Small post processor

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1. Clear complete workspace

For new Matlab projects best practise is to clear the complete workspace and the command window. It is also a good habit to close all remaining figures since Matlab does not automatically open a new window each time a plot call is invoked.

The above mentioned clears are performed in the function ClearWs. In addition some basic parameters like the name of the data directory or the dimensionality of the problem are also defined.

2. Read data files

During the evaluation of the function ReadData all data files neseccary for the calculation of the spectrum and the correlation coefficients are read, namely the velocity components. In addition the import operations are enclosed in a tic;...; toc block measuring the time needed for reading the ASCII data. What you should get from the tic/toc block is that most of the time is spend during data I/O (Input/Output operations), nearly 220s. The actual computation needs only about 8s. What you can easily calculate from this is that the computation of the spectrum is nearly 27 times faster then the data import. Why the computation of Fourier transforms is that fast we will come to that later. Although the ASCII data format ist not the prefered choice in terms of speed and size, we will use it since other methodologies require additional knowledge of data processing. Just for your information a very famous and highly protable data format is hdf5. It is a software library that runs on a range of computational platforms, from laptops to massively parallel systems and implements a high-level API (Application programming interface) with C, C++, Fortran 90, and Java interfaces. Besides its hierarchical structure it is highly optimized for parallel I/O operations and can be read by nearly all data processing tools.

```
1 display('Read data ...')
  [uvel, vvel, wvel, time_read] = ReadData(datadir, flag, 'uvel',
      'vvel', 'wvel');
3 % test=importdata('data/3D/CFX_velocity_field.dat');
4 % uvel=reshape(test(:,1),33,33,33);
 % vvel=reshape(test(:,2),33,33,33);
  % wvel=reshape(test(:,3),33,33,33);
  function [uvel, vvel, wvel, time] = ReadData(datadir, flag, . . .
2
                                               u_name, ...
                                               v_name, ...
3
                                               w_name)
      tic; % enable timer
      uvel=importdata([datadir,'/',flag,'/',u_name]);
6
      vvel=importdata([datadir,'/',flag,'/',v_name]);
      wvel=importdata([datadir,'/',flag,'/',w_name]);
8
      time = toc; % end timer
9
10 end
```

3. Set necessary parameters

For further computations it is important to define some parmeters of the DNS simulation such as

- Number of grid points in on direction n_p ,
- Physical length of one direction L_x ,
- Physical grid spacing $\triangle x$,
- Kinematic viscosity ν .

```
1 display('Set parameters ...')
2 [u,v,w,dim,Lx,dx,nu]=Params(uvel,vvel,wvel);
3 \% u=u-mean2(u);
4 % v=v-mean2(v);
5 % w=w-mean2(w);
function [u, v, w, dim, Lx, dx, nu] = Params (uvel, vvel, wvel)
       dim=385; % number of points in one dimension
      Lx = 0.4;
4
       dim=33;
        Lx=3.2e-2; % domain size
      Ly=Lx;
6
      Lz=Lx;
      dx=Lx/(dim-1); % grid spacing
      dy=dx;
      dz=dx;
10
      nu=1.7e-5; % viscosity
      u=reshape(uvel,dim,dim,dim); % reshape arrays to have
          them in 3D
      v=reshape(vvel, dim, dim, dim);
      w=reshape(wvel, dim, dim, dim);
14
       clear uvel vvel wvel
15
16 end
```

4. Compute 3D spectrum

The core of the code is contained in the function PowerSpec. It computes the three dimensional energy spectrum from the given velocity fields, obtained from a direct numerical simulation. Although the theoretical analysis is relatively demanding compared to one dimensional spectra its worth investing the effort. The theory of one dimensional spectra relies on the assumption that the propagation of spectral waves (κ_1) is in the direction of the observed velocity fields or to say it differently one dimensional spectra and correlation functions are Fourier transform pairs. The theory of correlation functions will be discussed in section 7. A key drawback of this theory is that the calculated spectrum has contributions from all wavenumbers κ , so that the magnitude of κ can be appreciably larger than κ_1 . This phenomenon is called aliasing. In order to avoid these aliasing effects is also possible to produce correlations that involve all possible directions. The three dimensional Fourier transformation of such a correlation produces a spectrum that not only depends on a single wavenumber but on the wavenumber vector κ_i . Though the directional information contained in κ_i eliminates the aliasing problem the complexity makes a physical reasoning impossible. For homogeneous isotropic turbulence the situation can be considerably simplified. From the knowledge that the velocity field is isotropic it can be shown that the velocity spectrum tensor is fully determined by

$$\Phi_{ij}(\kappa) = A(\kappa)\delta_{ij} + B(\kappa)\kappa_i\kappa_j, \tag{1}$$

where $A(\kappa)$ and $B(\kappa)$ are arbitrary scalar functions. Since we assume incompressible fluids (mathematically expressed by $\nabla \cdot u = 0$ or $\kappa_i u_i = 0$ the following condition holds

$$\kappa_i \, \Phi_{ij}(\boldsymbol{\kappa}) = 0. \tag{2}$$

It can be shown that this yields a relation between A and B by means of

$$B(\kappa) = -\frac{A(\kappa)}{\kappa^2} \tag{3}$$

In the end this gives a relation between the three dimensional energy spectrum function $E(|\kappa|)$ and the velocity spectrum tensor Φ_{ij} .

$$\Phi_{ij} = \frac{E(|\boldsymbol{\kappa}|)}{4\pi (|\boldsymbol{\kappa}|)^2} \left(\delta_{ij} - \frac{\kappa_i \kappa_j}{(|\boldsymbol{\kappa}|)^2} \right)$$
(4)

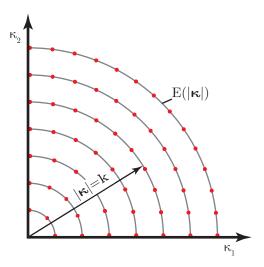


Fig. 1: Illustration of the two dimensional shell integration

The question is now how the remaining variable (A or B) can be determined. Regarding the turbulent kinetic energy we know that

$$k = \int_{-\infty}^{\infty} E(|\boldsymbol{\kappa}|) \, dk = \sum_{\boldsymbol{\kappa}} E(\boldsymbol{\kappa}) = \sum_{\boldsymbol{\kappa}} \frac{1}{2} \langle u^*(\boldsymbol{\kappa}) \, u(\boldsymbol{\kappa}) \rangle = \iiint_{-\infty}^{\infty} \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}) \, d\boldsymbol{\kappa}. \quad (5)$$

Comparing the second and last expression we get

$$E(|\boldsymbol{\kappa}|) = \iint \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}) \, dS(\kappa). \tag{6}$$

This integral can be solved analytically by utilizing again the assumption of isotropy. For these kind of flows the energy spectrum function can be regarded as the sum of kinetic energy (in wave number space) on different energy levels. Each of these energy levels is denoted by a spherical shell in wave number space. Since the surface of a sphere is completly determined by its radius the surface integral can be solved analytically. The idea of this integration is illustrated in Fig. 1. As a result of this one gets

$$E(|\boldsymbol{\kappa}|) = \iint \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}) \, dS(\kappa) = 4\pi (|\boldsymbol{\kappa}|)^2 \, \Phi_{ii}(|\boldsymbol{\kappa}|). \tag{7}$$

Introducing this relation to equations (1) and (3) one arrives at an expression for the variable B.

$$B = -\frac{E(|\kappa|)}{4\pi(|\kappa|)^2} \tag{8}$$

Together with the approximation of the integral of Φ (equation (5))

$$\iiint_{-\infty}^{\infty} \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}) \, d\boldsymbol{\kappa} \approx \frac{1}{2} \sum_{\boldsymbol{\kappa}} \Phi_{ii}(\boldsymbol{\kappa}) \, (\Delta \kappa)^3, \tag{9}$$

where $\Delta \kappa$ refers to the step size in wave number space, the final expression of the three dimensional discrete energy spectrum can be derived.

$$E(|\kappa|) = 2\pi (|\kappa|)^2 \frac{\langle u^*(\kappa) u(\kappa) \rangle}{(\Delta \kappa)^3}$$
 (10)

The calling sequence for the computation of the energy spectrum reads

```
1 display('Compute spectrum...')
  [spectrum, k, bin_counter, time_spec] = PowerSpec(u, v, w, Lx,
      dim);
  function [spectrum, k, bin_counter, time] = PowerSpec(u, v, w,
                                                          L, dim)
2
      tic;
3
       uu_fft=fftn(u);
       vv_fft=fftn(v);
       ww_fft=fftn(w);
       muu = abs(uu_fft)/length(u)^3;
      mvv = abs(vv_fft)/length(v)^3;
      mww = abs(ww_fft)/length(w)^3;
11
      muu = muu.^2;
12
      mvv = mvv.^2;
      mww = mww.^2;
14
15
       rx=[0:1:dim-1] - (dim-1)/2;
16
       ry=[0:1:dim-1] - (dim-1)/2;
```

```
rz=[0:1:dim-1] - (dim-1)/2;
18
19
       test_x=circshift(rx',[(dim+1)/2 1]);
20
       test_y=circshift(ry',[(dim+1)/2 1]);
       test_z=circshift(rz',[(dim+1)/2 1]);
22
       [X,Y,Z] = meshgrid(test_x,test_y,test_z);
24
       r=(sqrt(X.^2+Y.^2+Z.^2));
25
26
       dx=2*pi/L;
27
       k=[1:(dim-1)/2].*dx;
28
       spectrum=zeros(size(k,2),1);
29
       bin_counter=zeros(size(k,2),1);
30
       for N=2: (dim-1)/2-1
31
           picker = (r(:,:,:)*dx \le (k(N+1) + k(N))/2) & ...
                     (r(:,:,:)*dx > (k(N) + k(N-1))/2);
33
           spectrum(N) = sum(muu(picker)) + ...
34
                           sum (mvv (picker)) + . . .
35
36
                           sum (mww (picker));
           bin_counter(N) = size(find(picker==1),1);
37
       end
       % compute first value of spectrum
39
       picker = (r(:,:,:)*dx <= (k(2) + k(1))/2);
40
       spectrum(1) = sum(muu(picker))+...
41
                      sum (mvv (picker)) + . . .
                      sum (mww (picker));
43
       bin_counter(1) = size(find(picker==1),1);
44
       % compute last value of spectrum
45
       picker = (r(:,:,:)*dx > (k(end) + k(end-1))/2 \& ...
46
                  r(:,:,:)*dx <= k(end));
47
       spectrum(end) = sum(muu(picker))+...
48
                        sum (mvv (picker)) + . . .
49
                        sum (mww (picker));
50
       bin_counter(end) = size(find(picker==1),1);
51
       %compute final spectrum
52
       spectrum = spectrum*2*pi.*k'.^2./(bin_counter.*dx.^3);
54
       time=toc;
55
  end
```

5. Compute dissipation and turbulent kinetic energy

The function **SpecProp** calculates the kinetic energy both from the velocities and the previously computed spectrum. The latter one is calculated by

$$k = \int_{-\infty}^{\infty} E(|\boldsymbol{\kappa}|) \, \mathrm{d}|\boldsymbol{\kappa}| \tag{11}$$

A second integral, also evaluated in this routine, gives the value of the Dissipation

$$\epsilon = 2 \int_{-\infty}^{\infty} \nu(|\boldsymbol{\kappa}|)^2 E(|\boldsymbol{\kappa}|) \, \mathrm{d}|\boldsymbol{\kappa}|, \tag{12}$$

where ν refers to the kinematic viscosity. The calling sequence reads

6. Kolmogorov properties

According to the Kolomogorov hypotheses the length scale η , characteristic velocity u_{η} and the characteristic time scale τ of the smallest swirls in the flow are computed within the function **KolmoScale**. From a dimensionality

analysis Kolmogorov derived

$$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4},\tag{13}$$

$$u_{\eta} = (\epsilon \, \nu)^{1/4} \,, \tag{14}$$

$$u_{\eta} = (\epsilon \nu)^{1/4}, \qquad (14)$$

$$\tau_{\eta} = \left(\frac{\nu}{\epsilon}\right)^{1/2}. \qquad (15)$$

For further reading concerning his theory it is referred to Pope [1], Hinze [2] and Tennekes and Lumley [3].

```
1 display('Compute Kolmogorov scales...')
2 [eta, u_eta, tau] = KolmoScale (nu, Dissipation);
  function [eta, u_eta, tau] = KolmoScale (nu, Dissipation)
      eta = (nu^3/Dissipation)^(1/4);
      u_{eta} = (nu*Dissipation)^(1/4);
      tau = (nu/Dissipation)^(1/2);
  end
```

7. Compute correlations

From a general perspective correlation functions are a measure of how much two physical quantities are connected. So how is this helpful for the analysis of turbulent flows? For seemingly chaotic and random procescees it would be beneficial if we had a measure of how the velocity at point A is influenced by the velocity at point B. A maybe more intuitive quantity that can be calculated from the correlation functions is the integral lengthscale which gives a measure of the largest eddies in the flow. In fluid dynamics one generally differentiates between two forms of correlation functions, the longitudinal and the transversal or lateral correlation function. The difference between both forms is illustrated in figure 2. In general the correlation between two components of an isotropic homogeneous velocity field is expressed by

$$R_{ij} = \langle u_i(\mathbf{x} + r) \, u_j(\mathbf{x}) \rangle \,. \tag{16}$$

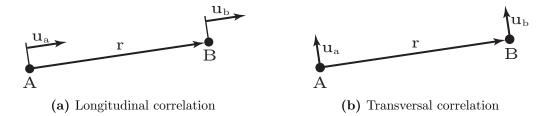


Fig. 2: Illustration of different correlation functions

The correlation coefficients are computed by normalizing R_{ij} with the square root of the product of the two variances σ_i^2 and σ_i^2 .

$$r_{ij} = \frac{\langle u_i(\mathbf{x} + \mathbf{r}) u_j(\mathbf{x}) \rangle}{\sqrt{\sigma_i^2 \sigma_j^2}}$$
(17)

As illustrated in figure 2 the longitudinal and lateral correlation depend on the direction of \mathbf{r} , i.e.

$$f(r) = \frac{\langle u_1(\mathbf{x} + r\mathbf{e}_1) u_1(\mathbf{x}) \rangle}{\sigma_1}$$

$$g(r) = \frac{\langle u_2(\mathbf{x} + r\mathbf{e}_1) u_2(\mathbf{x}) \rangle}{\sigma_2}$$
(18)

$$g(r) = \frac{\langle u_2(\mathbf{x} + r\mathbf{e}_1) u_2(\mathbf{x}) \rangle}{\sigma_2}$$
 (19)

From several theoretical analysis it is well known that correlations can be efficiently computed by means of multiplying the Fourier transform of a quantity with its complex conjugate. Using the FFT approach this gives an enormeous speed advantage.

$$R_{ij} = \mathfrak{F}^{-1} \left\{ \mathfrak{F} \left\{ u_i \right\}^* \cdot \mathfrak{F} \left\{ u_i \right\} \right\} \tag{20}$$

```
1 display('Compute Correlations...')
2 [R11,R22,r,R1,R2,R3]=Correlation(u,v,w,Lx,dim);
```

The content of Correlation reads

```
function [R11, R22, r, R1, R2, R3] = Correlation (u, v, w, Lx, dim)
     scaling = 1;
```

```
NFFT = 2. nextpow2 (size(u)); %power of 2 fitting
          length of u
       u_fft=fftn(u,NFFT)./scaling;
4
       NFFT = 2.^nextpow2(size(v));
       v_fft=fftn(v,NFFT)./scaling;
       NFFT = 2.^nextpow2(size(w));
       w_fft=fftn(w,NFFT)./scaling;
       Rij_x=(u_fft.*conj(u_fft)); % compute velo.
10
          correlation tensor
       Rij_y=(v_fft.*conj(v_fft));
11
       Rij_z=(w_fft.*conj(w_fft));
12
       % x-component
14
       NFFT = 2.^nextpow2(size(u_fft));
       R1=ifftn(Rij_x,NFFT)/std2(u)^2/dim^3;
16
17
       % y-component
18
       NFFT = 2.^nextpow2(size(v_fft));
       R2=ifftn(Rij_y,NFFT)/std2(v)^2./dim^3;
20
       % z-component
       NFFT = 2.^nextpow2(size(w_fft));
22
       R3=ifftn(Rij_z,NFFT)/std2(w)^2./dim^3;
24
       R11 = (reshape(R3(1,1,:),NFFT(1),1)+R2(1,:,1)'+R1
          (:,1,1))/3;
       R11 = R11(1:size(u_fft)/2+1);
26
       R1_22 = (R1(1,:,1) + R3(1,:,1))/2;
28
       R2_22 = (R2(:,1,1)+R3(:,1,1))/2;
       R3_22 = (reshape(R1(1,1,:), size(u_fft,1),1)+...
30
                reshape(R2(1,1,:),size(u_fft,1),1))/2;
31
32
      R22 = (R1_22' + R2_22 + R3_22)/3;
       R22 = R22(1:size(u_fft)/2+1);
34
       r = linspace(0, Lx/2, size(u_fft, 1)/2+1)/(Lx/2);
36
  end
```

References

- [1] S. B. Pope, Turbulent Flows, Cambridge University Press, 1 edition, 2000.
- [2] J. O. Hinze, Turbulence, Mcgraw-Hill College, 2 edition, 1975.

[3] H. Tennekes, J. L. Lumley, A first course in turbulence, The MIT Press, 1972.

8. Plotting

```
display('Save results...')
close all
comte=importdata('Comte-Bellot.txt');
kC=comte.data(:,1).*100;
EC=comte.data(:,2)./100^3;
kp=importdata('data/3D/CTRL_TURB_ENERGY');
h=loglog(vkp(:,1),vkp(:,3),'*-b');hold on
set(h,'LineWidth',1);
h=loglog(k,spectrum,'r-s');
set(h,'LineWidth',1);
h=loglog(kC,EC,'*-g');
set(h,'LineWidth',1);
legend('VKP','Dietzsch','Comte-Bellot')
saveas(gcf,'spectrum.eps','psc2')
```