + u_i p_{,i}) dx = \int_\Omega u_i f_i dx \tag{121}$$

$$\int_\Omega u_i u_{i,t} dx = \frac{1}{2}\frac{d}{dt}\int_\Omega u^2(x) dx = \frac{d}{dt}e(u), \tag{122}$$

$$\int_\Omega u_j u_i u_{i,j} dx = \frac{1}{2}\int_\Omega u_j (u_i^2)_{,j} dx = -\frac{1}{2}\int_\Omega u_i^2 u_{j,j} dx = 0 \tag{123}$$

$$-\int_\Omega \nu u_i u_{i,jj} = \nu\int_\Omega u_{i,j}^2 dx = \nu E(u) \tag{124}$$

$$\int_\Omega u_i p_{,i} = -\int_\Omega u_{i,i} p dx = 0 \tag{125}$$

Leaving us the following expression for the change of kinetic energy using the enstrophy and integrated force f times fluid velocity u,

$$\frac{d}{dt}e(u) = -\nu E(u) + \int_{\Omega} f_i u_i dx \tag{126}$$

Assuming zero external body force, we have the following simple expression for the rate of change of total kinetic energy, which equals the total turbulent energy dissipation rate ϵ, since no external energy enters or leaves the system

$$\frac{d}{dt}e(u) = -\nu E(u) = -\epsilon \tag{127}$$

This is very applicable in calculations, since we may want to extract the ϵ to be able to calculate the integral scale, the Taylor microscale, the Kolmogorov microscale and other derived quantities like the Reynolds numbers corresponding to these scales.

6 Analysis

The simulations were initiated using the energy spectrum described in section 5.9. They were excecuted using a time stepsize-increase method which was basically to output the solution at chosen times, and then increase the time stepsize, running the problem from the last output with the new timestep. I adjusted between four and six times for a single test. The results are compared to the reference solution using a normalization process to reduce the initial energy-damping problems experienced. More about the initial energy-damping will be found in chapter 6.2.*********TOO SOON ENDING*****

6.1 Presentation of results

The main subject was to investigate the kinetic energy decay of homogeneous, isotropic turbulent velocity fields simulated using the software developed at FFI, a 3d spectral element discretization based solver for partial differential equations, specially aimed at Navier-Stokes equations, utilizing variational multiscale turbulence modeling. The following setup was used for the main simulations.

Exp. #	M	N	model	large	alpha
0.0	8	8	smag-les	N/A	0.50
0.1	8	8	vms-les	0.000	0.00
0.2	8	8	vms-les	0.500	0.00
0.3	8	8	vms-les	0.750	0.00
0.4	8	8	vms-les	0.875	0.00
1.0	4	16	smag-les	N/A	0.50
1.1	4	16	vms-les	0.000	0.00
1.2	4	16	vms-les	0.500	0.00
1.3	4	16	vms-les	0.625	0.00
1.4	4	16	vms-les	0.750	0.00
1.5	4	16	vms-les	0.875	0.00

I will now present some figures. The energy plots are scaled such that maximum value i one for all the graphs. The time axis is not scaled. I present the data using reduced numberof graphs in each plot, therefore not all graphs of solutions will be presented. I have removed some of the graphs for parameter "large" between 0.5 and 0.875, to make it easier to see the separation between the graphs, which is quite small already. There ewill be three figures. The first will show the time evolusion of kinetic energy using a $K_1 = K_2 = K_3 = 8, N_1 = N_2 = N_3 = 8$ grid, displaying three graphs in addition to the DNS reference. The simulation using no vms model, vms with large scale fraction equal to zero, and large-scale fraction equal to 0.875, figure 3.

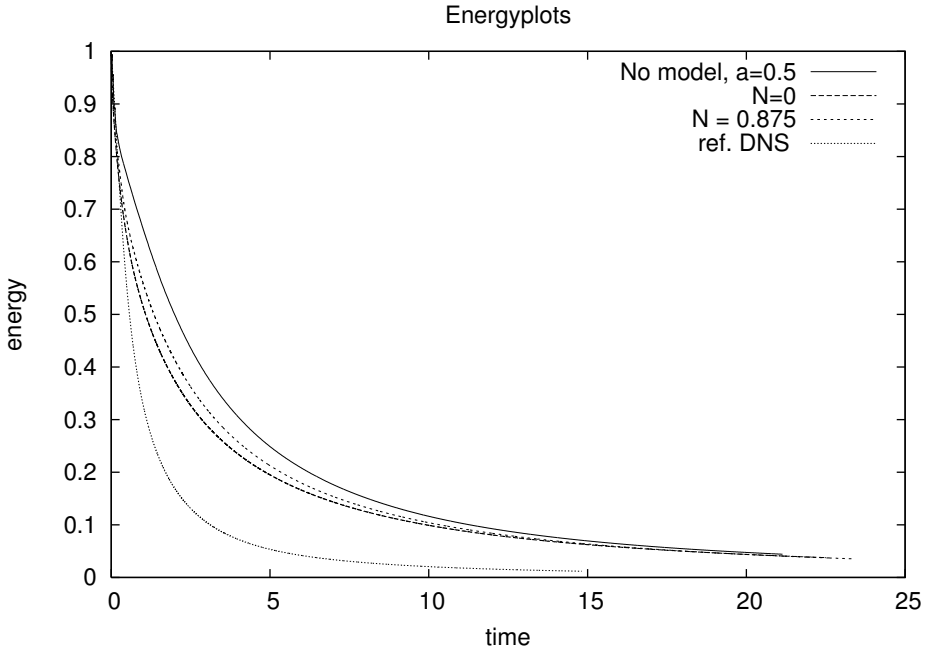

Figure 3: $(8 * 8)^3$ grid

The second figure will be of the $K_1 = K_2 = K_3 = 4, N_1 = N_2 = N_=16$ grid, showing three graphs. One without the vms model, and then two using vms with large-scale fractions 0.5 and 0.875, figure 4.

There is a significantly lower dissipation of energy in both the figures. The enrgy does not decay nearly as fast as it should. When the discrepancy is as large as this, we may need to go back to the drawing board. However, the relative behaviour of the simulation energy evolutions show that the higher large-scale fraction, the faster decay. That may indicate that the model is better than having no model at all. Since the discrepancies are so large, I choose not to make statements about the vms-les method, but conclude that there are significant discrepancy, and the software must be checked.

6.2 Initial Damping

I found problems with the software when initializing the velocity field. Giving a highly turbulent field, initiated with the energy spectrum in wavenumber-space, with a highest wavenumber-vector norm $|k_{max}|$, and a grid described by $h = (K, N)$, that is: K elements in each of the three spatial dimensions, and each element having polynomial degree and number of GLL integration points N, the problem is approximately this: The total kinetic energy suffers a great loss that increases monotonically when N is increased. The total

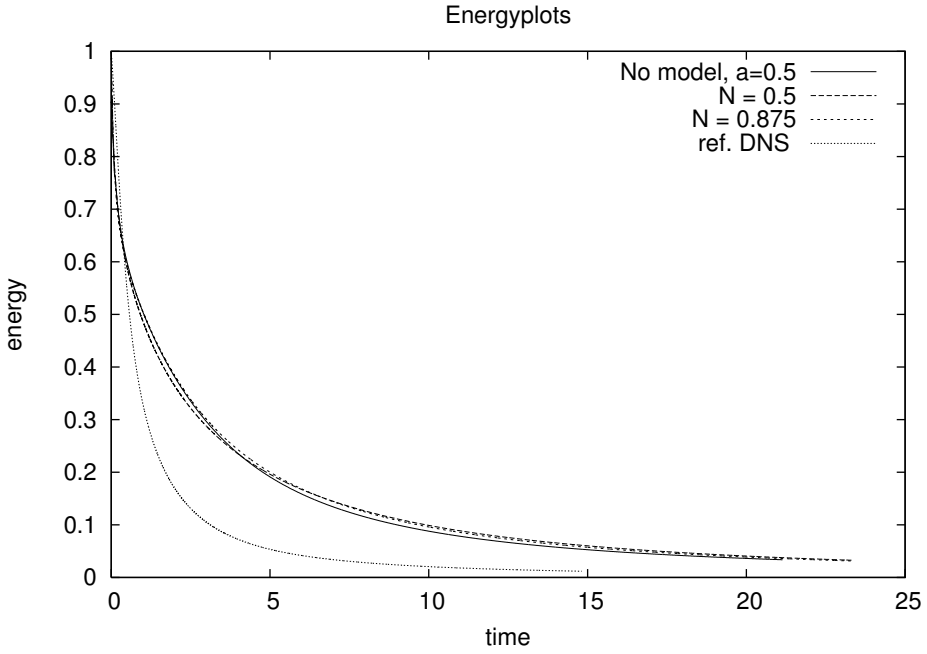

Figure 4: $(4 * 16)^3$ grid

kinetic energy sees to be kept from falling too much if the number of elements, K, is relatively high, and the energy will increase monotonically if K is increased. What is the possible explanation? There are many suggestions in the air. Some say that the initial iteration procedure, the implicit first order method, may be the cause of the great damping. If the damping in the method is anti proportional to the number of elements, then we might have a solution. The main stability and accuracy issue when dealing with implicit methods is that most of them are stable, regardless of the grid and the complexity of the underlying differential equation. The critical issue is accuracy. The accuracy of the method that is used, is the

6.2.1 Filtering and over-integration

The importance of filtering and over-integration is easily seen by the user when running tests. The lower level of filtering, the more iterations needed in the various sub-step procedures in the software algorithm. A short example, I was supposed to run a simulation using the standard initial spectrum for the Fourier-transformed velocity field. I was going to test the dependence of filtering. Without the filter, the program kept running and there was a slight increase in the number of iterations as time went by, even if the characteristic behaviour of the velocity field in the liquid was to decrease its energy, such that compute time should technically decrease, and problems

would be increasingly less complex, and would need fewer iterations. My supervisors had experienced no poitive effects of using both ove-integration and filtering in their previous channel simulations, as such they were sceptical about the combined use. It turned out, without the vms model, the over-integration alone was not enough. I had to put on filtering, at the level of 0.5. After that adjustment, simulations behaved better. When using the vms model, no filtering was applied.

7 Conclusion

To conclude this thesis, I sum up the results.

- The simulations were executed according to plan, not all tests that we wanted to do were completed, but we have the main simulations. There is a problem in comparison with the reference solution, which needs to be sorted out before any real knowledge about the performance of the methods is obtained.

- The homogeneous, isotropic velocity was in fact shown to yield appreciable behaviour at time equal to zero. I thought there was a stong connection between the variation of the grid parameters and the initial velocity, but due to a delay of first output, this was a misunderstanding, and led the author to address the wrong problems. The real problem seems to be that the initial turbulent field is damped out very fast. For girds with a high polynomial degree, the damping was most intensive. This problem has no obvious solution, I recommend the developers to look in to that and try to solve the problem.

- A good deal of knowledge about the software has been obtained. It takes some months to fully understand a large program. I recommend that there is produced more documentation about he code, to get workers faster in to development stage.

- The homogeneous, isotropic turbulence simulation has yet to produce adequate results. A final validation of the code must be able to address the problems encountered with the initial damping of kinetic energy.

Having said that, I believe the method is very powerful. We have seen results from channel simulations showing very good agreement with reference benchmark solutions. I believe the problem that was incountered in my work has to do with the sudden insantiation of a violently turbulent field also. If the field was gradually increased or artificially forced into being turbulent fy external forcing function, the initial value problem should be overcome without much difficulty.

References

[1] AMSglossary, *http://amsglossary.allenpress.com/glossary/search?id=turbulence-length-scales1*, April 2008.

[2] G.K. Batchelor, *Theory of homogeneous turbulence*, Cambridge University Press, Cambridge, U.K.; New York, U.S.A., 1970.

[3] S. Scott Collis, *Multiscale methods for turbulence simulation and control*, September 2002.

[4] G. Comte-Bellot and S. Corrsin, *Simple eulerian time correlation of full- and narrow-band velocity signals in grid-generated, isotropic turbulence*, J. Fluid Mechanics **48** (1971), 273–337.

[5] Bassi Emmanuelle, *Dictionary version 2.16.0*.

[6] L. Euler, *Principes gńeraux du mouvement des fluides*, Mem. Acad. Sci. Berlin **11** (1755), 274–315.

[7] Charles L. Fefferman, *Existence and smoothness of the navier-stokes equation*, http://www.claymath.org/millennium/Navier-Stokes_Equations/navierstokes.pdf, May 2000.

[8] Joel H. Ferziger, *Direct and large eddy simulatino of turbulence*, CRM Proceedins and Lecture Notes **16** (1998), 53–97.

[9] Massimo Germano, Ugo Piomelli, and William H. Moin, Parviz and-Cabot, *A dynamic subgrid-scale eddy viscosity model*, Physics of Fluids A **3** (1991), no. 7, 1760–1765.

[10] Juergen O. Hinze, *Turbulence*, 2nd ed., McGraw-Hill Book Company, New York, NY, 1975.

[11] Thomas J.R. Hughes, Luca Mazzei, and Kenneth E. Jansen, *Large eddy simulation and variational multiscale method*, Computing and Visualisation in Science **3** (2000), 47–59.

[12] John. K. Hunter and Bruno Nachtergaele, *Applied analysis*, World Scientific Publishing Co. Pte. Ltd, 2001.

[13] Hyung Suk Kang, Stuart Chester, and Charles Meneveau, *Decaying turbulence in an active grid-generated flow and comparisons with large-eddy simulation*, J. Fluid Mechanics **480** (2003), 129–160.

[14] David Kincaid and Ward Cheney, *Numerical analysis -mathematics of scientifc computing*, 3 ed., Brooks / Cole, 2002.

[15] Andrey Nikolaevich Kolmogorov, *The local structure of turbulence in incompressible viscous fluid for very large reynolds numbers*, Proceedings of the Royal society in London **434** (1991), no. 1890, 9–13.

[16] Landau L. D. and Lifshitz E. M., *Fluid mechanics 2nd edition*, Butterworth-Heniemann, 1987.

[17] John C. Mankins, *Technology readiness levels*, April 1995, White Paper.

[18] Stefano Mussachio, January 2004, http://www.ph.unito.it/ smusacch/tesi/node16.html.

[19] C. L. M. H. Navier, *Memoire sur led lois du mouvement des fluides*, Mem. Acad. Sci. Inst. France **6** (1845), 389–440.

[20] Lewis F. Richardson, *Weather forecast by numerical process*, Cambridge University Press, Cambridge, 1922.

[21] C. Schütte and Folkmar Bornemann, *Approximation properties and limits of the quantum-classical molecular dynamics model*, In algorithms for Maromolecular Modelling, P. Deufihard, J. Hermans, B. Leimkuhler, A. mark, S. Reich, and R. D. Skeel, eds., Springer-Verlag, berlin, Heidleberg, New York, to appear.

[22] J. Smagorinsky, *General circulatino experiments with the primitive equations*, Monthly Weather Review **91** (1963), no. 3, 99–164.

[23] G.G. Stokes, *On the theorie of interna friction of fluids in motion*, Trans. Camb. Philos. Soc. **8** (1845), 287–305.

[24] Dubois Thierry, Jauberteau Francois, and Temam Roger, *Dynamic mulilevel methods and the numerical simulation of turbulence*, Cambridge University Press, 1999.

[25] Carl-Erik Wasberg, Thor Gjesdal, Bjørn Anders Pettersson Reif, and Øyvind andreassen, *Variational multiscale turbulence modelling in a high-order spectral element method*, 2008, Preprint submitted to Journal of Computational Physics, 23 April 2008.

[26] Wikipedia, *Definition*, June, http://en.wikipedia.org/wiki/Definition.

[27] Christian Wollblad, *DNS of homogeneous isotropic turbulence and the importance of boundaries*, 2001, Diploma Work 01/14.