LES of Turbulent Flows: Lecture 4

Dr. Jeremy A. Gibbs

Department of Mechanical Engineering University of Utah

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1 One last review of turbulence (beat it into your heads)

2 Numerical simulations

3 Equations of motion



- Unsteadiness: $u = f(\vec{x}, t)$
- Three-dimensional: $\vec{x} = f(x_i)$ for any turbulent flow
- High vorticity: $\omega = \nabla \times \vec{u}$
- Mixing effect: turbulence acts to reduce gradients
- Continuous spectrum of scales: energy cascade described broadly by Kolmogorov's hypotheses



Review: Kolmogorov's similarity hypothesis

Kolmogorov's 1^{st} hypothesis

- Smallests scales receive energy at a rate proportional to the dissipation of energy rate
- With this, he defined the Kolmogorov (dissipation) scales:

length scale

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

time scale

$$\tau = \left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}}$$

velocity scale

$$v = \frac{\eta}{\nu} = (\nu \epsilon)^{\frac{1}{4}}$$



Review: Kolmogorov's similarity hypothesis

• Using these scales, we can define the ratios of the largest to smallest scales:





Kolmogorov's 2nd hypothesis

- In turbulent flow, a range of scales exists at very high Re where statistics of motion in a range l ($\ell_o \gg \ell \gg \eta$) have a universal form that is determined only by ϵ (dissipation) and independent of ν (kinematic viscosity).
- Kolmogorov formed his hypothesis and examined it by looking at the PDF of velocity increments Δu .



Review: Kolmogorov's similarity hypothesis

- We can examine this through E(k), where $E(k)dk = \mathsf{TKE}$ contained between k and k + dk.
- What are the implications of Kolmogorov's hypothesis for E(k)? K41 \Rightarrow $E(k) = f(k,\epsilon)$
- By dimensional analysis, Kolmogorov showed:

$$E(K) = c_k \epsilon^{2/3} k^{-5/3}$$

Kolmogorov's -5/3 power law.



Review: Kolmogorov's similarity hypothesis



- We now have a description of turbulence and the range of energy containing scales (the dynamic range) in turbulence.
- In computational fluid dynamics (CFD), we need to discretize the equations of motion using either difference approximations (finite differences) or as a finite number of basis functions (e.g., Fourier transforms).
- Essentially, a continuous solution is approximated by a finite set of values corresponding as closely as possible with the values of the solution on a grid of discrete positions in space.



- To capture all of the dynamics (degrees of freedom) in a turbulent flow, we must consider the required amount of discrete values needed for an accurate approximation.
- We need a grid fine enough to capture the smallest *and* the largest scales of motion (η and ℓ_o).



- From K41, we know that $\ell_o/\eta \sim \text{Re}^{3/4}$ and there exists a continuous range of scales between η and ℓ_o .
- We will assume that we need n grid points per increment η.
 Note that n can vary, but a value of 3 to 5 is often suggested.
- Thus, in each direction, the number of required grid points is

$$N_i = \frac{\ell_o}{(\eta/n)} = n \ \frac{\ell_o}{\eta} \sim n \ \mathrm{Re}^{3/4}$$

 Remember that turbulence is 3D, so the total number of grid points needed to accurately estimate the flow is

$$N = \left(n \operatorname{Re}^{3/4}\right)^3 = \boxed{n^3 \operatorname{Re}^{9/4}}$$



• Let's revisit our example of a typical atmospheric boundary layer flow:

$$U_o \sim 10 \text{ m s}^{-1}, \ \ell_o \sim 10^3 \text{ m}, \ \nu \sim 10^{-5} \text{ m}^2 \text{ s}^{-1}$$

which gives us,

$$\mathsf{Re} = \frac{U_o \ell_o}{\nu} \sim \frac{(10 \text{ m s}^{-1})(10^3 \text{ m})}{10^{-5} \text{ m}^2 \text{ s}^{-1}} \sim 10^9$$

• thus, the number of grid points required to fully resolve this flow (assuming n = 3) is

$$N = 9 \times (10^9)^{9/4} \sim 1.6 \times 10^{21} \dots \dots \dots$$

Note: current capabilities of modern computing allow for grid sizes with $\mathcal{O}(10^{11})$ points.



• What does a simulation of a typical atmospheric boundary layer flow using a grid with 1.6×10^{21} points buy? (recall $\eta \sim 0.18$ mm)

$$l_i = \eta * (1.6 \times 10^{21})^{1/3} \sim 2 \text{ km}$$

This means we can simulate a $2~{\rm km}\times 2~{\rm km}\times 2~{\rm km}$ cube. Think how big the atmosphere is and then be depressed.



- When will we be able to directly simulate all the scales of motion in a turbulent flow?
- A couple of studies used historical data from the literature to build a model that predicts this question (see Voller and Porté-Agel, 2002 and Bou-Zeid, 2014 handouts).
- VP02 derived a model based on Moore's Law

$$P = A \ 2^{0.6667 \text{Y}}$$

where A is the computer power at reference year Y=0.



- VP02 used a reference year of 1980 and used A = 100 and A = 10,000.
- The best fit was

$$N(t) = 691 \times 2^{0.697({\rm year}-1980)}$$





TABLE II

Expected Year (\pm 5) That the Given Direct Simulation Will Be Possible

If Grid Size Increases Are Bound by Eq. (2)

| Simulation | Domain length scale | Resolution length scale | Grid points required | Expected year (±5 years) |
|----------------|---------------------|-------------------------|----------------------|--------------------------|
| 2-D casting | 0.1 m | 1 μm (dendrite tip) | 1010 | 2015 |
| 2-D casting | 1 m | 1 µm (dendrite tip) | 10 ¹² | 2025 |
| 3-D casting | 0.1 m | 1 µm (dendrite tip) | 1015 | 2040 |
| Boundary layer | 100 m | 1 mm | 1015 | 2040 |
| 2-D casting | 0.1 m | 1 nm (lattice space) | 1016 | 2045 |
| 3-D casting | 1 m | 1 μm (dendrite tip) | 1018 | 2055 |
| 2-D casting | 1 m | 1 nm (lattice space) | 1018 | 2055 |
| Boundary layer | 1 km | 1 mm | 1018 | 2055 |
| Boundary layer | 10 km | 1 mm | 10 ²¹ | 2070 |
| 3-D casting | 0.1 m | 1 nm (lattice space) | 1024 | 2085 |
| 3-D casting | 1 m | 1 nm (lattice space) | 10 ²⁷ | 2100 |



 BZ14 updated VP02 using data between 2002 and 2014. It turns out that VP02 was too optimistic. Be more depressed.





- The Re of relevant flows are orders of magnitude too large for current computational resources.
- Thus, DNS will not be a suitable tool for a long time (relevant to our brief time on Earth).
- The only alternative is to simplify the description of a flow and try to model the small scales instead of resolving them.
- This makes the problem less demanding computationally, but harder in many aspects due to the modeling requirement.
- Before we delve into methods that accomplish this reduction of complexity, we need to understand how we describe a flow.



- Turbulent flow (and fluid dynamics in general) can be mathematically described by the Navier-Stokes equations (see Bachelor, 1967 for a derivation, see also Pope chapter 2).
- The primary goal of CFD (and LES) is to solve the discretized equations of motion.
- We use the continuum hypothesis (*i.e.*, $\eta \gg$ mean free path of molecules) so that

$$u_i = u_i(x_j, t)$$
 and $\rho = \rho(x_j, t)$



Equations of motion: conservation of mass

• Conservation of mass

$$\left. \frac{dm}{dt} \right|_{sys} = 0$$

• We can use Reynolds Transport Theorem (RTT, see any fluids book)

$$\left.\frac{dm}{dt}\right|_{sys} = \frac{\partial}{\partial t} \underbrace{\int_{CV} \rho dV}_{\text{rate of increase in CV}} + \underbrace{\int_{CS} \rho \vec{V} \cdot d\vec{A}}_{\text{net flux leaving CV}} = 0$$

Another way of saying that: Production + Input = Change (in time) + Output (PICO).



• We can use Gauss's theorem and shrink the control volume to an infinitesimal size:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

This is the differential form of the conservation of mass.



Equations of motion: conservation of momentum

• Conservation of momentum (Newton's 2nd law)

$$\sum \vec{F} = \left. \frac{d(m\vec{V})}{dt} \right|_{sys}$$

We can again apply RTT and Gauss's theorem

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i \rho u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(2\mu S_{ij} - \frac{2}{3}\mu \delta_{ij} \frac{\partial u_i}{\partial x_i} \right) - \frac{\partial P}{\partial x_i} + \rho g_i$$

where

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

is the rate of strain (deformation) tensor.

This is the differential form of the conservation of momentum.



Equations of motion: conservation of energy

• Conservation of energy (1st law of thermodynamics)

$$\dot{Q} - \dot{W} = \left. \frac{dE}{dt} \right|_{sys}$$

If we use $e = c_v T$ (specific internal energy and $q_i = -K\partial T/\partial x_i$ (where c_v is the specific heat, T is temperature, and q_i is the thermal flux), then we arrive at

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x_i} \left[u_i(P+E) \right] = \\\rho \dot{q} + \frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_i} \left[u_j \left(2\mu S_{ij} - \frac{2}{3}\mu \delta_{ij} \frac{\partial u_i}{\partial x_i} \right) \right]$$

This is the differential form of the conservation of energy.



Let's consider incompressible flow (*i.e.*, the density of a fluid element does not change during its motion)

• Conservation of mass

$$\frac{\partial u_i}{\partial xi} = 0$$

i.e., divergence of the flow velocity is zero.

• Conservation of momentum

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + F_i$$



Let's consider incompressible flow (*i.e.*, the density of a fluid element does not change during its motion)

• Conservation of scalar (temperature, species, etc)

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_i \theta}{\partial x_j} = \nu_\theta \frac{\partial^2 \theta}{\partial x_j^2} + Q$$

where

$$u_{\theta} = rac{
u}{\mathsf{Sc}} = rac{
u}{\mathsf{Pr}}$$

and Sc is the Schmidt number (used for scalars) and Pr is the Prandtl number (used for temperature).



• Recall that

and

$$Sc = \frac{\nu}{D} = \frac{\text{viscous diffusion rate}}{\text{molecular diffusion rate}}$$
$$Pr = \frac{\nu}{\alpha} = \frac{\text{viscous diffusion rate}}{\text{thermal diffusion rate}}$$



Equations of motion: non-dimensional

- We can non-dimensionalize these equations by using a velocity scale (U_o) and length (ℓ_o) scale. For example, the free-stream velocity and the boundary layer depth.
- Conservation of mass

$$\frac{\partial u_i^*}{\partial x_i^*} = 0$$

• Conservation of momentum:

$$\frac{\partial u_i^*}{\partial t*} + \frac{\partial u_i^* u_j^*}{\partial x_j^*} = -\frac{\partial P^*}{\partial x_i^*} + \frac{1}{\operatorname{Re}} \frac{\partial^2 u_i^*}{\partial x_j^{*2}} + F_i^*$$

where Re is based on our velocity and length scales.



• For any general scalar

$$\frac{\partial \theta^*}{\partial t^*} + \frac{\partial u_i^* \theta^*}{\partial x_j^*} = \frac{1}{\operatorname{Sc}\,\operatorname{Re}} \frac{\partial^2 \theta^*}{\partial x_j^{*2}} + Q^*$$

generally, Sc ~ 1 and Pr ~ 0.72 (for air).



Properties of Navier-Stokes equations

- <u>Reynolds number similarity</u> for a range of Re, the equations of motion can be considered invariant to transformations of scale.
- Time and space invariance The equations are invariant to shifts in time or space, *i.e.*, we can define the shifted space variable

$$\hat{x} = \bar{x}/L$$
, where $\bar{x} = x - X$

- <u>Rotational and reflection invariance</u> The equations are invariant to rotations and reflections about a fixed axis.
- <u>Invariance to time reflections</u> The equations are invariant to reflections in time. They are the same going backward or forward in time.
- <u>Galilean invariance</u> The equations are invariant to constant velocity translations

$$\hat{x} = x - Vt$$



- As an example of using Reynolds number similarity to make DNS available.
- Recall our example of atmospheric scales that gave a Re of 10⁹? We cannot afford this, but if we change the viscosity ν from 10⁻⁵ to 1, then Re = 10⁴ which is doable.
- In fact, all dimensional scales match those of a typical laboratory experiment.
- We can use Reynolds number similarity to apply findings of our flow using the modified Re to that of a typical atmosphere.



Reynolds number similarity



Figure: Velocity from DNS of a low-level jet. (a) and (b) have different slope angles.



Reynolds number similarity



Figure: TKE from DNS of a low-level jet. (a) and (b) have different slope angles.

- You see that by changing the scaling, we still get results that seem to match the behavior of a flow with a larger Re.
- This is an example of using Reynolds number similarity.

