Spectral Simulation of Turbulence

and Tracking of Small Particles

Homogeneous Turbulence

- Statistical (time average) properties (RMS velocity fluctuations, dissipation rate) are independent of position.
- Homogeneous turbulence can be modeled with randomly stirred turbulence in a cubic periodic box.
- The turbulence in a periodic box is homogeneous, but not isotropic. (Diagonals and edges are different.)

Navier-Stokes Equation with Random Stirring Force

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p / \rho + \mathbf{f} + \upsilon \nabla^2 \mathbf{u}$$

Periodic Cubic Box

$$\mathbf{u}(x + mL, y + nL, z + pL) = \mathbf{u}(x, y, z)$$

The velocity is a periodic function of x, y, and z with period L.

Time Discretization – "Time Splitting"

- Each time step involves three sub-steps.
- First sub-step: the non-linear term is computed explicitly.
- Second sub-step: the pressure term is computed implicitly.
- Third sub-step: the viscous term is computed implicitly.

Rotational Form of Navier-Stokes Equation

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{u} \times \boldsymbol{\omega} - \nabla \Pi + \mathbf{f} + \nu \nabla^2 \mathbf{u}$$

$$\boldsymbol{\omega} = \nabla \times \mathbf{u}$$

$$\Pi = \frac{p}{\rho} + \frac{1}{2} u^2$$

First Fractional Step

$$\tilde{\mathbf{u}} = \mathbf{u}_{\mathrm{p}} + (\mathbf{u}_{\mathrm{p}} \times \boldsymbol{\omega}_{\mathrm{p}} + \mathbf{f}_{\mathrm{p}})\Delta t$$

p is the time step

Second Fractional Step

$$\hat{\mathbf{u}} = \tilde{\mathbf{u}} - (\nabla \Pi)\Delta t$$

$$\nabla^2 \Pi = \nabla \cdot \tilde{\mathbf{u}} / \Delta t$$

Third Fractional Step

$$\mathbf{u}_{p+1} = \hat{\mathbf{u}} + \upsilon \nabla^2 \mathbf{u}_{p+1}$$

Fourier Representation of the velocity and pressure fields

- We represent the velocity and pressure fields by three-dimensional Fourier series.
- Since Fourier series are periodic, the velocity and pressure fields are periodic.
- Calculations with the velocity and pressure are in “physical space”. Calculations with the Fourier coefficients are in “spectral space”

Three-Dimensional Fourier Series

$$\mathbf{u}(x,y,z,t)=\sum_{l=-(N/2)}^{(N/2)-1}\sum_{m=-(N/2)}^{(N/2)-1}\sum_{n=-(N/2)}^{(N/2)-1}\mathbf{U}(l,m,n,t)e^{2\pi i(lx+my+nz)/L}$$

$$\Pi(x,y,z,t)=\sum_{l=-(N/2)}^{(N/2)-1}\sum_{m=-(N/2)}^{(N/2)-1}\sum_{n=-(N/2)}^{(N/2)-1}P(l,m,n,t)e^{2\pi i(lx+my+nz)/L}$$

$$N=2^q$$

Fast Fourier Transform

- FFT = Fast Fourier Transform, Cooley & Tookey (1966)
- If a Fourier series involving N terms is computed directly, the number of operations is proportional to N^2
- With the FFT algorithm, the number of operations is proportional to $N \log_2 N$

Procedure for Calculating the Velocity and Pressure

- The first fractional step is performed with the velocity field on a 3D grid with N^3 points (physical space).
- The Fourier coefficients of the pressure are computed in spectral space.
- The Fourier coefficients of the velocity are computed in spectral space.

FFT's Needed for Each Time Step

- At the end of a time step, we have the Fourier coefficients of the velocity. Therefore, we need a 3D FFT to compute the velocity and vorticity for the first fractional step of the next time step.
- After computing the first intermediate velocity field (the "~" field), do an inverse 3D FFT to obtain the Fourier coefficients.

Pressure Step

$$\hat{\mathbf{u}} = \tilde{\mathbf{u}} - (\nabla\Pi)\Delta t$$

$$\nabla^2\Pi = \nabla \cdot \tilde{\mathbf{u}} / \Delta t \equiv g$$

In spectral space:

$$\hat{U}(l,m,n,t) = \tilde{U}(l,m,n,t) - \frac{2\pi i}{L} P(l,m,n,t)\Delta t$$

$$-\frac{4\pi^2}{L^2}(l^2 + m^2 + p^2)P(l,m,n,t) = G(l,m,n,t)$$

Viscous Step

$$\mathbf{u}_{p+1} = \hat{\mathbf{u}} + \upsilon \nabla^2 \mathbf{u}_{p+1}$$

In spectral space.

$$\mathbf{U}_{p+1}(l,m,n,t) = \hat{\mathbf{U}}(l,m,n,t) - \upsilon \Delta t \left(\frac{4\pi^2}{L^2}\right)(l^2 + m^2 + n^2)\mathbf{U}_{p+1}$$

Channel Flow-Inhomogeneous Turbulence

- Pressure driven flow between two flat, infinite, parallel plates.
- Let us assume that the flow is in the *x*-direction and that the walls are located at $z=h$ and $z=-h$.
- Assume that the flow is periodic in *x* and *y* and use Fourier series in those directions, but use a **Chebyshev** series in z.

Chebyshev Polynomials

- The convergence of Chebyshev series is independent of the boundary conditions, unlike Fourier series, because Chebyshev polynomials are solutions of a singular Sturm-Liouville problem.
- We can still use FFT methods for Chebyshev series.

Chebyshev Polynomials

$$T_n(z/h) = \cos(n\theta)$$

$$\theta = \cos^{-1}(\frac{z}{h})$$

Spectral Representation for Channel Flow

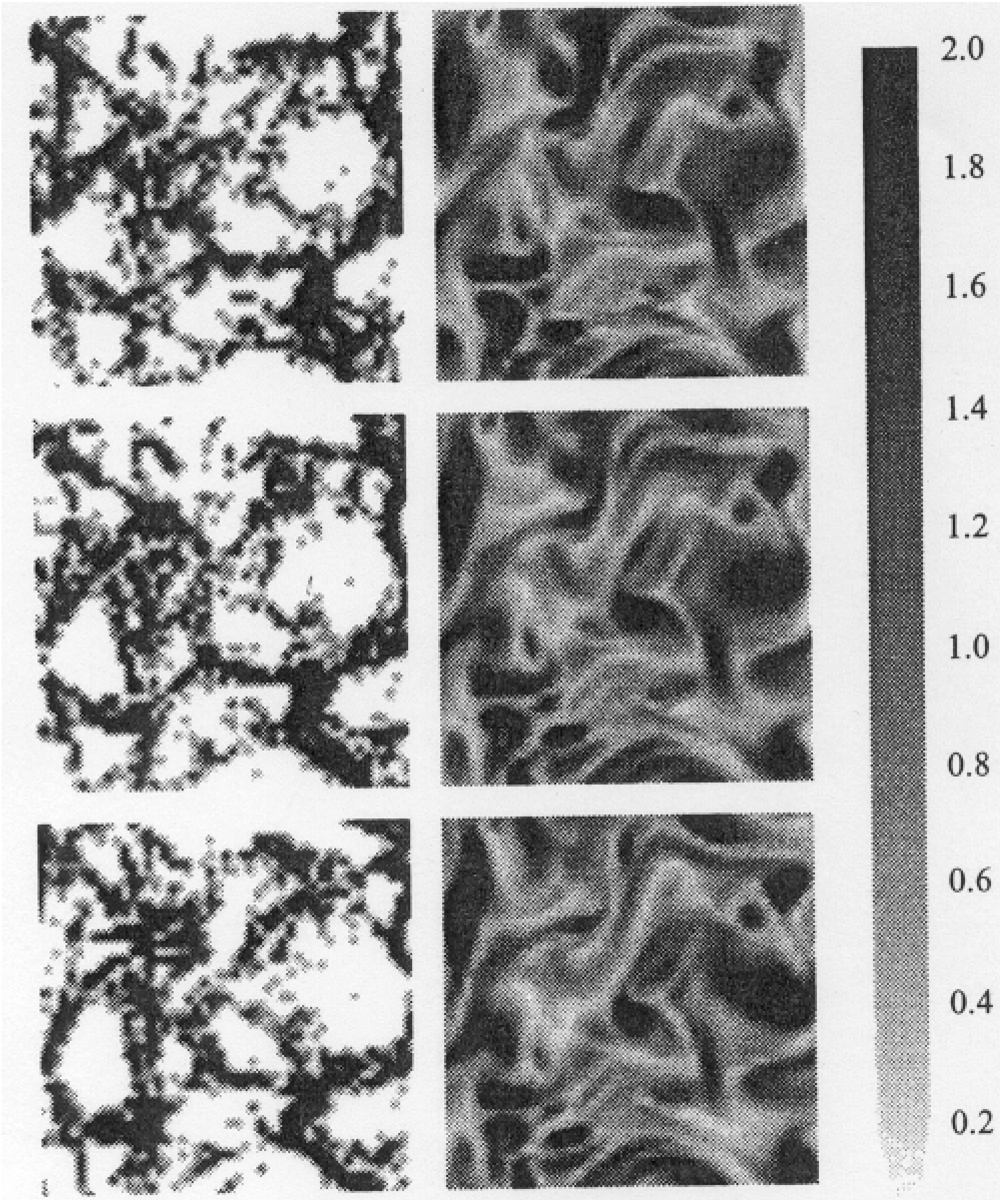
$$\mathbf{u}(x,y,z,t) = \sum_{l=-(N/2)}^{(N/2)-1} \sum_{m=-(N/2)}^{(N/2)-1} \sum_{n=0}^{N} \mathbf{U}(l,m,n,t) e^{2\pi i (lx+my)/L} T_n(z/h)$$

$$\Pi(x,y,z,t) = \sum_{l=-(N/2)}^{(N/2)-1} \sum_{m=-(N/2)}^{(N/2)-1} \sum_{n=0}^{N} P(l,m,n,t) e^{2\pi i (lx+my)/L} T_n(z/h)$$

$$N = 2^q$$

Tracking of Small Particles

- Low concentrations of small particles have little effect on the underlying flow: “one-way coupling”
- To track a particle, we need to know the forces acting on it.
- We solve 6 ODE’s in time for each particle’s coordinates and velocity components.



The particles may be seen on the left and the magnitude of the fluid vorticity is shown on the right. The particles are centrifuged out of regions of high vorticity into regions of low vorticity.

Equation of Motion for Small, Spherical Particles

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\tau}(\mathbf{v} - \mathbf{u}) - g\mathbf{k}$$

$$\tau = (\frac{\mathbf{9}}{\mathbf{2}})(\frac{\rho_f}{\rho_p})(\frac{a^2}{\upsilon})C_c$$

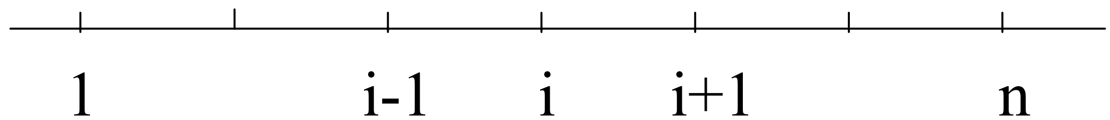
Cunningham Correction Factor

- The Cunningham factor, C_c, depends on the molecular mean-free path and the diameter of the particle
- Under normal conditions, the Cunningham factor is close to unity for aerosols that are larger than 1 micron.

Calculation of Aerosol Trajectories

- To compute the trajectory of an aerosol particle, we need to solve 6 simultaneous ODE's for the coordinates and velocity components of the particle.
- Since the drag force involves the fluid velocity at the location of the particle, it is necessary to interpolate the fluid velocity on the closest grid points.

Hermite Interpolation in 1D



$$f(x) = f_i H_1(\xi) + f_{i+1} H_2(\xi) + f_i^{'} G_1(\xi) + f_{i+1}^{'} G_2(\xi)$$

$$\xi = \frac{x - x_i}{h}$$

$$H_1(\xi) = (1 - \xi)^2 (1 + 2\xi)$$

$$H_2(\xi) = \xi^2 (3 - 2\xi)$$

$$G_1(\xi) = (1 - \xi)^2 \xi h$$

$$G_2(\xi) = (\xi - 1)\xi^2 h$$

Accuracy

- The grid spacing is denoted by h on the previous slide.
- The error involved in the interpolation of the function *f* is $O(h^4)$.
- Note that the interpolation reduces to the correct values for the function **and** its first derivatives at the ends of the grid interval.

Two or Three-Dimensional Hermite Interpolation

- In 2D, one needs the values of the function, the first derivatives of the function, and the second mixed derivative of the function at the four neighboring points (16 numbers).
- In 3D, the third mixed derivative is used. A total of 64 numbers are needed.

Advantages of Hermite Interpolation

- Hermite interpolation has the advantage that it avoids discontinuities as a particle crosses the (artificial) boundaries between grid cells.
- In two-dimensions, one needs to know the velocity components, their first derivatives, and their second mixed derivative at the 4 closest grid points.