An introduction to Fluid-Thermo Dynamics modelling using an open-source CFD software

Dr. Najmeh Foroozani

Computational Studies and Molecular Dynamic Simulations workshop

University of Ibadan, Ibadan

April 2019

The lectures aims to convey the following information/message to the students:

♦ <u>Fluid Mechanics (FM) - Day 1</u>

→ Definition

→ Statistical descriptions

→ Equations of turbulent flows

♦ <u>Approaches to study fluid mechanics - Day 2</u>

→ Numerical *vs* Analytical *vs* Experimental

→ Numerical modeling (CFD)

♦ <u>Heat transfer</u> - Day 3

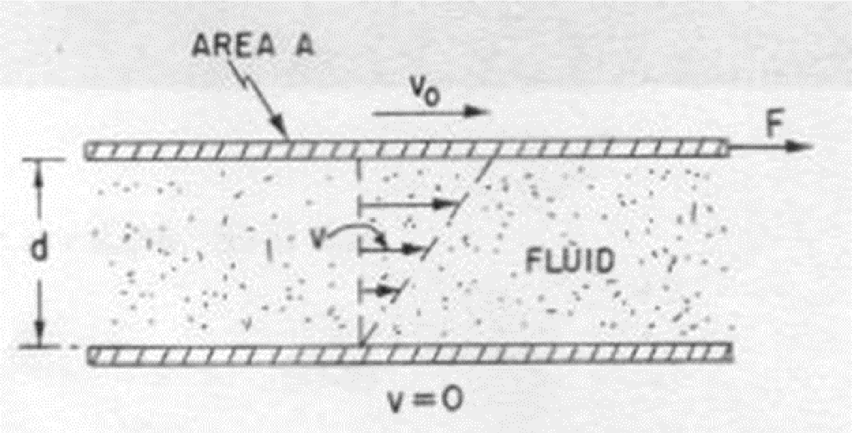
♦ Introduction to NEK5000 & Hands -on

Fluid Mechanics and the Governing Equations

What is a Fluid?

‘’**Fluid:** A substance that deforms continuously when acted on by a shearing stress of any size’’.

- If you apply a shearing force to a fluid it will move— the shear forces are described by the viscosity. Consider a layer of fluid between two plates, one stationary and one moving at a slow speed $v_{0.}$



shear stress $\tau = \frac{F}{A} = \mu \frac{\partial u}{\partial y}$ Newtonian fluid

Fluids

"A substance that deforms continuously when acted on by a shearing stress of any size".

Important characteristics of fluid, from a fluid mechanics point of view, are density (ρ), pressure (P),viscosity (μ), surface tension (τ) and compressibility.

Steady/Unsteady

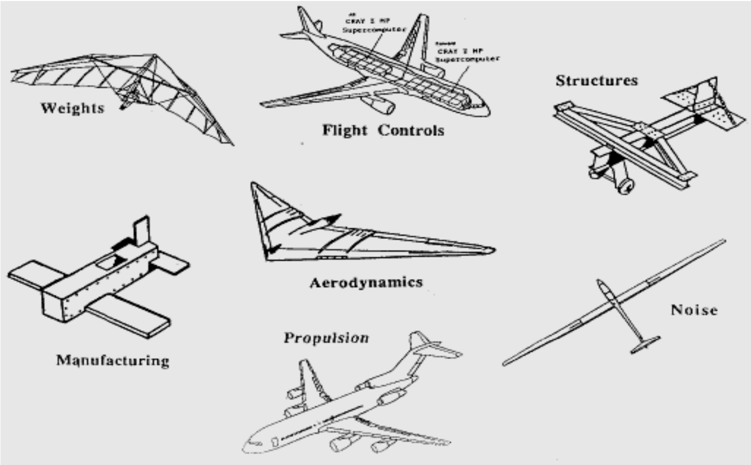
Uniform/non-Uniform

Laminar/Turbulent

Compressible/Incompressible

1, 3 and 3 Dimensional flow

Why is the study of FM important?



More examples…

Natural flows and weather
© Vol. 16/Photo Disc.

Boats
© Vol. 5/Photo Disc.

Aircraft and spacecraft
© Vol. 1/Photo Disc.

Power plants
© Vol. 57/Photo Disc.

Human body
© Vol. 110/Photo Disc.

Cars
Photo by John M. Cimbala.

Wind turbines
© Vol. 17/Photo Disc.

Piping and plumbing systems
Photo by John M. Cimbala.

Industrial applications
Courtesy UMDE Engineering, Contracting, and Trading. Used by permission.

Some application areas of fluid mechanics.

Ways to study FM

To study Fluid Mechanics…

Analytically

Solutions are available for only very few problems.

Experimentally

Combined with empirical correlations have traditionally been the main tool – an expensive one

Numerically

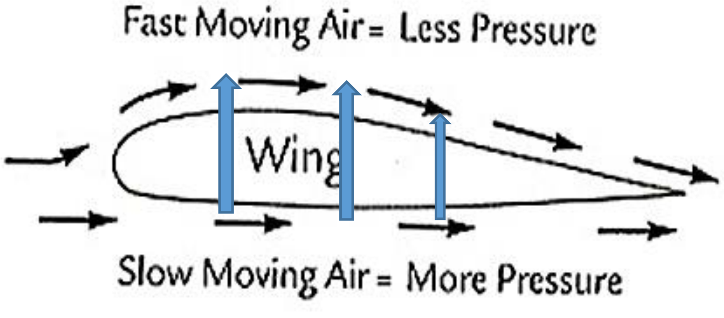
Potentially provides an unlimited power for solving any flow problems

Aerodynamics

Lift and wings

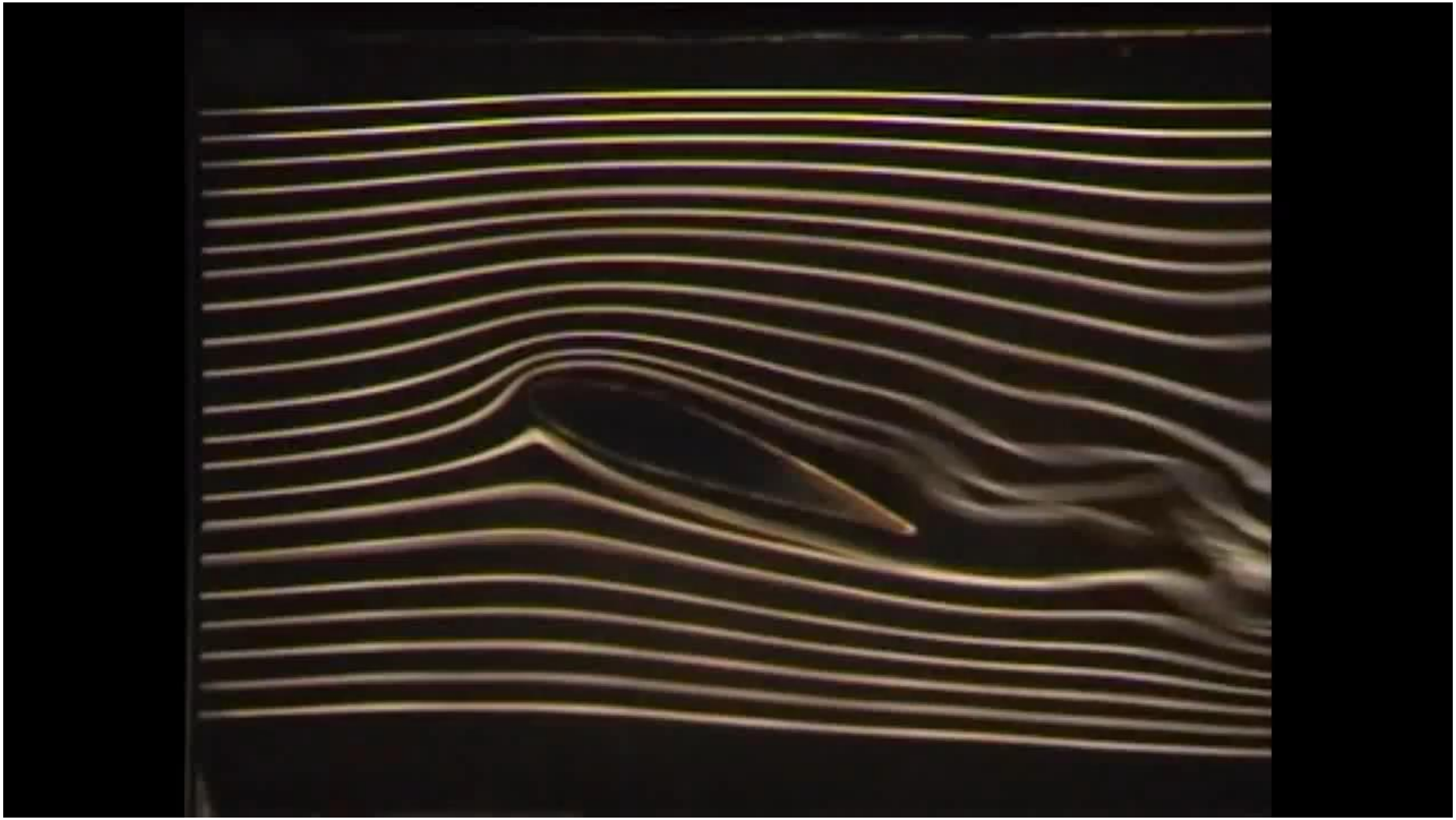
In order for an aircraft to rise into the air, a force must be created that equals or exceeds the force of gravity. This force is called lift. In heavier-than-air craft, lift is created by the flow of air over an airfoil. The shape of an airfoil causes air to flow faster on top than on bottom. The fast flowing air decreases the surrounding air pressure. Because the air pressure is greater below the airfoil than above, a resulting lift force is created

LIFT

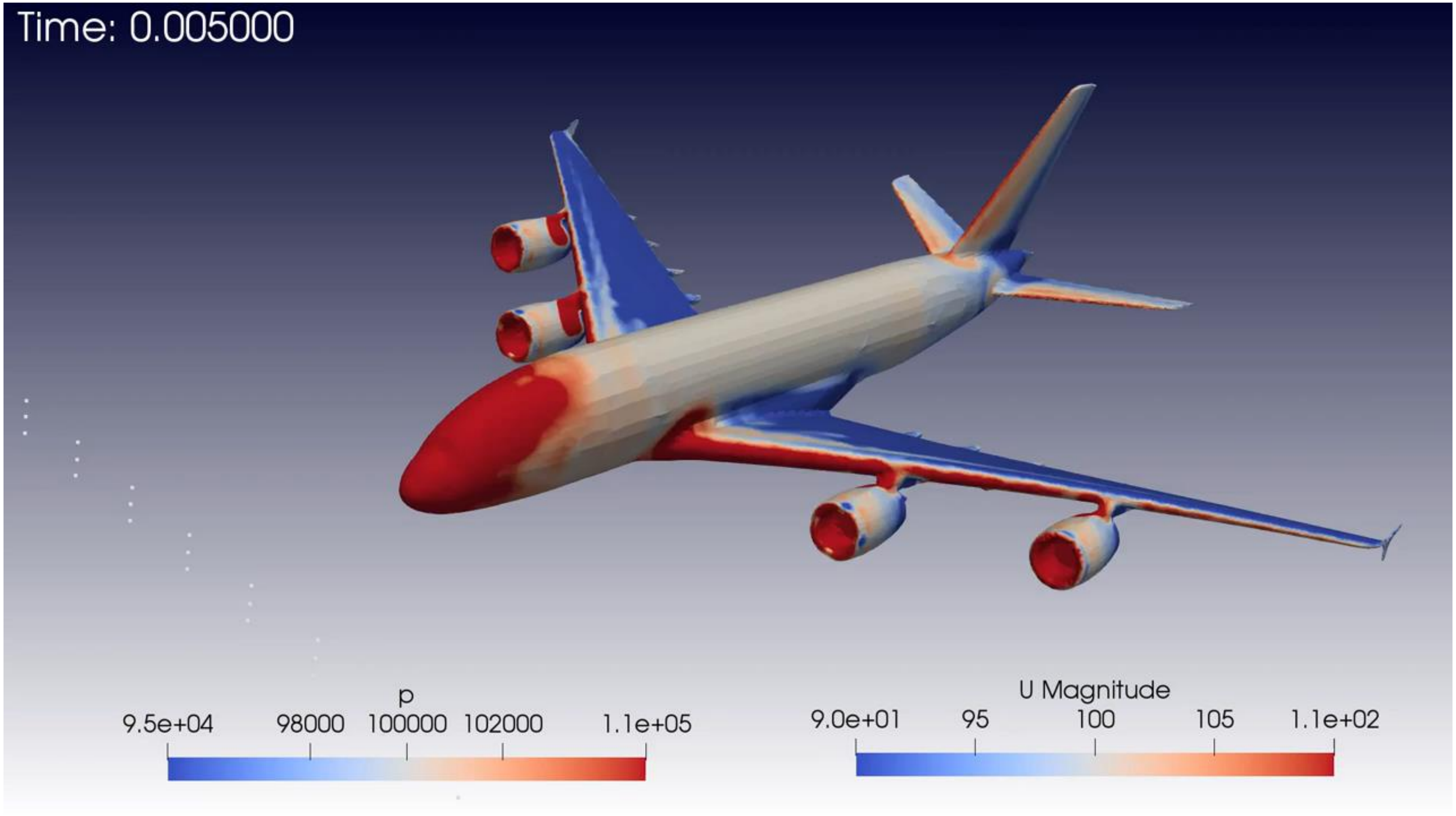


When a fluid is moving faster, it has lower pressure. This principle explains the lift created by an airplane's wing.

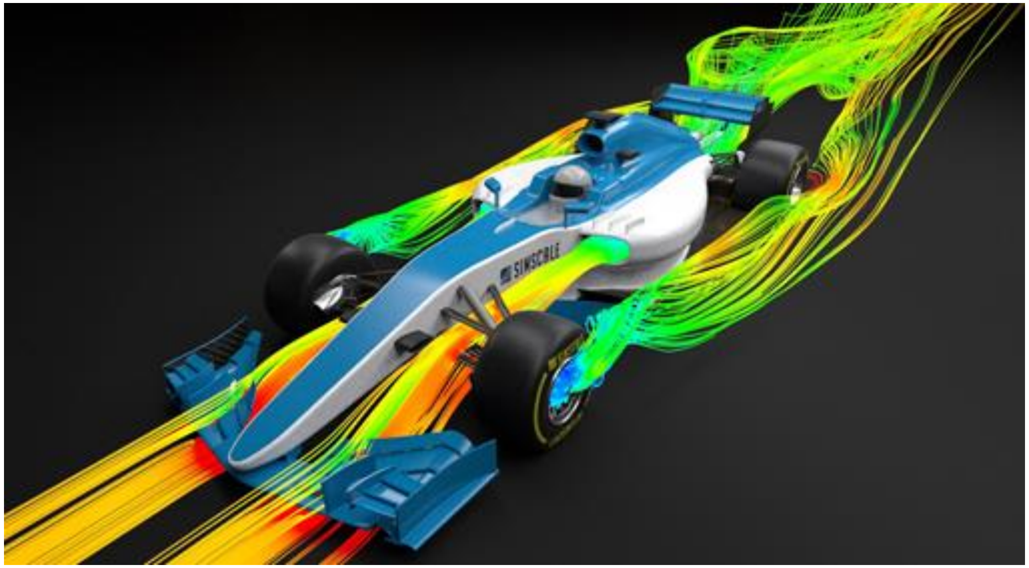
Airflow across a wing



EX1. Aircraft Simulation



EX2. Using CFD Simulations to Optimize Race Car Design



A race car's aerodynamic efficiency is driven by shape parameters such as angles, radius and dimensions. Engineers need to be able to refine the vehicle's shapes throughout the design process, and [Computational Fluid Dynamics (CFD) simulations] allow them to do just that.

Flow visualization

CFD *vs* Experiment

	Simulation(CFD)	Experiment
Cost	Cheap	Expensive
Time	Short	Long
Scale	Any	Small/Middle
Information	All	Measured Points
Repeatable	All	Some
Security	Safe	Some Dangerous

Disadvantage

1) Deals with a mathematical description not with reality
2) mathematical description can be inadequate
3) multiple solutions can exist
4) Enough spatial resolution to solve numerical equations

Validation of numerical modelling

Numerical modelling results always need validation. They can be:

- Compared with experiments
- Compared with analytical solutions
- Checked by intuition/common sense
- Compared with other codes (only for coding validation!)

Fundamental equations of motion;

➢ The fundamental equations of fluid dynamics are based on the following universal laws of conservation:

1) Conservation of mass
2) Conservation of momentum (Newton's 2nd law)
3) Conservation of energy

1) Physical principle: Mass is conserved

$$\frac{D\rho}{Dt} + \rho(\boldsymbol{\nabla}.\boldsymbol{u}) = 0,$$

A fluid is usually called incompressible if its density does not change with pressure

$$(\frac{D\rho}{Dt} = 0)$$

$$\nabla.\boldsymbol{u} = 0,$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

Whether or not the flow is steady.

Fundamental equations of motion;

u, v and w are the velocities in the x, y and z direction. ρ is the density, g is gravitational force, p pressure, μ is the viscosity

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=$$

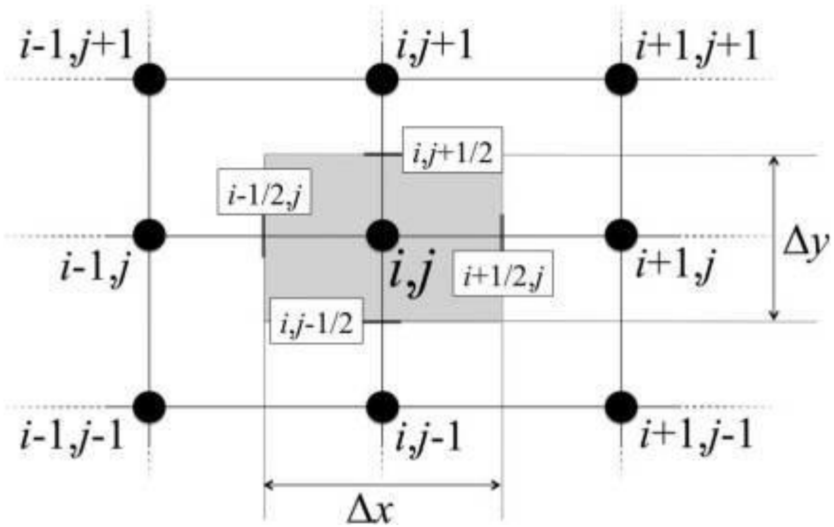
$$\rho g_x-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left[2\mu\frac{\partial u}{\partial x}+\lambda\nabla\cdot\mathbf{V}\right]+\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]+\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)\right]$$

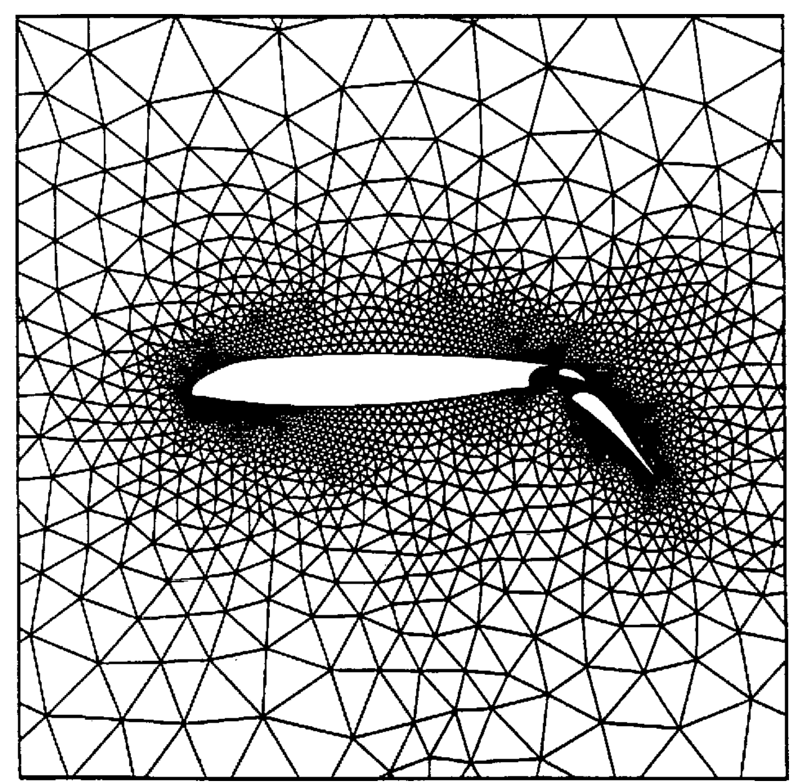
$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=$$

$$\rho g_y-\frac{\partial p}{\partial y}+\frac{\partial}{\partial y}\left[2\mu\frac{\partial v}{\partial y}+\lambda\nabla\cdot\mathbf{V}\right]+\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)\right]+\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]$$

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=$$

$$\rho g_z-\frac{\partial p}{\partial z}+\frac{\partial}{\partial z}\left[2\mu\frac{\partial w}{\partial z}+\lambda\nabla\cdot\mathbf{V}\right]+\frac{\partial}{\partial x}\left[\mu\left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)\right]+\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y}\right)\right]$$


i-1,j+1
i,j+1
i+1,j+1
i,j+1/2
i-1/2,j
Δy
i-1,j
i,j
i+1/2,j
i+1,j
i,j-1/2
i-1,j-1
i,j-1
i+1,j-1
Δx



Fundamentals of Boundary Layer

Boundary layer

- The boundary layer (BL) is a relatively thin layer of fluid close to the surface of a body that is immersed in a flow of fluid.

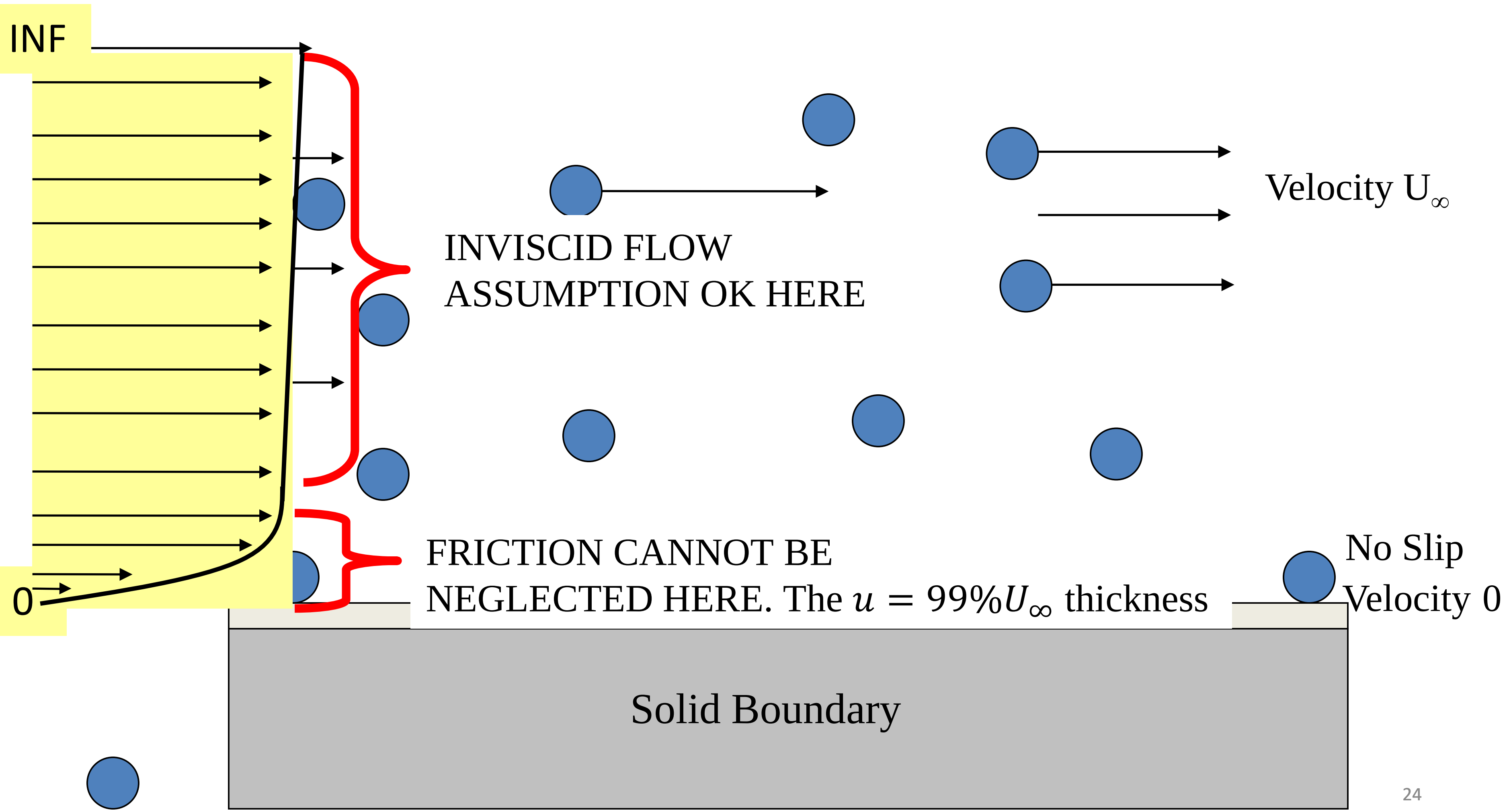
- The important thing to note is that within the boundary layer the effects of viscosity are important. Therefore even if the freestream may have a high Reynolds Number and therefore be considered inviscid, the same is not true inside the BL.

- The laminar boundary is a very smooth flow, while the turbulent boundary layer contains swirls or "eddies." The laminar flow creates less skin friction drag than the turbulent flow, but is less stable. Boundary layer flow over a wing surface begins as a smooth laminar flow. As the flow continues back from the leading edge, the laminar boundary layer increases in thickness.

Why viscosity is so important in fluid mechanics?

This so-called "**no-slip**" condition is a very important one that must be satisfied in any accurate analysis of fluid flow phenomena.

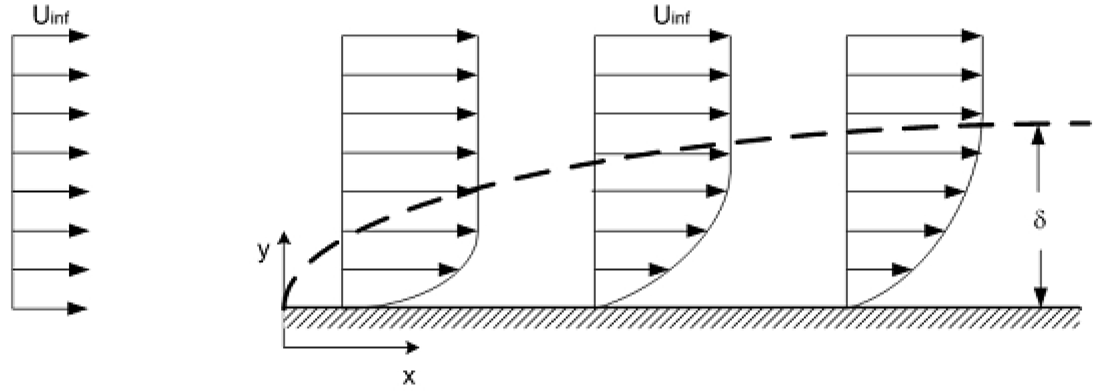
Boundary layer over a flat plate



Velocity Boundary Layer (BL)

Boundary Layer is a layer which is a boundary of two regions:

1. The near-wall region in which:
   - The flow is rotational
   - The Bernoulli's Equation fails
   - Viscous effect is important
2. Flow region far from body in which:
   - The flow is irrotational
   - The Bernoulli Eq. holds
   - Viscous effect is damped



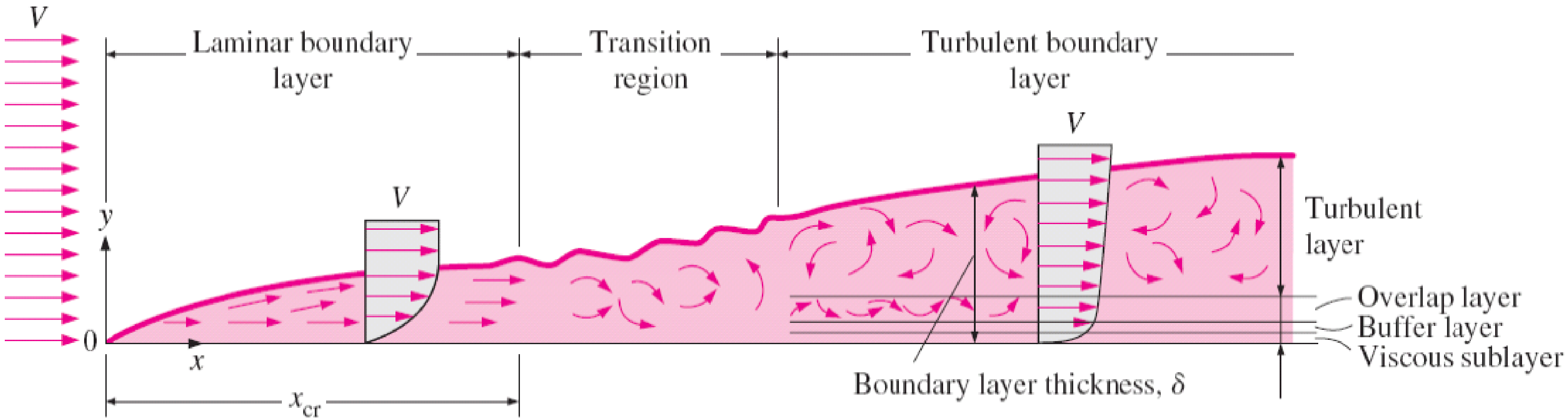
BL Flow regimes

- Similar to other viscous flows we have 3 flow regimes

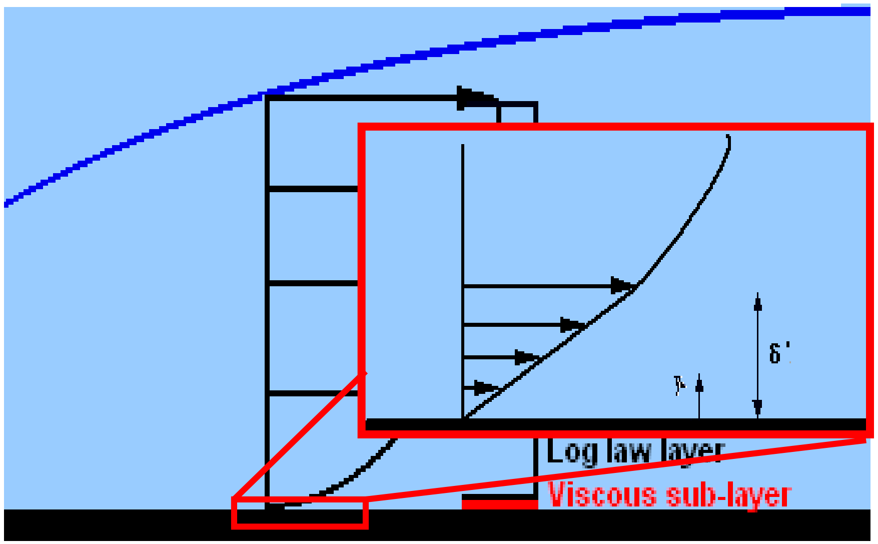
  Laminar: over starting point of the body

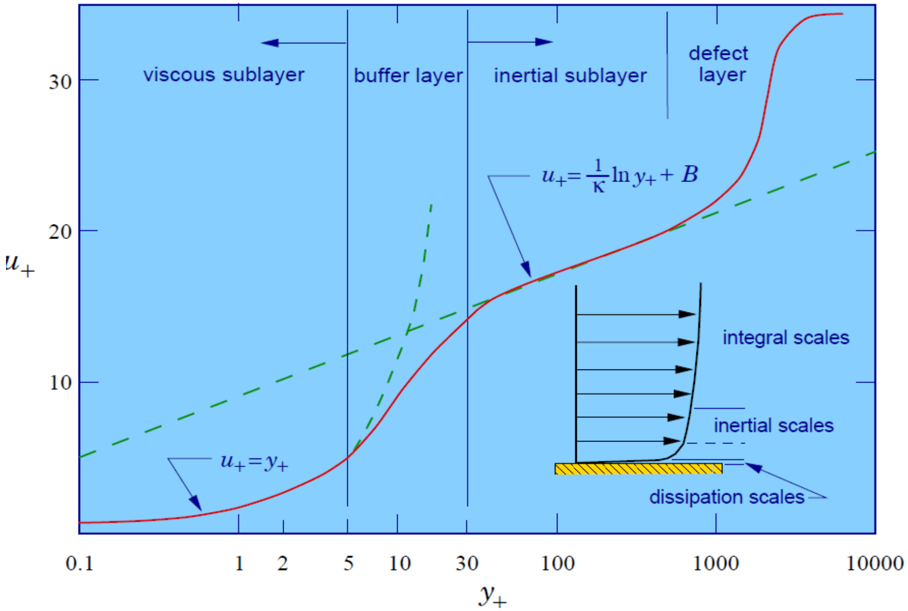
  Transition: mid-locations of the body

  Turbulent: ending parts of the body



The universal law of the wall





$y^+ = \frac{y u_\tau}{\nu}$ $\quad u^+ = \frac{u}{u_\tau}$ where

$u_\tau = \sqrt{\frac{\tau_{wall}}{\rho}}$

u^+: local velocity

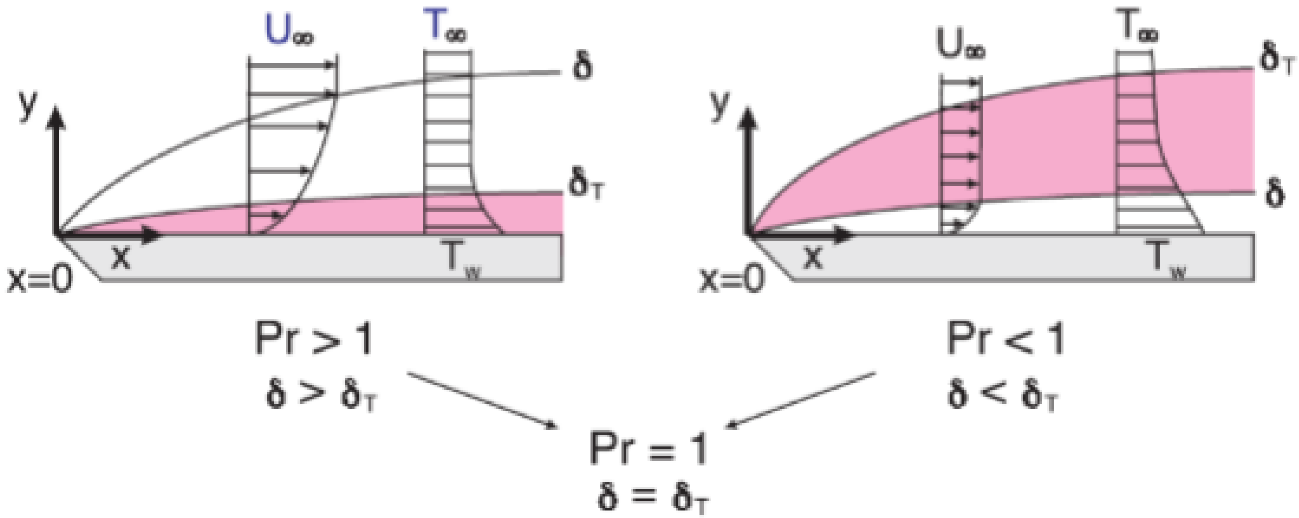
u_τ: friction velocity

τ_{wall}: wall shear stress

Dimensionless velocity profiles plotted in the near-wall coordinates. The linear section in the semi-log plot is called the **universal law of the wall layer**, or log law layer, for equilibrium turbulent boundary layers (TBL).

Thermal Boundary layer

If the surface and flow temperatures differ, there will be a region of the fluid through which the temperature varies from Ts at surface to T∞ in the outer flow. This region, called the thermal boundary layer, may be smaller, larger, or the same size as that through which the velocity varies.



Prandtl Number

- The relative thickness of the velocity and the thermal boundary layers is best described by the *dimensionless* parameter **Prandtl number**, defined as:

$$Pr = \frac{Molecular\ diffusivity\ of\ momentum}{Molecular\ diffusivity\ of\ heat} = \frac{\nu}{\kappa}$$

- Heat diffuses very quickly in liquid metals (Pr«1) and very slowly in oils (Pr»1) relative to momentum.

- Consequently the thermal boundary layer is much thicker for liquid metals and much thinner for oils relative to the velocity boundary layer.

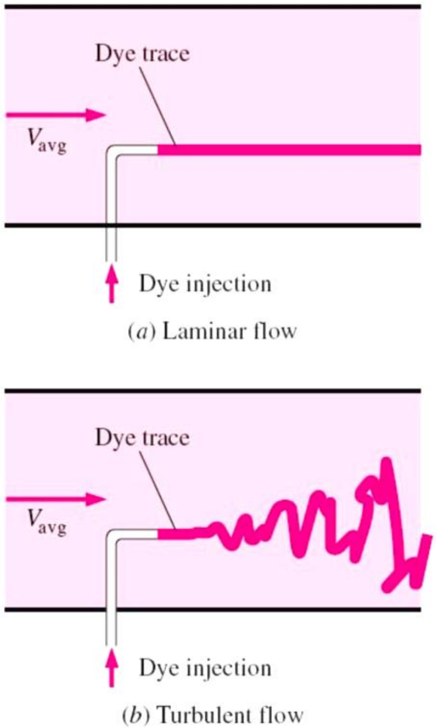
Some notes on turbulent flow

Laminar and turbulent flows

- Laminar flow — the flow is characterized by <u>*smooth streamlines*</u> and *highly-ordered motion.*

- Turbulent flow — the flow is characterized by *velocity fluctuations* and *highly-disordered motion.*

- The **transition** from laminar to turbulent flow does not occur suddenly.



(*a*) Laminar flow

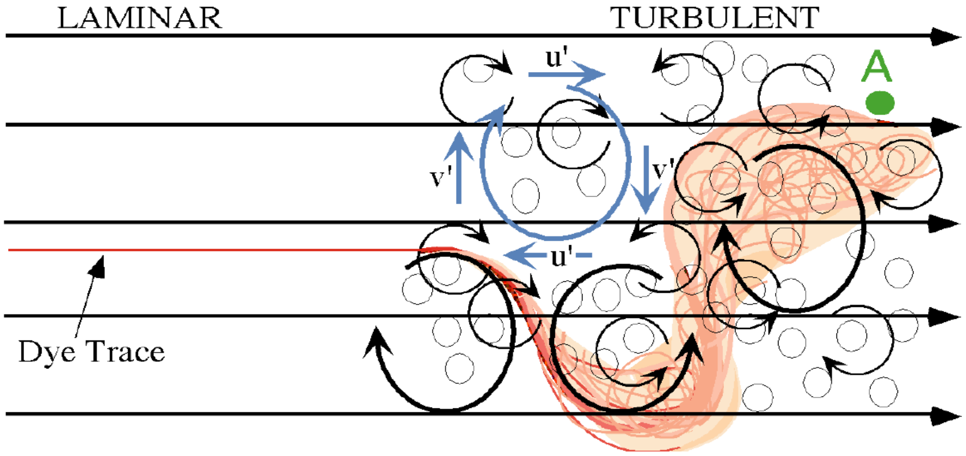
(*b*) Turbulent flow

Reynolds number (*Re*)

- This is not an universal definition of turbulent field, rather it is known from experiments and observations that a flow becomes turbulent when *"Re"* is large enough;

$$Re = \frac{inertia\ force}{viscous\ force}, \qquad Re = \frac{\rho U L}{\mu} = \frac{UL}{\nu}, \quad \text{where} \quad \upsilon = \frac{\mu}{\rho}$$

- U: typical inertial velocity scale of the flow
- L: typical inertial length scale of the flow
- ν: kinematic viscosity of the fluid
- μ: dynamic viscosity of the fluid
- ρ: density of the fluid



An example

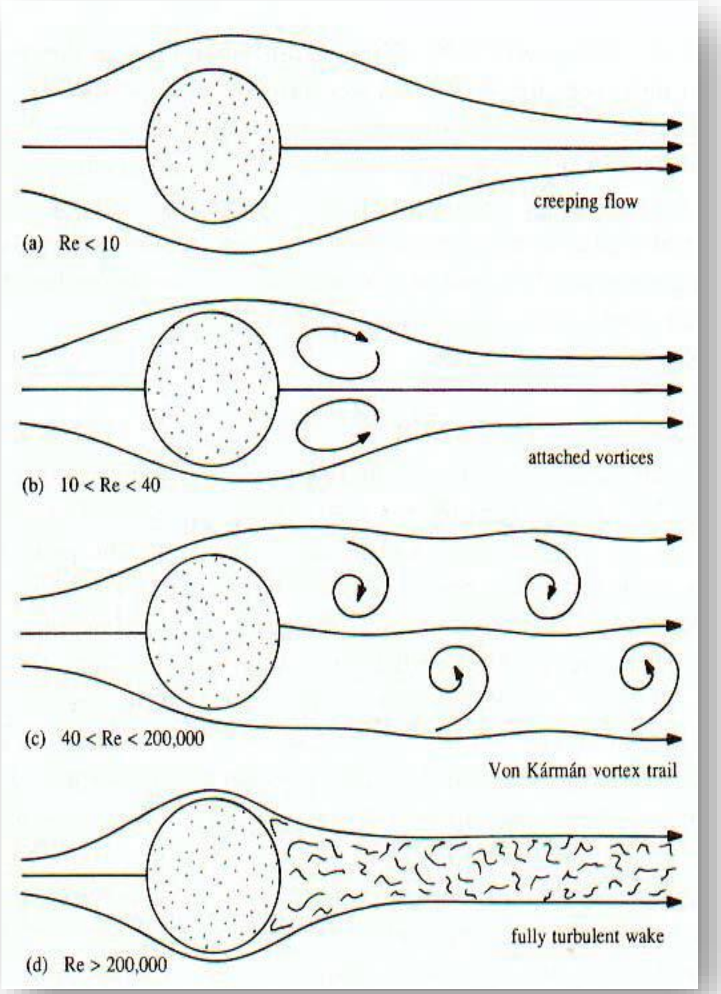
✓ The flow pattern around some an obstruction in the flow depends on the Reynolds Number, *Re*, and on the shape of an object. For a cylindrical obstruction, the following patterns are observed.

– At **low *Re*** (*Re* < 10) the flow is laminar and the streamlines are smooth.

– At **higher *Re*** (> 10), eddies start to develop, but the flow pattern is steady and not chaotic.

– At *Re* > 40, the eddies repeatedly grow and are shed periodically to form a "vortex street".

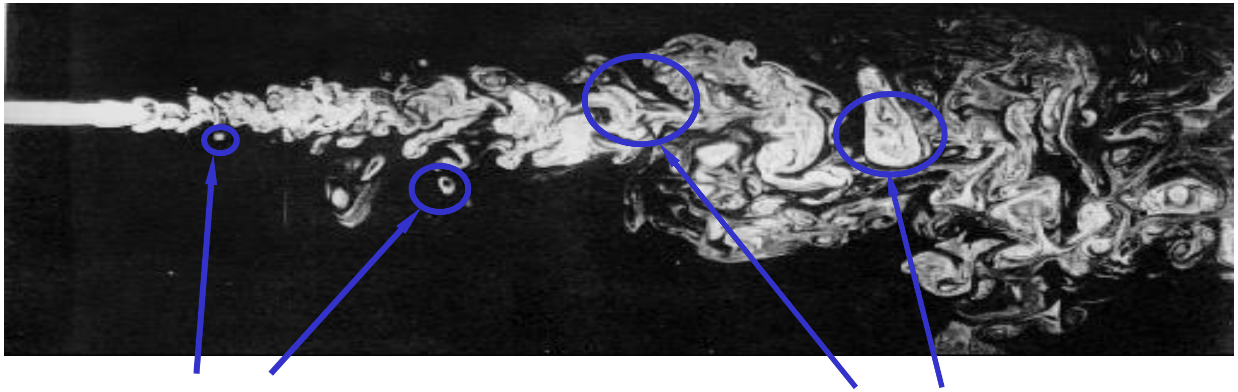
– Turbulence starts to develop at around *Re* ~ 1000, and the flow in the wake of the cylinder becomes more and more chaotic.



Flow pass a cylinder

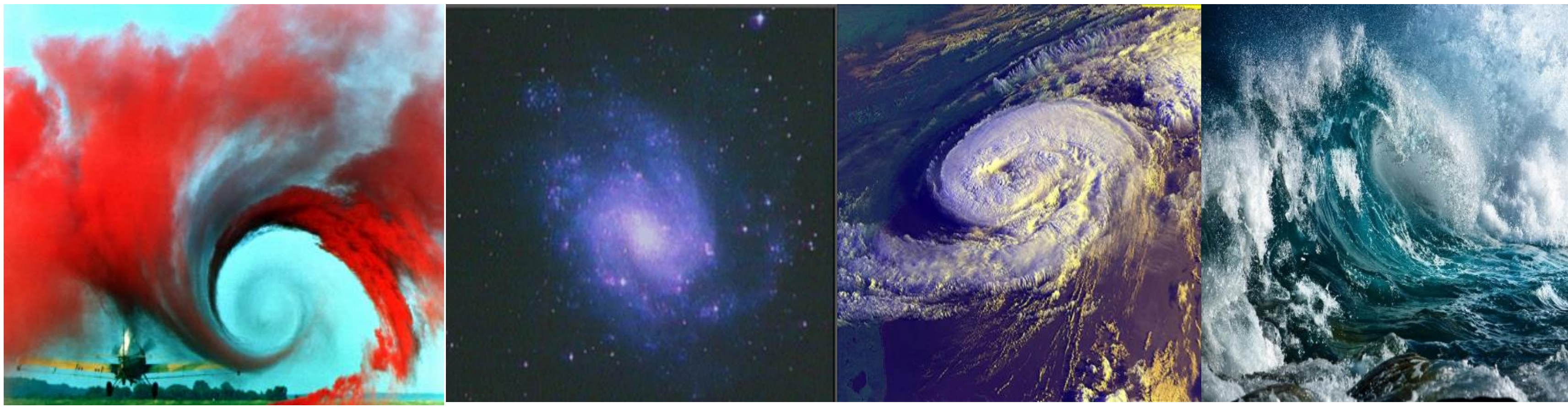
Some defining characteristics of turbulence

- ✓ It is chaotic
- ✓ It is characterized by the presence of large amount of vorticity
- ✓ It is dissipative
- ✓ It is characterized by strong mixing
- ✓ A turbulent field is also continuum (in the continuum mechanics sense)



Why study turbulence?

- Fluids and fluid instabilities, including turbulence, appear in a wide range of natural contexts as well as engineering systems.



- The problem of turbulence has been studied by many of the greatest physicists and engineers of the 19th and 20th centuries, and yet we do not understand in complete detail how or why turbulence occurs, nor can we predict turbulent behavior with any degree of reliability, even in very simple (from an engineering perspective) flow situations. Thus, study of turbulence is motivated both by its inherent intellectual challenge and by the practical utility of a thorough understanding of its nature.

What is turbulence?

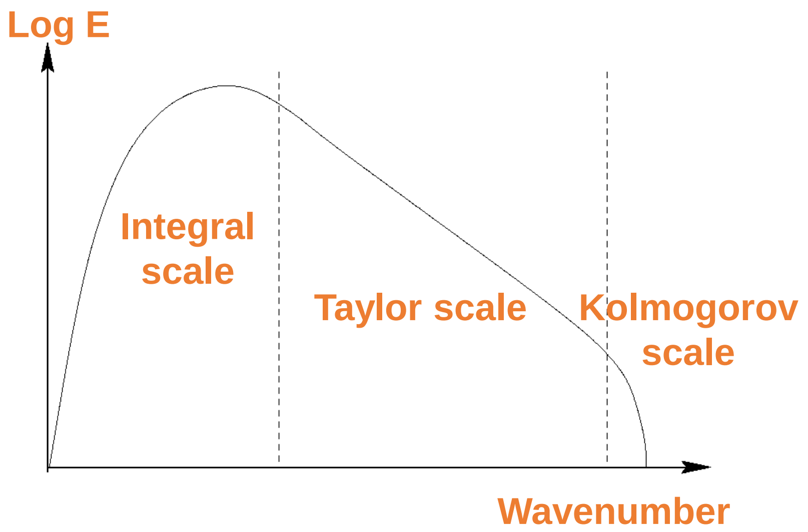
- Turbulent flows have the following characteristics:
  - One characteristic of turbulent flows is their **irregularity** or randomness. A full deterministic approach is very difficult. Turbulent flows are usually described statistically. Turbulent flows are always **chaotic**. But not all chaotic flows are turbulent. Waves in the ocean, for example, can be chaotic but are not necessarily turbulent.
  - The **diffusivity** of turbulence causes rapid mixing and increased rates of momentum, heat, and mass transfer. A flow that looks random but does not exhibit the spreading of velocity fluctuations through the surrounding fluid is not turbulent. If a flow is chaotic, but not diffusive, it is not turbulent. The trail left behind a jet plane that seems chaotic, but does not diffuse for miles is then not turbulent.
  - Turbulent flows always occur at **high Reynolds numbers**. They are caused by the complex interaction between the viscous terms and the inertia terms in the momentum equations.
  - Turbulent flows are **rotational**; that is, they have non-zero vorticity. Mechanisms such as the stretching of three-dimensional vortices play a key role in turbulence.

--continued

- Turbulent flows are **dissipative**. Kinetic energy gets converted into heat due to viscous shear stresses. Turbulent flows die out quickly when no energy is supplied. Random motions that have insignificant viscous losses, such as random sound waves, are not turbulent.
- Turbulence is a **continuum** phenomenon. Even the smallest eddies are significantly larger than the molecular scales. Turbulence is therefore governed by the equations of fluid mechanics.
- Turbulent flows are flows. Turbulence is a **feature of fluid flow**, not of the fluid. When the Reynolds number is high enough, most of the dynamics of turbulence are the same whether the fluid is an actual fluid or a gas. Most of the dynamics are then independent of the properties of the fluid.

Kolmogorov energy spectrum

- Energy cascade, from large scale to small scale.
- E is energy contained in eddies of wavelength l.
- Length scales:
  - Largest eddies. Integral length scale ($k^{3/2}/e$).
  - Length scales at which turbulence is isotropic. Taylor microscale $(15nu'^2/e)^{1/2.}$
  - Smallest eddies. Kolmogorov length scale $(n^3/e)^{1/4}$. These eddies have a velocity scale $(n.e)^{1/4}$ and a time scale $(n/e)^{1/2}$.



ε is the energy dissipation rate (m^2/s^3)

k is the turbulent kinetic energy (m^2/s^2)

ν is the kinematic viscosity (m^2/s)

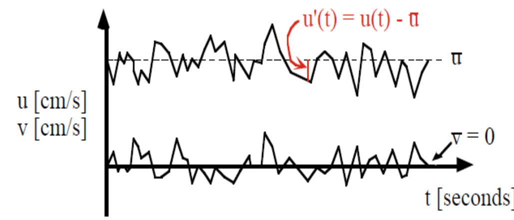
Mean and fluctuating field

- A proper statistical description of turbulence takes advantage of the **Reynolds decomposition**. An instantaneous field can be decomposed into the:

  mean field + fluctuating (zero-mean) field

Mean flow; Time averaging $\bar{u}(\vec{x}) = \frac{1}{T}\int_{t}^{t+T} u(\vec{x},t)dt$

Space averaging
$$\begin{cases} \bar{u}(t) = \frac{1}{V}\int_{V} u(\vec{x},t)dV & \\ \bar{u}(x_1,t) = \frac{1}{L_2L_3}\int_{x_2x_3} u(\vec{x},t)dx_2dx_3 & x_1 \perp S \\ \bar{u}(x_1,x_2,t) = \frac{1}{L_3}\int_{x_3} u(\vec{x},t)dx_3 & x_1,x_2 \perp x_3 \end{cases}$$



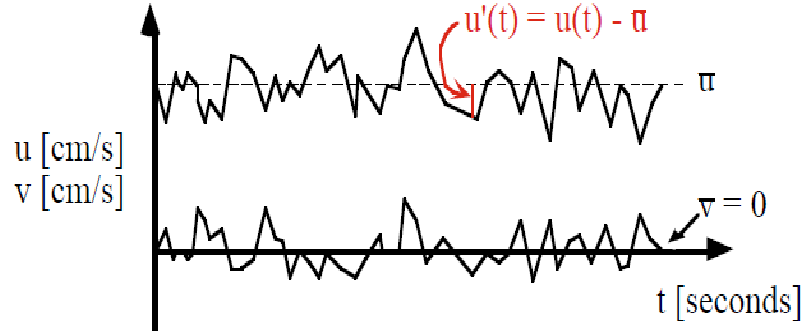
Ensemble averaging $\bar{u}(\vec{x},t) = \sum_{n=1}^{M} \bar{u}_n(\vec{x},t)$

We can write; $u(\vec{x},t) = U(\vec{x}) + u'(\vec{x},t)$

note : $U' = \frac{1}{T}\int_{t}^{t+T} u'(\vec{x},t)dt = 0$

Mean and fluctuating field

- Similar fluctuations for pressure, temperature and species concentration values.



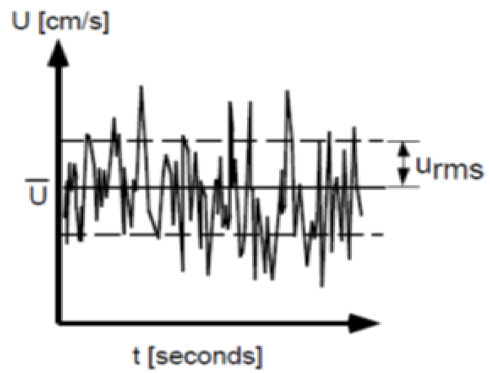
Turbulent Fluctuation: $u'(t) = u(t) - \bar{u}$: continuous record

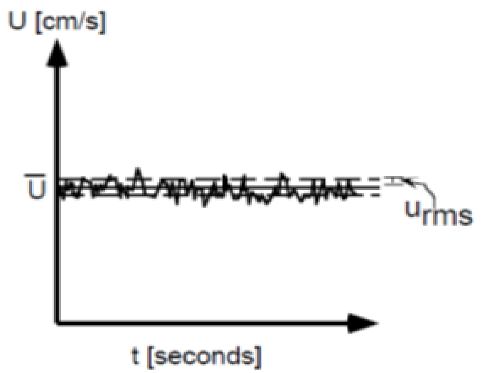
$u'_i = u_i - \bar{u}$: discrete points

Turbulence Strength: $u_{rms} = \sqrt{\overline{u'(t)^2}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(u'_i)^2}$

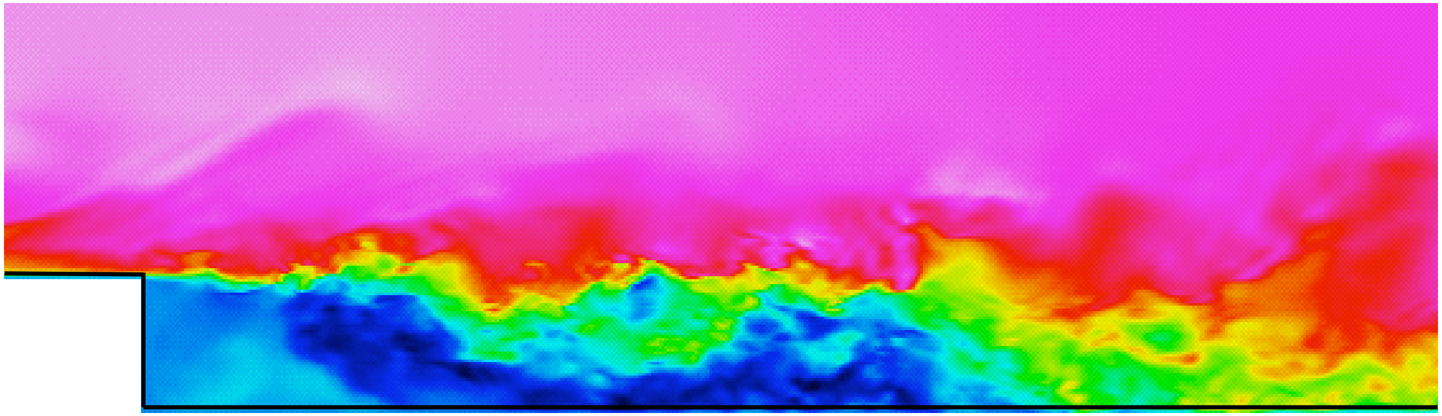
continuous record — discrete, equi-spaced

Turbulence Intensity: $u_{rms}/\bar{u}$

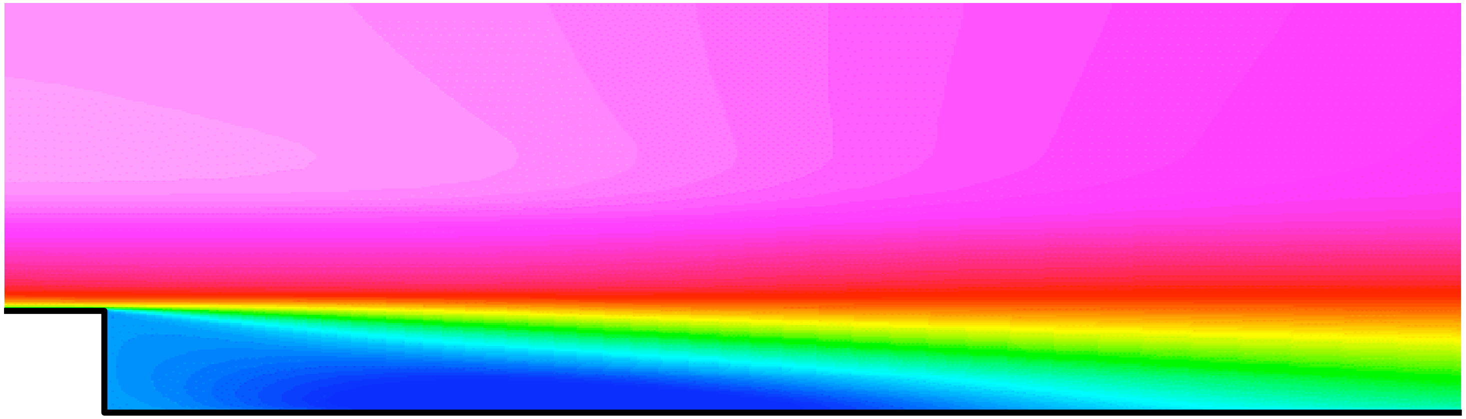




Instantaneous velocity contour



Time-averaged velocity contour



Decomposition

Flow property φ. The mean Φ is defined as :

$$\Phi = \frac{1}{\Delta t} \int_0^{\Delta t} \varphi(t)\, dt$$

Δt should be larger than the time scale of the slowest turbulent fluctuations.

Time dependence : $\varphi(t) = \Phi + \varphi'(t)$

Write shorthand as : $\varphi = \Phi + \varphi'$

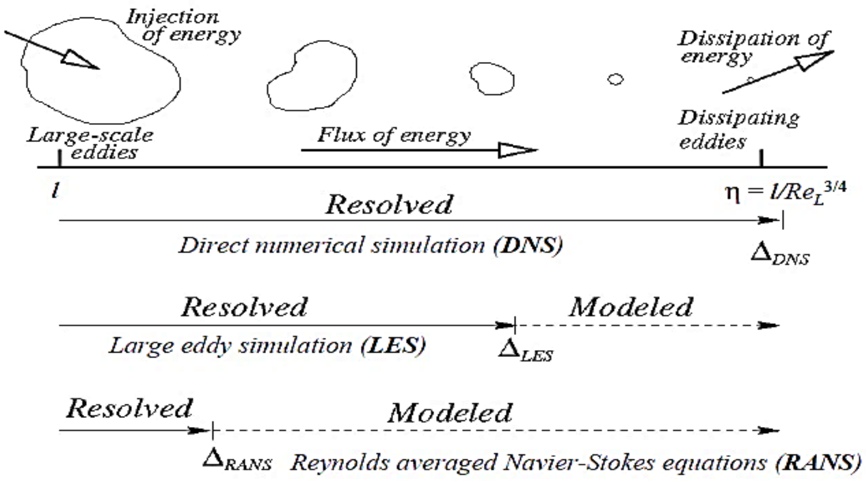
$$\overline{\varphi}' = \frac{1}{\Delta t} \int_0^{\Delta t} \varphi'(t)\, dt = 0 \quad \text{by definition}$$

Information regarding the fluctuating part of the flow can be obtained from the root – mean - square (rms) of the fluctuations :

$$\varphi_{rms} = \sqrt{\overline{(\varphi')^2}} = \left[\frac{1}{\Delta t} \int_0^{\Delta t} (\varphi')^2\, dt \right]^{1/2}$$

Energy Transfer/Turbulent scales

- The large eddies are unstable and break up, transferring their energy to somewhat smaller eddies.
- These smaller eddies undergo a similar break-up process and transfer their energy to yet smaller eddies.
- This ***energy cascade*** – in which energy is transferred to successively smaller and smaller eddies – continues until the Reynolds number $\mathrm{Re}(l) \equiv u(l)l/\nu$ is sufficiently small that the eddy motion is stable, and molecular viscosity is effective in dissipating the kinetic energy.
- At these small scales, the kinetic energy of turbulence is converted into heat.



Statistical tools

- We now define some statistical quantities, useful to understand the main features of a turbulent field

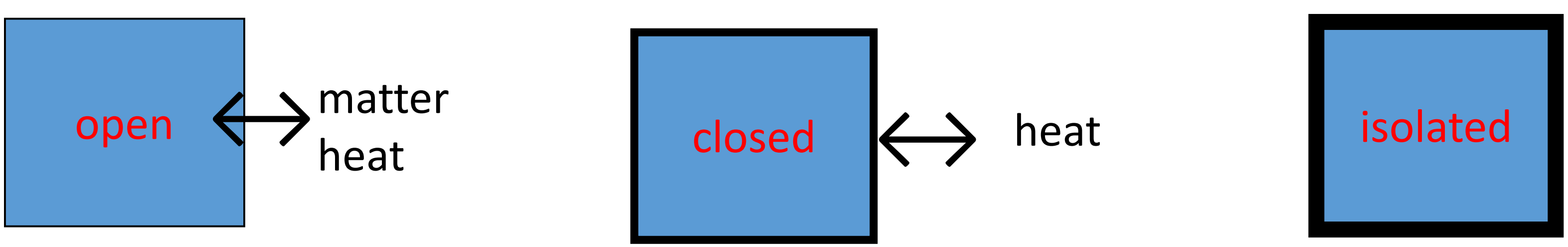
- ✓ The Probability Density Function, PDF
- ✓ The Joint PDF
- ✓ The central moments of the PDF
- ✓ The correlation function
- ✓ Spectra

Heat transfer

Thermodynamics

- "The branch of science that deals with energy levels and the transfer of energy between systems and between different states of matter"

- System – the PART of the universe that is under consideration. It is separated from the rest of the universe by it's boundaries
  - Open system → when matter CAN cross the boundary
  - Closed system → when matter CANNOT cross the boundary
  - Isolated → Boundary seals matter and heat from exchange with another system



How does heat travel?

Heat transfer is the physical act of thermal energy being exchanged between two systems by dissipating heat

1. Conduction: (solids--mostly) Heat transfer without mass transfer.
2. Convection: (liquids/gas) Heat transfer with mass transfer.
3. Radiation: Takes place even in a vacuum.

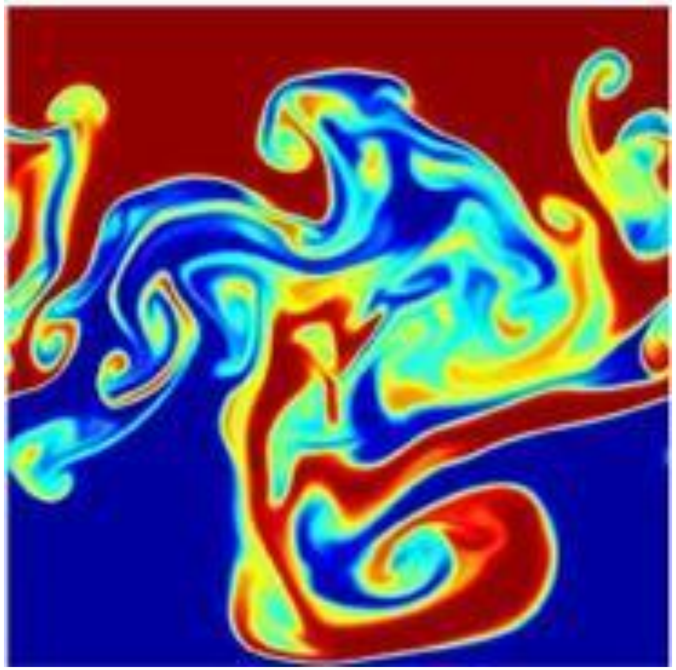
Conduction: is the flow of internal energy from a region of higher temperature to one of lower temperature by the interaction of the adjacent particles (atoms, molecules, ions, electrons, etc.) in the intervening space

Factors affecting the rate of heat transfer by conduction:

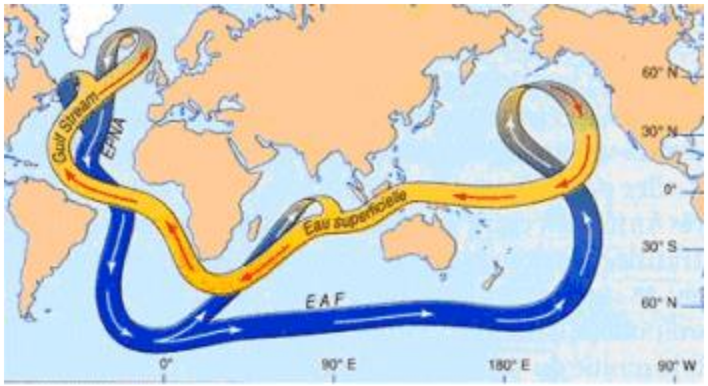
- temperature difference
- length
- cross-sectional area
- material

Convection

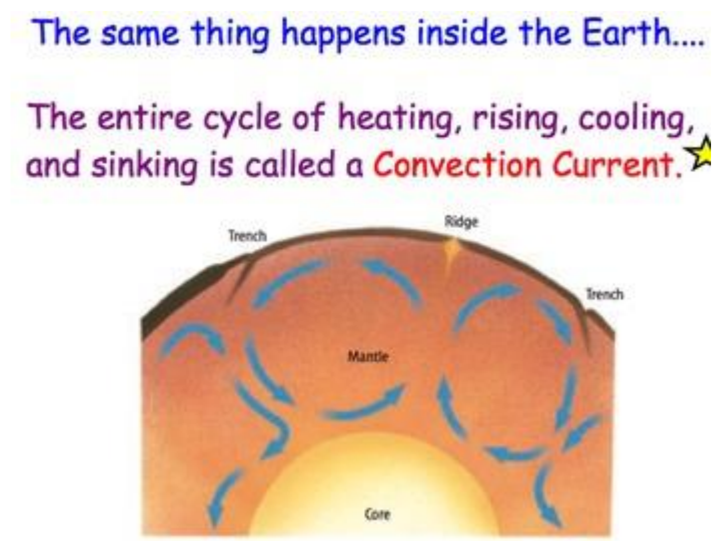
- Typically very complicated.
- Very efficient way to transfer energy.
- Vortex formation is very common feature.
- liquid convection
- vortex formation
- Sunspot
- solar simulation

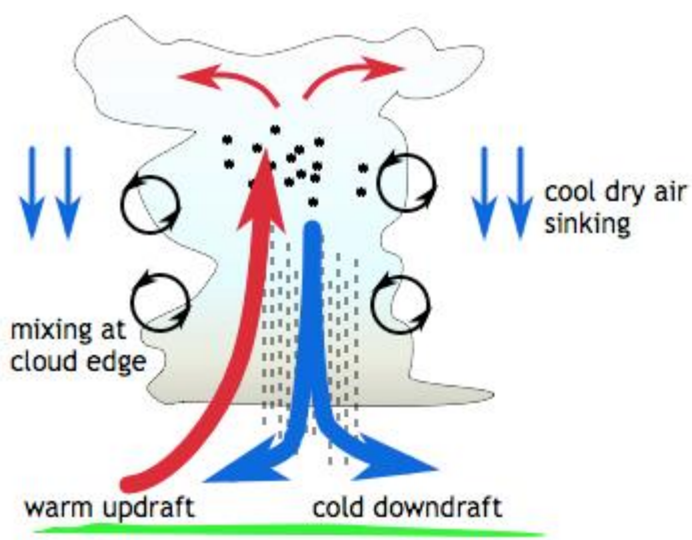


Convection example



Ocean current

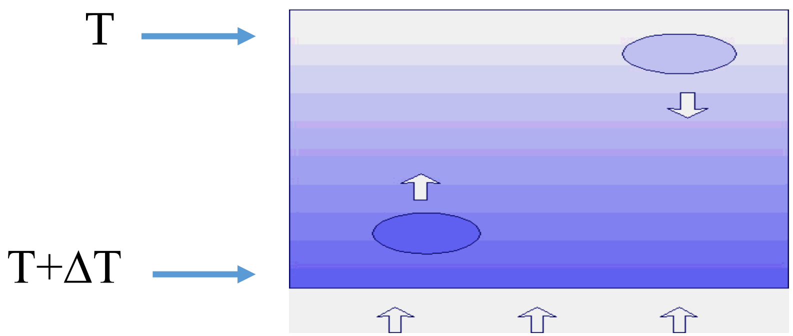




Thermal convection

Buoyancy-driven flows

Thermal expansion causes hot fluid to rise and cold fluid to sink at the presence of gravity.

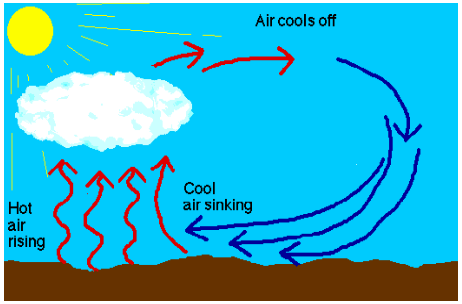


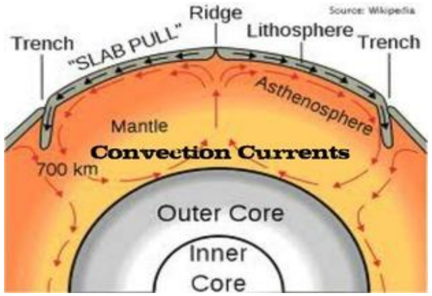
α: Fluid thermal expansion coefficient

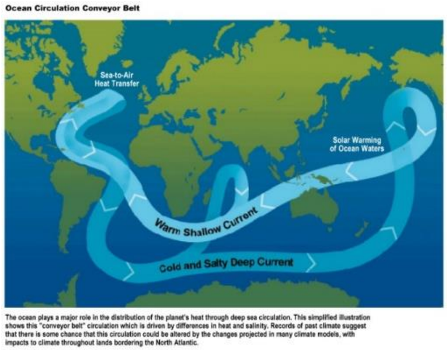
υ: Fluid kinematic viscosity

κ: Fluid thermal diffusivity

Heat transfer mediated by a fluid takes place in countless phenomena in industrial and natural systems, for example ....

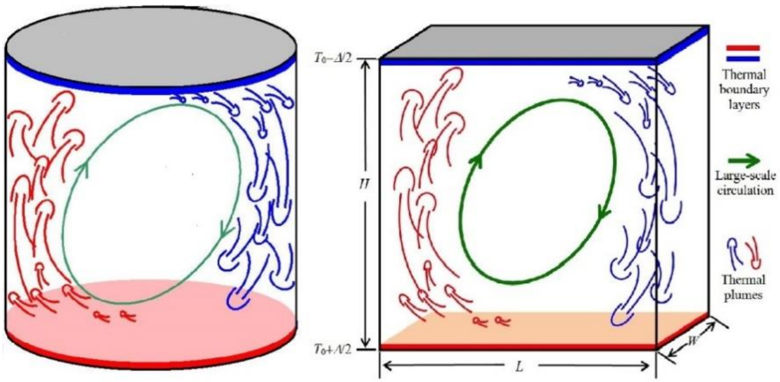






RBC system

- Rayleigh-Bénard (RB) system: A fluid layer of depth H heated from below and/or cooled from above.



- The fluid starts moving only when $Ra > Ra_c$

(buoyancy must "exceed" viscous drag and heat diffusion)

- Control parameters for convection;

1) $\boldsymbol{Ra} = \frac{\alpha g \Delta T H^3}{\nu\kappa}$ "forcing" parameter

2) $\boldsymbol{Pr} = \frac{\nu}{\kappa}$ fluid properties

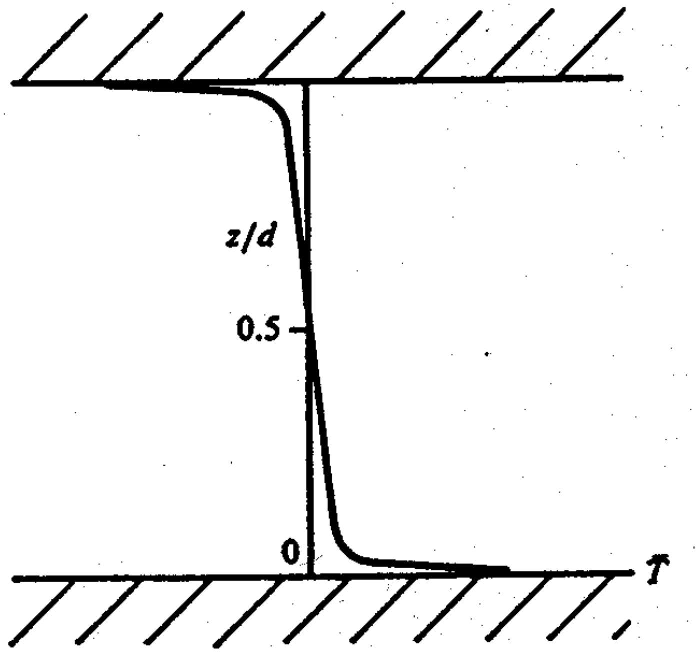
3) $\boldsymbol{\Gamma} = \frac{L}{H}$ geometry parameter

Nusselt number $Nu = \frac{QH}{\kappa \Delta T}$

Reynold number $Re = \frac{UH}{\nu}$

Ra=f(Nu, Pr, Γ, shape)

- Very high Ra: thermal boundary layers at the upper and lower walls are highly stressed regions giving rise to plumes



The temperature gradient is all at the wall!

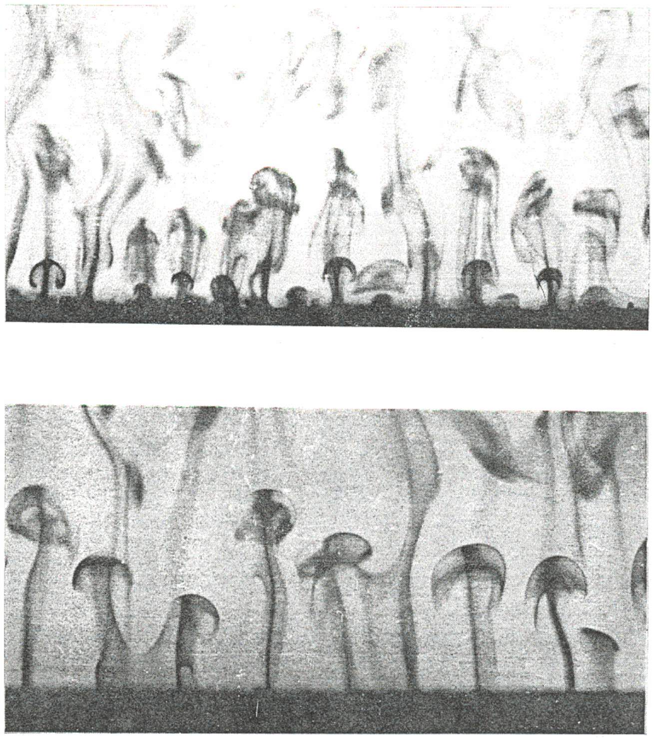


FIGURE 1. Photographs of thermals rising from a heated horizontal surface.

Plume Sparrow, Husar & Goldstein
J. Fluid Mech. **41**, 793 (1970)

Rayleigh-Bénard convection

- ✓ Simple model of convection
- ✓ Thermal convection- transfer of heat trough a fluid
- ✓ Parcel will rise to the level of natural buoyancy
- ✓ The hot layer try to rise while the cold later try to sink
- ✓ Breaks up into convection cells
- ✓ In the form of rolls, hexagon, cell etc.

Equations of motion

- We solve the 3D equations of motion in the Boussinesq approximation. For the Nondimensionalization we use

$$\mathrm{H},\ U_f = \sqrt{g\alpha\Delta T H},\ \Delta T$$

1) $$\boldsymbol{\nabla}.\boldsymbol{u} = 0$$

2) $$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}.\boldsymbol{\nabla})\boldsymbol{u} = -\boldsymbol{\nabla} p + \sqrt{\frac{Pr}{Ra}}\boldsymbol{\nabla}^2\boldsymbol{u} + T\boldsymbol{e}_z$$

3) $$\frac{\partial T}{\partial t} + (\boldsymbol{u}.\boldsymbol{\nabla})T = \frac{1}{\sqrt{RaPr}}\boldsymbol{\nabla}^2 T$$

Thermal boundary layer thickness as a function of Ra;

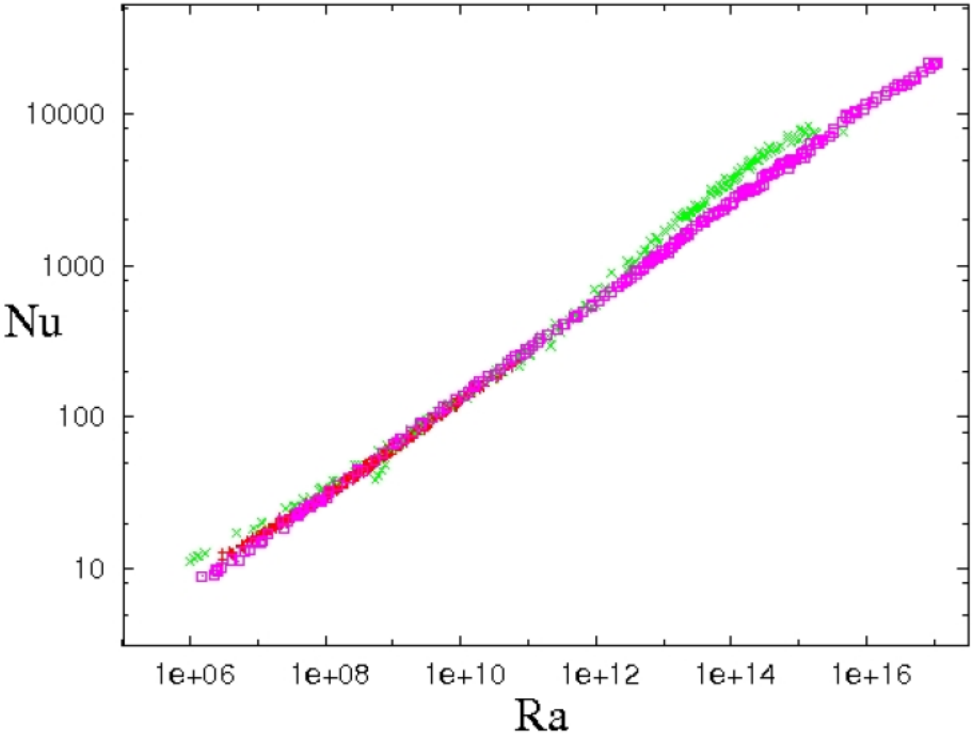
$$\begin{cases} \dfrac{\lambda_\theta}{H} = \dfrac{1}{2Nu} \\ \dfrac{\lambda_u}{H} \sim \dfrac{1}{4\sqrt{RaPr}} \end{cases}$$

$$\begin{cases} N_\theta \approx 0.35Ra^{0.15} \quad 10^6 \le Ra \le 10^{10} \\ N_u \approx 0.13Ra^{0.15}, \quad 10^6 \le Ra \le 10^{10} \end{cases}$$

RBC system

State-of-the-Art Experiments (high Ra)

Cryogenic helium, cylindrical cell *Γ=1/2*



Niemela et al. (2000), Chavanne et al. (2001), Roche et al. (2002)

Statistical tools

Statistical tools

Statistical tools

Statistical tools