DNS of Turbulent Flow with Particle Tracking

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Outline

- Definitions of DNS and LES
- Background on turbulence
- DNS techniques
- Pseudospectral method
- Aerosol particle motion
- Homogeneous turbulence
- Turbulent channel flow

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Definitions

- Direct Numerical Simulation (DNS): solution of the continuity and Navier-Stokes equation without modeling.
- Large Eddy Simulation (LES): approximate solution of the continuity and Navier-Stokes equation on a "coarse grid" with some modeling.

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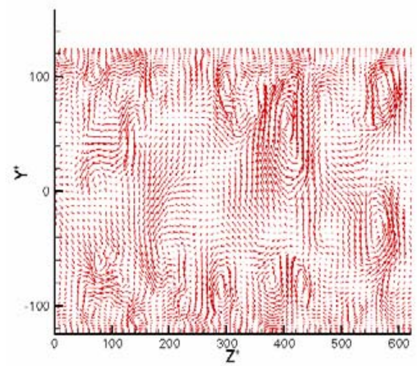
Turbulent channel flow (mean flow into page)



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Characteristics of turbulent flow

- Velocity at each point is time-dependent
- Flow contains "eddies" that form and disappear continually
- Large range of length scales
- Large range of time scales
- Good at mixing chemicals, heat, momentum
- Re>>1

Computer time for DNS

$$CPU\ time \propto Re^3 = (Re^{3/4})^3 (Re^{3/4})$$

We must resolve he smallest eddies
and the shortest time scales.

Numerical Solution of PDE's

- The solutions are computed at a discrete set of times. This is called "time discretization".
- The dependent variables are computed on "grid points". This is called "spatial discretization." For DNS, the distance between grid points should be smaller than the smallest eddies.

Example: Unsteady Thermal Conduction

- Governing equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

where α is the thermal diffusivity

Time Discretization

$$\frac{\partial T}{\partial t} = \frac{T(x,t_{n+1}) - T(x,t_n)}{\Delta t}$$

$$T(x,t_{n+1}) = T(x,t_n) + (\alpha \Delta t)\frac{\partial^2 T}{\partial x^2}$$

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Low Order Explicit Methods

Euler forward

$$\frac{\partial^2 T}{\partial x^2} = \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n} + O(\Delta t)$$

Adams - Bashforth

$$\frac{\partial^2 T}{\partial x^2} = \frac{3}{2}\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n} - \frac{1}{2}\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n-1}} + O(\Delta t^2)$$

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Low Order Implicit Methods

Euler backward

$$\frac{\partial^2 T}{\partial x^2} = \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n+1}} + O(\Delta t)$$

Crank - Nicolson

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}\left(\left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_{n+1}} + \left.\frac{\partial^2 T}{\partial x^2}\right|_{t=t_n}\right) + O(\Delta t^2)$$

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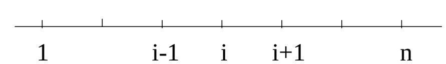
Spatial Discretization: 1D Uniform Grid.



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Central Difference Approximation

$$\frac{\partial T}{\partial x} = \frac{T_{i+1} - T_{i-1}}{2\Delta x} + O(\Delta x^2)$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta x^2} + O(\Delta x^2)$$

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Discretized Equation

$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^{n+1} + T_{i-1}^{n+1} - 2T_i^{n+1}\right)$$

"Tridiagonal" system of linear algebraic equations subject to boundary conditions at i=1 and i=N. Solve with Thomas algorithm.

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Numerical Stability

The tridiagonal system is implicit so it is stable for all values of the time step and grid spacing. The only restriction is accuracy.

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Fluid Mechanics

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

$$\nabla \cdot \mathbf{u} = 0$$

Navier-Stokes and continuity equations.

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Time Discretization

The time discretization is the same as for the 1-D temperature equation.

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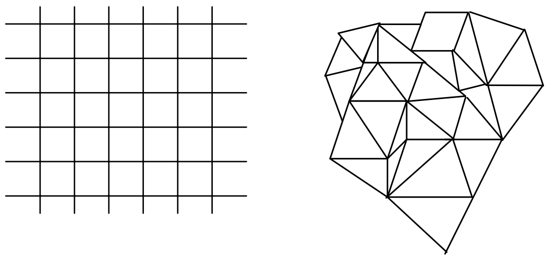
Spatial Discretization (2D)



Structured grid   Unstructured grid

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Structured Grids

- Each point can be labeled by a pair (2D) or a triplet (3D) of integers without ambiguity.
- Usually, structured grids are used with Cartesian or “body-fitted” curvilinear coordinate systems and the grid points lie on coordinate curves.

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Methods for Single Phase DNS

- Finite difference
- Finite volume
- **Pseudospectral**
- Finite element (boundary element, spectral element)
- Lattice Boltzmann

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Pseudospectral Method

- Easy to formulate discretized equations.
- Exponential spatial convergence (less resolution is needed than for FDM or others).
- Limited to very simple geometries (periodic box, channel flow between infinite flat walls).

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DNS of turbulent flows with particles

- Let us consider turbulent flows with solid or fluid particles in gases or liquids.
- For spherical particles that are smaller than the "Kolmogorov length", there are approximate equations of motion for the particles.
- In the "dilute" regime, small suspended particles have no "feedback" on the flow.

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One-way Coupling Regime

- "One-way coupling" means that the suspended particles have no effect on the flow of the fluid.
- For aerosol particles, this condition may be expressed by requiring that the mass loading of the particles is very small compared to unity.

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Aerosol Mass Loading

$$m_l = \phi \frac{\rho_p}{\rho_g} \qquad \frac{\rho_p}{\rho_g} = O(10^3)$$

where φ is the volume fraction,
ρ_p is the particle density,
ρ_g is the gas density.

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Particle Equation of Motion for Small Spherical Particles

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{F}}{m}$$

The force includes the drag, lift, gravitational, and Brownian forces.

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Particle position vector

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}$$

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$$

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Particle Tracking

- We solve Newton's law and the equation for the particle position vector as a set of 6 (in 3D) ODE's in time.
- Since the particles do not lie on grid points at any given time, it is necessary to use interpolation methods to compute the fluid velocity at the location of a particle.

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Interpolation Methods

- Trilinear (simple, but introduces discontinuities at grid "cell" boundaries.)
- Legendre (more accurate, although discontinuities still exist).
- Hermite (complicated, but no discontinuities).

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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.)

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Navier-Stokes Equation with Random Stirring Force

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

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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.

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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.

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Rotational Form of Navier-Stokes Equation

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

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

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

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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

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Second Fractional Step

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

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

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Third Fractional Step

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

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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"

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Three-Dimensional Fourier Series

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

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

$$N=2^q$$

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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 $N\log_2 N$

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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.

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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.

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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:

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

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

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Viscous Step

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

In spectral space.

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

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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.

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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.

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Chebyshev Polynomials

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

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

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Spectral Representation for Channel Flow

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

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

$$N = 2^q$$

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Aerosol Particle Trajectories in Homogeneous Turbulence

- The particles are initially randomly seeded in the flow.
- Since the particles have inertia, they are centrifuged out of regions of high vorticity.
- The particles have a higher average sedimentation velocity once they are no longer “trapped” in regions of high vorticity.

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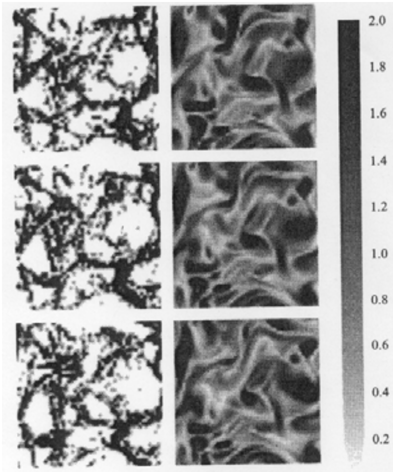


The particles may be seen on the left and the magnitude of the fluid vorticity is shown on the right. The particles are centrifuged out of regions of high vorticity into regions of low vorticity.

Equation of Motion for Small, Spherical Particles

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

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

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

1 i-1 i i+1 n

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

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

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

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

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

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

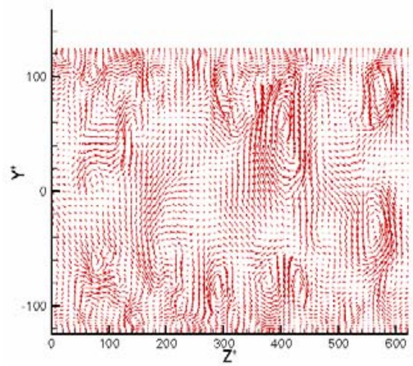
Accuracy

- 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.

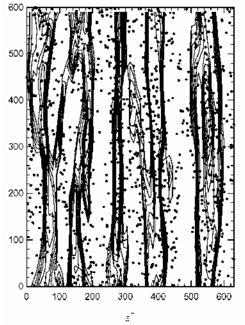
Aerosol Trajectories in a DNS of Turbulent Channel Flow

- The aerosols are randomly seeded initially.
- The channel flow is vertical so that gravity cannot directly cause deposition.
- As time proceeds, particles collect near the walls because of "turbophoresis".
- In the near wall region, particles collect in "low speed streaks."

Turbulent Channel Flow



Aerosol Particles Accumulate in Low Speed Streaks



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References for DNS

- Orszag, S.A. & Patterson, G.S. 1972. Physical Review Letters **28**, 76-79.
- Kim, J. Moin, P., & Moser, R. 1972. Journal of Fluid Mechanics **177**, 133-166.
- Lyons, S.L., Hanratty, T.J., & McLaughlin, J.B. 1991. International Journal for Numerical Methods in Fluids **13**, 999-1028.

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References for Particle-Tracking

- Yeung, P.K. & Pope, S.B. 1988. Journal of Computational Physics **79**, 373-416.
- Balachandar, S. & Maxey, M.R. 1989. Journal of Computational Physics **83**, 96-125.
- McLaughlin, J.B. 1994. International Journal of Multiphase Flow **20**, 211-232.

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