Pseudospectral Simulation of 3D Turbulence

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1 Introduction

In this lab we will learn how to use a three-dimensional *pseudospectral simulation*, a widely used numerical tool for the study of fluid turbulence. The equation we will be solving is the three-dimensional incompressible Navier–Stokes equation. A key step requires solving for the pressure by inverting a Laplace operator for the pressure P:

$$\boldsymbol{\nabla}\cdot[\boldsymbol{f}-(\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}]=\nabla^2 P, \tag{1}$$

where $\boldsymbol{f}$ represents an external stirring force. One of the most efficient methods for doing this is the pseudospectral method, which exploits the Fast Fourier Transform algorithm. Strictly speaking, this method is only appropriate for periodic boundary conditions. However, in practice it can be used even when the physical boundary conditions are nonperiodic, as long as the turbulence *decorrelation length* is smaller than the box size.

In order to set up our simulation, we will first need to determine a consistent set of forcing and dissipation parameters so that a fully developed turbulent state is obtained, in which net forcing balances net dissipation.

2 Theory

We begin with the three-dimensional isotropic incompressible Navier–Stokes equation for the velocity field in the case where the density ρ is constant and, by proper choice of units, equal to 1:

$$\frac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}=-\boldsymbol{\nabla}P+\nu_H(-1)^{p_H-1}\nabla^{2p_H}\boldsymbol{u}+\boldsymbol{f}. \tag{2}$$

where on the right hand side we have included small-scale dissipation ($p_H \geq 1$) and $\boldsymbol{f}$ is a random (white-noise in time) solenoidal force. [A compressive component to $\boldsymbol{f}$ would have no effect, because of Eq. (1).] Upon taking the spatial Fourier Transform $\boldsymbol{u}_{\boldsymbol{k}}=\int \boldsymbol{u}(\boldsymbol{x})e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\,d\boldsymbol{x}$ of Eq. (2) we obtain

$$\frac{\partial \boldsymbol{u}_{\boldsymbol{k}}}{\partial t}=\boldsymbol{S}_{\boldsymbol{k}}-\nu_H k^{2p_H}\boldsymbol{u}_{\boldsymbol{k}}+\boldsymbol{f}_{\boldsymbol{k}}. \tag{3}$$

where $\boldsymbol{S}_{\boldsymbol{k}}$ denotes the nonlinear terms, $\boldsymbol{f}_{\boldsymbol{k}}=F_k(\mathbf{1}-\boldsymbol{k}\boldsymbol{k}/k^2)\cdot\boldsymbol{\xi}_{\boldsymbol{k}}(t)$, and each of the components of $\boldsymbol{\xi}_{\boldsymbol{k}}(t)$ are independent Gaussian complex vector-valued random variables

with zero mean and unit variance. We will use a *dealiased* pseudospectral method to solve Eq. (3); this means that the convolution sum in $\boldsymbol{S_k}$ is computed in the spatial domain, with the help of the convolution theorem.

3 Simulation

In order to determine reasonable parameters for our numerical simulation of Eq. (3), we introduce the *energy*, or *total mean-squared velocity*, E, defined as

$$E \doteq \frac{1}{2} \int |\boldsymbol{u_k}|^2 \, d\boldsymbol{k}, \tag{4}$$

where $d\boldsymbol{k} = k^2 \sin\theta \, dk d\theta d\phi$ is the volume element. (The notation "$\doteq$" denotes a definition.) Upon multiplying Eq. (3) by $\boldsymbol{u_k^*}$, symmetries cause the nonlinear (advective and pressure) contributions to vanish, so that in a steady state, the energy balance equation becomes just

$$0 = \overline{\frac{\partial E}{\partial t}} = -2 \int_0^\infty \nu_H k^{2p_H} E(k) \, dk + \mathrm{Re} \, \overline{\int f_{\boldsymbol{k}} \cdot \boldsymbol{u_k^*} \, d\boldsymbol{k}}, \tag{5}$$

where the over-bar denotes a time average and

$$E(k) \doteq \frac{1}{2} k^2 \int_0^{2\pi} \int_0^\pi \overline{|\boldsymbol{u_k}|^2} \sin\theta \, d\theta \, d\phi$$

is the angle-averaged energy spectrum. The energy dissipation, described by the first integral, occurs mostly at the small scales (high wavenumbers), where the viscous terms dominate. We characterize these scales by the *dissipation wavenumber* k_d. In this lab we use the factor F_k to restrict the forcing to a narrow band, $k \in [2, 4]$, centered on the *forcing wavenumber* $k_f = 3$. It turns out that it is crucial to include all contributions of the energy dissipation from the *inertial range*, which is the wavenumber interval between the low forcing wavenumber k_f and high dissipation wavenumber k_d. The theory of Kolmogorov [1941] predict that between k_f and k_d, Eq. (3) supports power law solutions of the form

$$E(k) = C \epsilon^{\frac{2}{3}} k^{-5/3}, \tag{6}$$

where

$$\epsilon \doteq 2 \int_{k_f}^{k_d} \nu_H k^{2p_H} E(k) \, dk, \tag{7}$$

the rate of energy dissipation, is constant. In other words,

$$\epsilon = 2C \nu_H \epsilon^{\frac{2}{3}} \int_{k_f}^{k_d} k^{2p_H - 5/3} \, dk, \tag{8}$$

which we may solve for ϵ.

We assume that Eq. (2) is ergodic, so that ensemble averages are equivalent to time averages. According to Novikov's theorem [1964], if we prescribe that $\boldsymbol{f_k}$ is an isotropic white-noise random process,

$$\langle \boldsymbol{f_k}(t) \cdot \boldsymbol{f}^*_{\boldsymbol{k}'}(t') \rangle = 2F_k^2 \delta(\boldsymbol{k} - \boldsymbol{k}')\delta(t - t'), \tag{9}$$

with F_k nonzero only for $k \in [2, 4]$, (the factor of 2 signifies that there are only two independent directions, once the incompressibility constraint has been taken into account), the second integral in Eq. (5) may be expressed in terms of the Green's function for Eq. (3). Equation (5) then simplifies to the balance

$$\epsilon = 8\pi \int_2^4 k^2 F_k^2 \, dk. \tag{10}$$

We may now finally describe the procedure that we will use to determine parameters for our pseudospectral run.

4 Procedure

1. Choose a resolution $N \times N \times N$ where N is an odd number. See the graphical user interface `xtriad3d` to the program `triad` for allowable values. The maximum wavenumber $k_{\max}$ will then be $(N - 1)/2$.

2. Choose k_d to be slightly less than (say 90% of) $k_{\max}$.

3. Pick a value for the white-noise forcing amplitude F_k (e.g. $F_k = 1$). Letting $p_H = 3$, $k_f = 3$, and the forcing width $\delta_f = 2$, solve Eq. (8) for the high wavenumber viscosity ν_H in terms of the energy dissipation rate ϵ. An approximate value for the universal constant C is 1.7.

4. Next, use Eq. (10) to determine ν_H.

5. Now try running the simulation with these parameters by typing `xtriad3d` at the command line prompt. Random initial conditions corresponding to a statistical-mechanical equipartition will be used by default. If you select the dynamic time-stepping option, you will not have to worry about calculating an optimal value for the time step. Just pick some small value like 10^{-6} as a starting time step; the dynamic time-stepping mechanism will then quickly determine the best value. The various graphs and movies may be viewed even while `triad` is running [the numbers in square brackets periodically displayed by `triad` correspond to 100 time steps or the movie sampling interval (if nonzero), whichever is less]. In the graph of the evolution of $E = \sum_{\mathbf{k}} E_{\mathbf{k}}$. The blue dotted line in the energy spectrum graph indicates the initial energy spectrum.