Computational Studies and Molecular Dynamic Simulations workshop

Dr. Najmeh Foroozani

University of Ibadan, Ibadan

April 2019

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

♦ Fluid Mechanics (FM) - Day 1

→ Definition

→ Statistical descriptions

→ Equations of turbulent flows

♦ Approaches to study fluid mechanics - Day 2

→ Numerical *vs* Analytical *vs* Experimental

→ Numerical modeling (CFD)

♦ Heat transfer - Day 3

♦ NEK5000

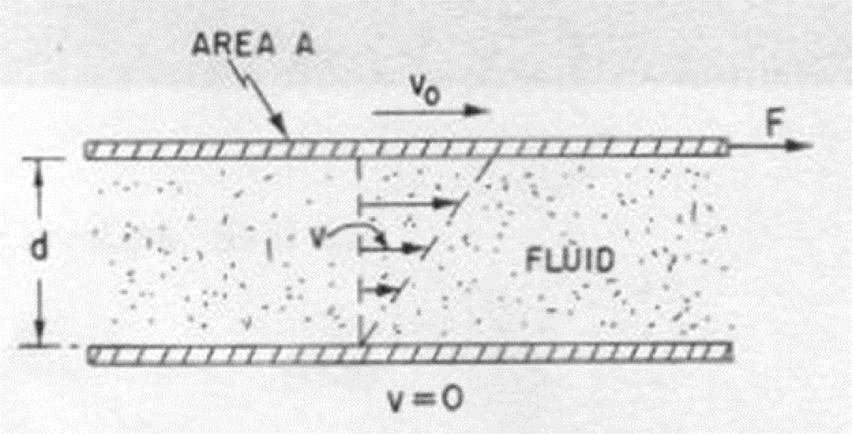
Fluid Mechanics and the Governing Equations

Fluids

Fluids are like graduate students….constantly under stress!!! (Joe Niemela)

‘’**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.

Internal/External flow

Viscous/Inviscid regions of flow

Laminar/Turbulent

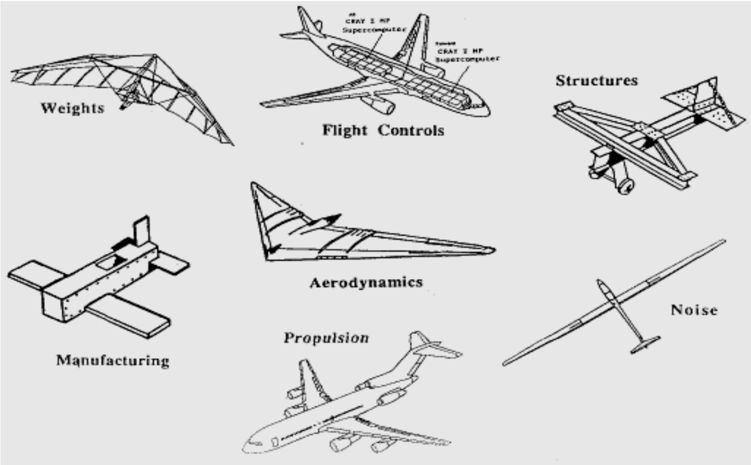
Forced/Neutral flow

Steady/Unsteady

Compressible/Incompressible

Newtonian/non-Newtonian

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

Introduction to CFD

- Computational fluid dynamics (CFD) is the science of predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related phenomena by solving the mathematical equations which govern these processes using a numerical process.

- We are interested in the forces (pressure , viscous stress etc.) acting on surfaces (Example: In an airplane, we are interested in the lift, drag, power, pressure distribution etc)

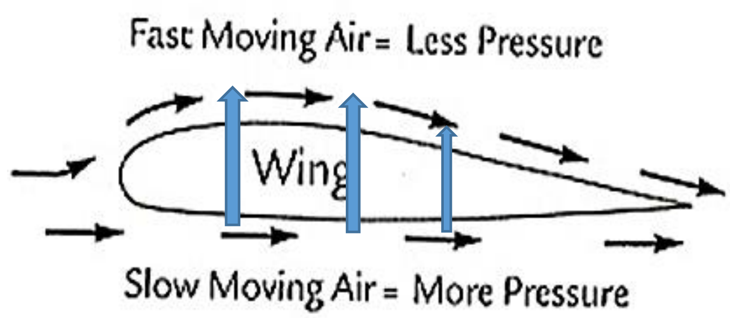
- We would like to determine the velocity field (Example: In a race car, we are interested in the local flow streamlines, so that we can design for less drag)

- We are interested in knowing the temperature distribution (Example: Heat transfer in the vicinity of a computer chip, cooling systems, …)

Aerodynamics

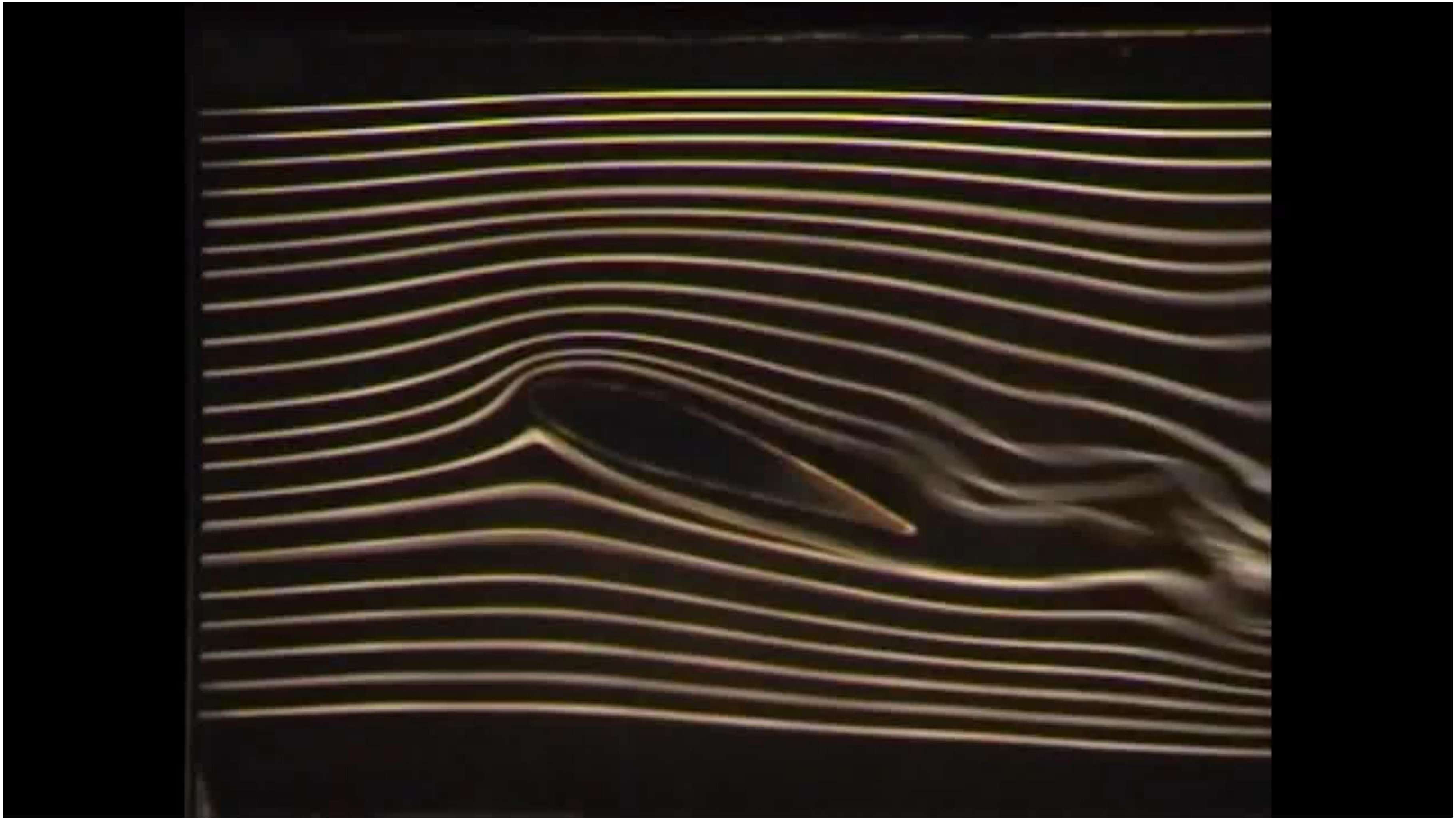
In order for an aircraft to rise into the air, a force must be created that equals or exceeds the force of gravity. This force is called lift. In heavier-than-air craft, lift is created by the flow of air over an airfoil. The shape of an airfoil causes air to flow faster on top than on bottom. The fast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

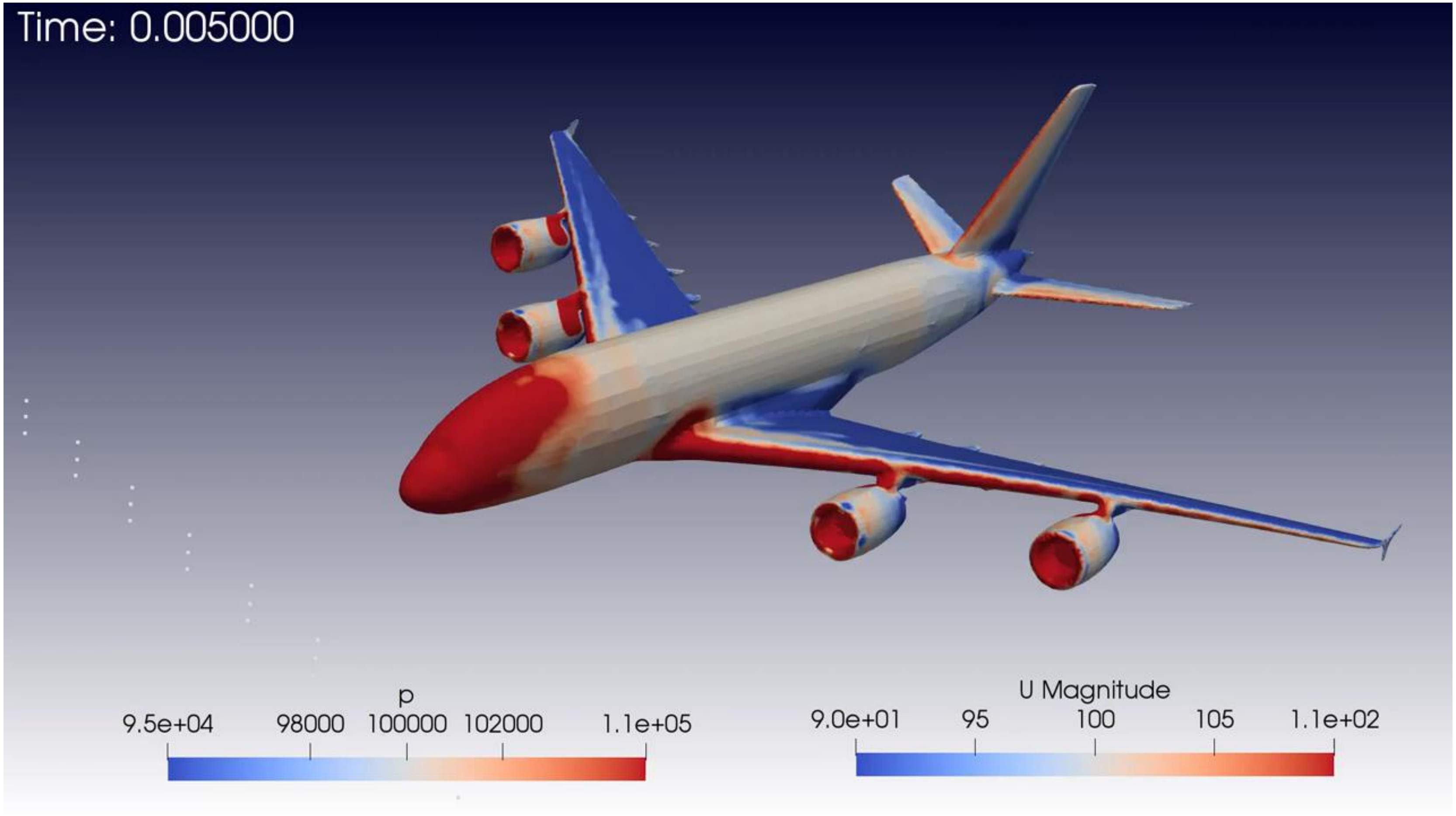


When a fluid is moving faster, it has lower pressure. This principle explains the lift created by an airplane's wing.

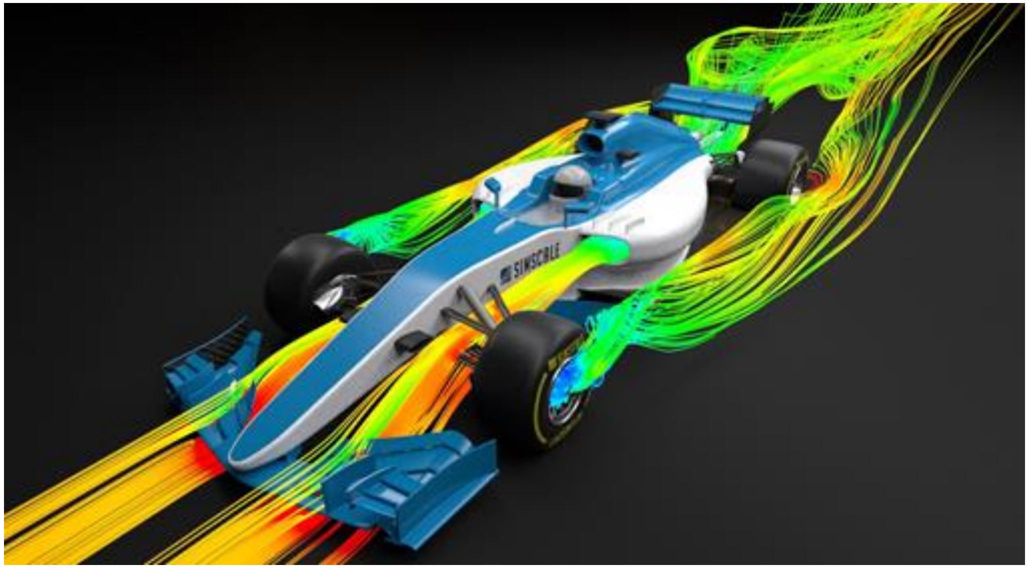
Airflow across a wing



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

A2 WIND TUNNEL

www.A2WT.com

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;

2) Physical principle: Energy is conserved

Applying the continuity equation, the simplified NS equation for incompressible fluids are then:

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

$$\frac{D\boldsymbol{u}}{Dt} = \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}.\boldsymbol{\nabla u} = -\frac{1}{\rho}\boldsymbol{\nabla} p + \boldsymbol{\nu \nabla}^2 \boldsymbol{u} + \frac{1}{\rho}\boldsymbol{F}$$ Vector form

3) Physical principle: Energy is conserved

$$\frac{\partial(\rho e_t)}{\partial t} + \boldsymbol{\nabla}.(\rho e_t \vec{u}) = k\boldsymbol{\nabla}.\boldsymbol{\nabla} T - \boldsymbol{\nabla} p.\boldsymbol{u} + (\boldsymbol{\nabla}.\tau).\boldsymbol{u}$$

Fundamentals of Boundary Layers

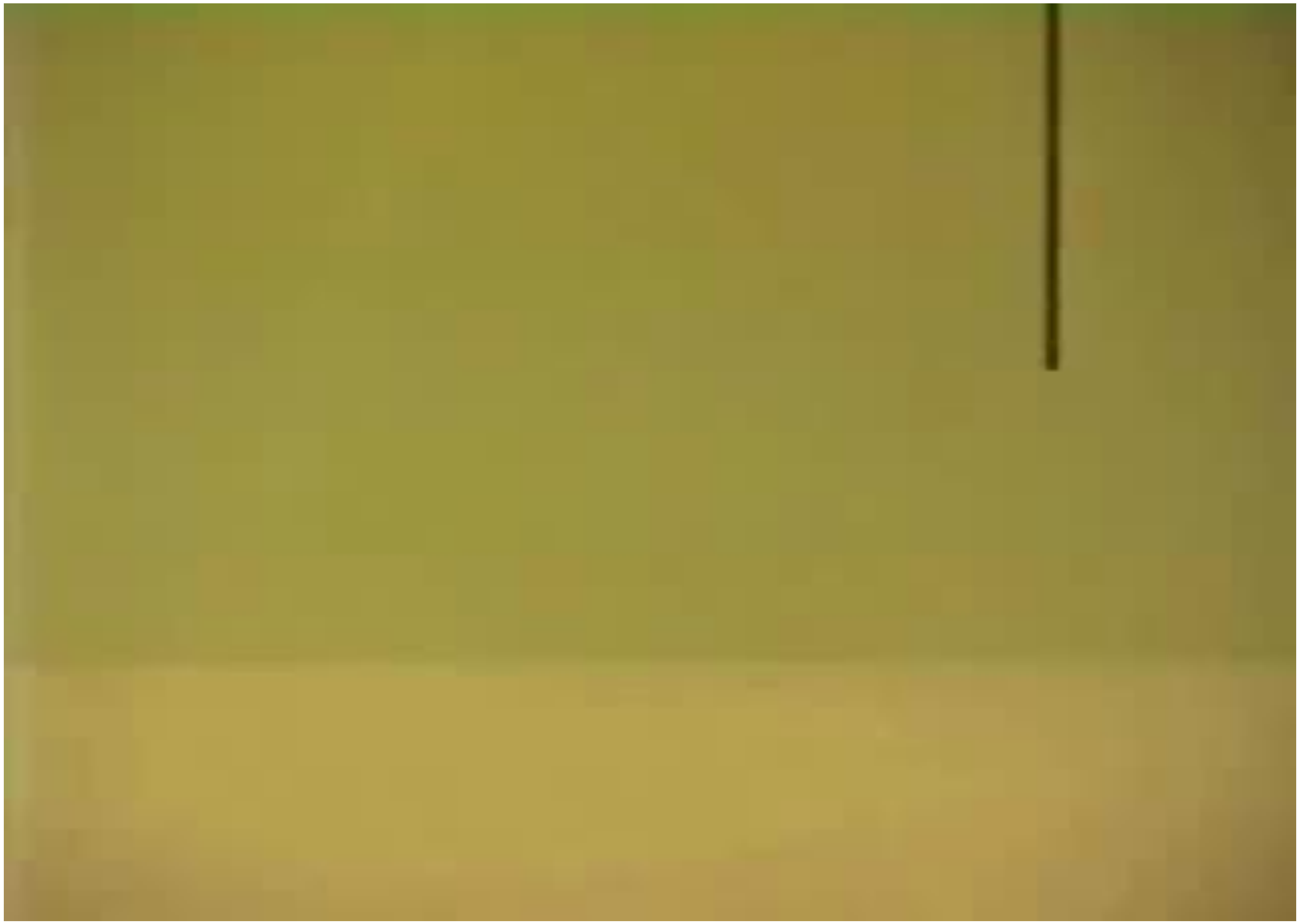
Boundary layer

- 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?

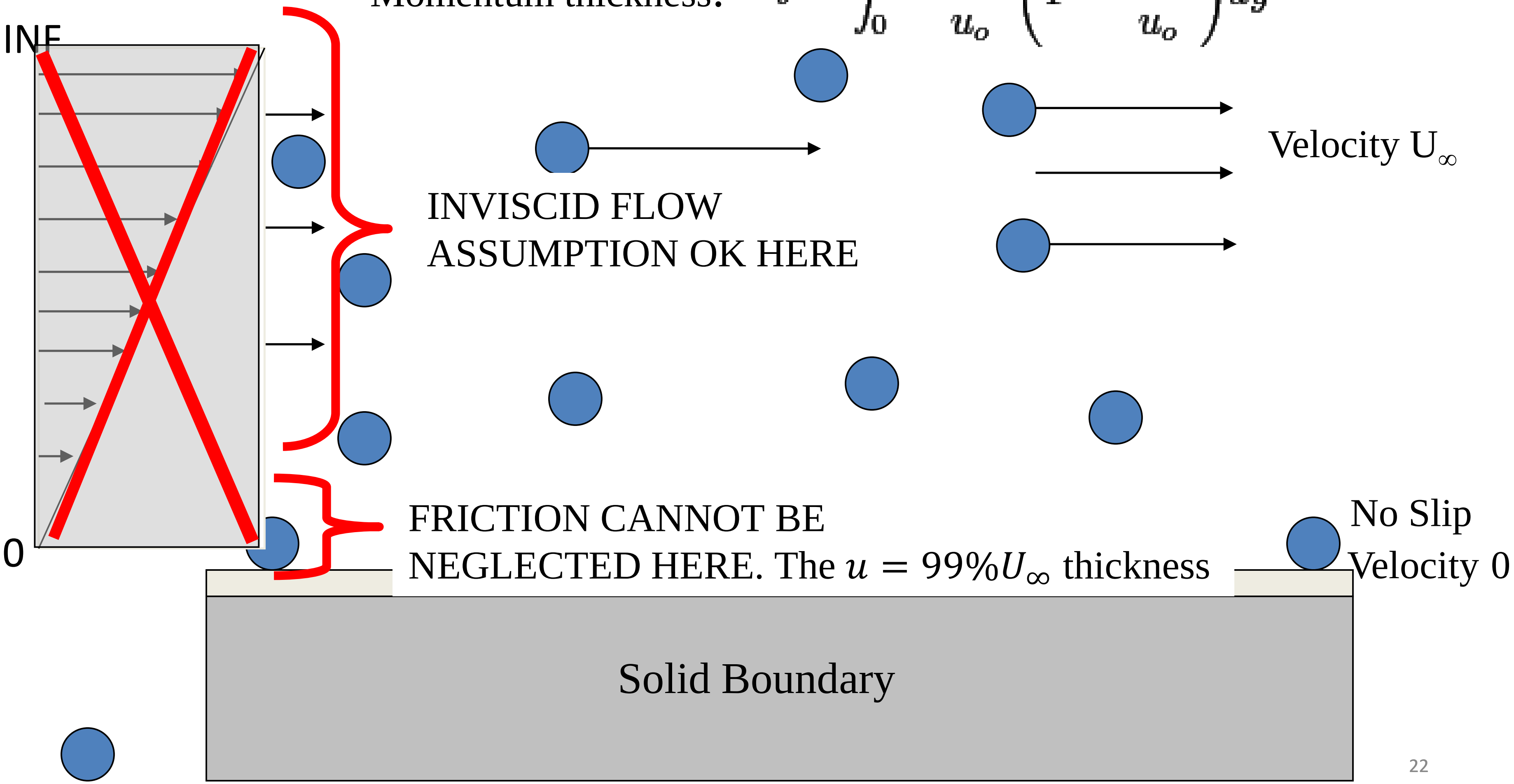


This so-called "**no-slip**" condition is a very important one that must be satisfied in any accurate analysis of fluid flow phenomena.

Boundary layer over a flat plate

Displacement thickness $\delta^* = \int_0^\infty \left(1 - \frac{u(y)}{u_0}\right) dy$

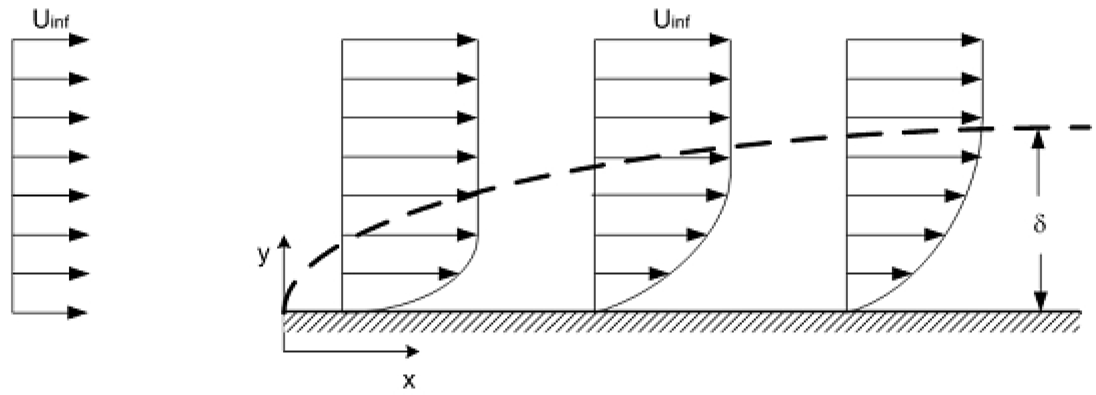
Momentum thickness: $\theta = \int_0^\infty \frac{u(y)}{u_o}\left(1 - \frac{u(y)}{u_o}\right) dy$



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



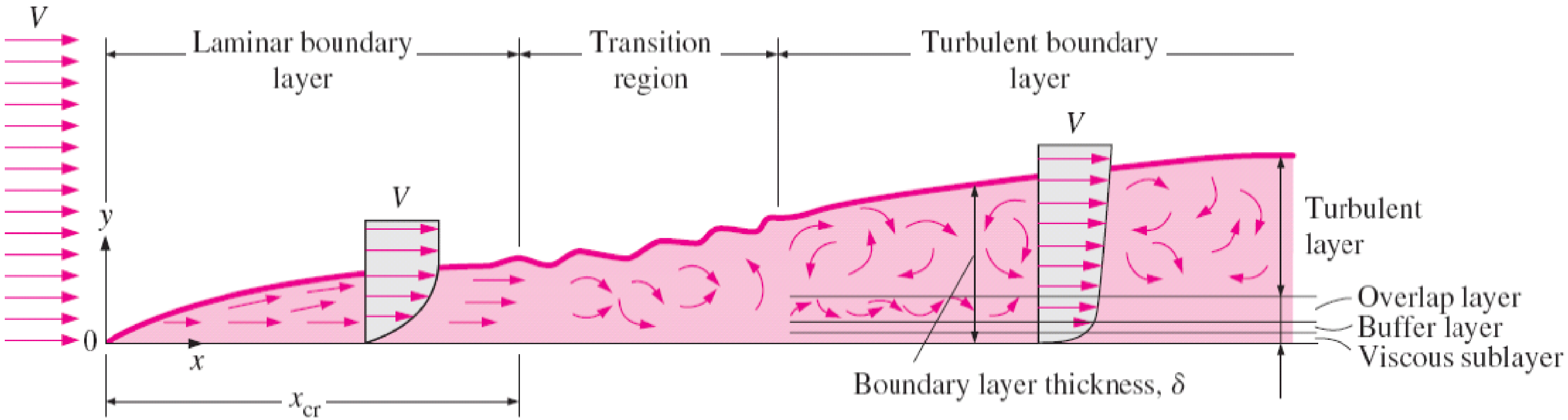
BL Flow regimes

- Similar to other viscous flows we have 3 flow regimes

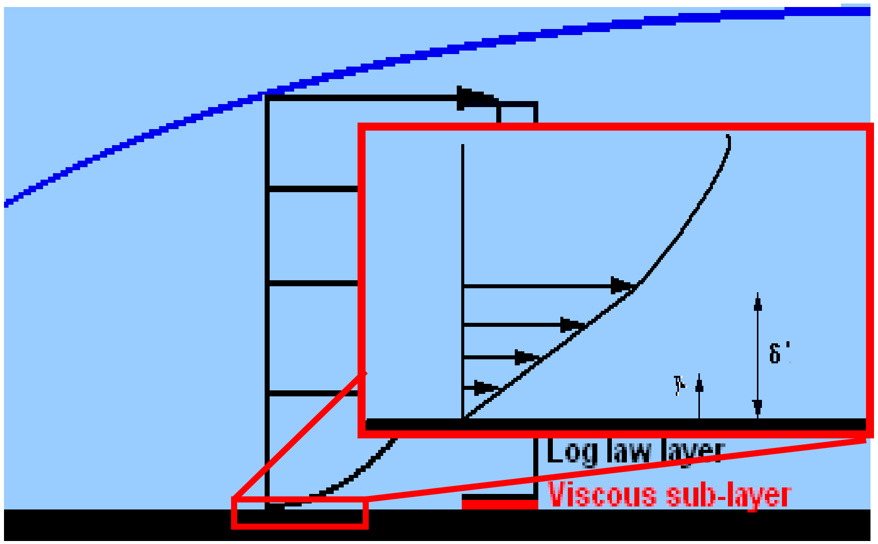
  Laminar: over starting point of the body

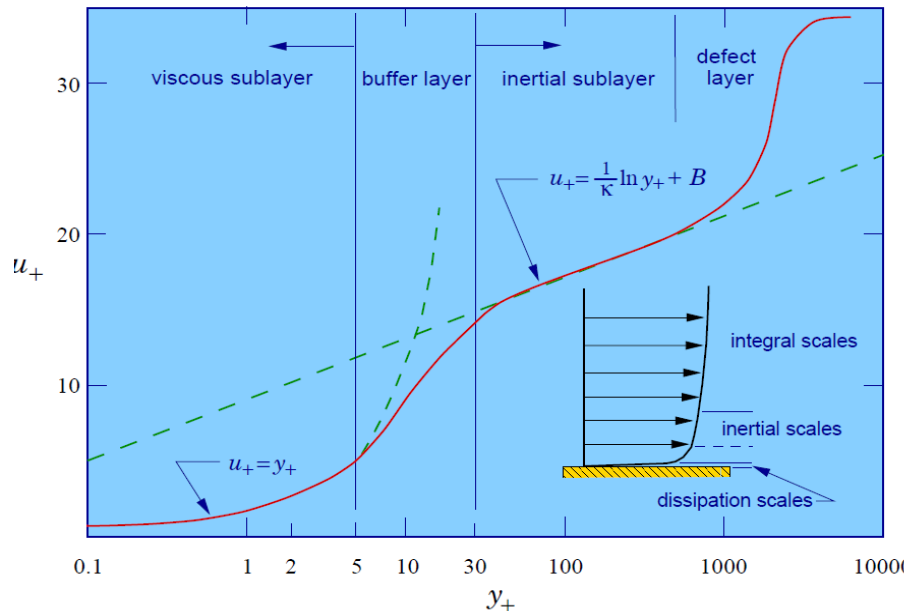
  Transition: mid-locations of the body

  Turbulent: ending parts of the body



The universal law of the wall





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

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

u^+: local velocity

u_τ: friction velocity

τ_{wall}: wall shear stress

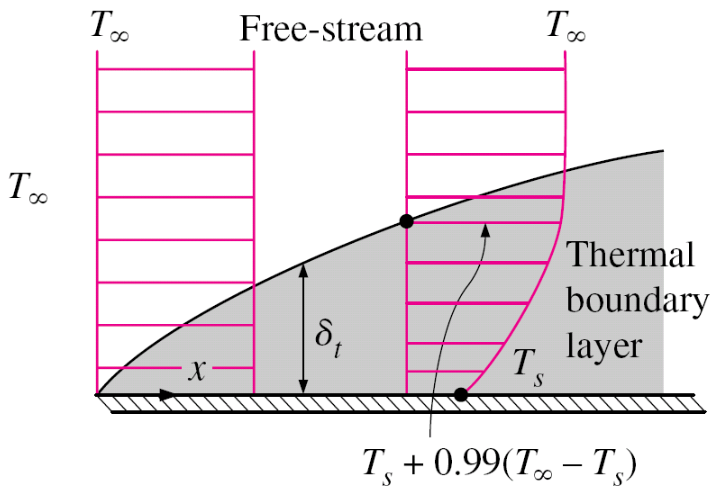
Dimensionless velocity profiles plotted in the near-wall coordinates. The linear section in the semi-log plot is called the **universal law of the wall layer**, or log law layer, for equilibrium turbulent boundary layers (TBL).

Thermal Boundary layer

A thermal boundary layer develops when a fluid at a specified temperature, flows over a surface that is at a different temperature.

The **thermal boundary layer ─** the flow region over the surface in which the temperature variation in the direction normal to the surface is significant.

The *thickness* of the thermal boundary layer *dt* at any location along the surface is defined as *the distance from the surface at which the temperature difference* *T*(*y*=*dt*)-*Ts*= *0.99(T∞-Ts*).



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.

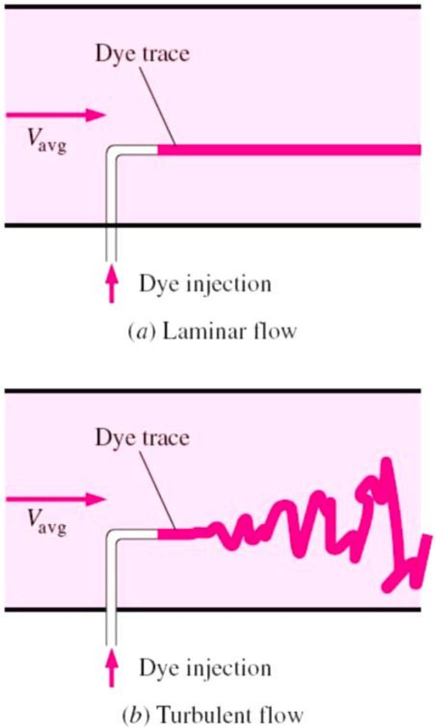
- Consequently the thermal boundary layer is much thicker for liquid metals and much thinner for oils relative to the velocity boundary layer.

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

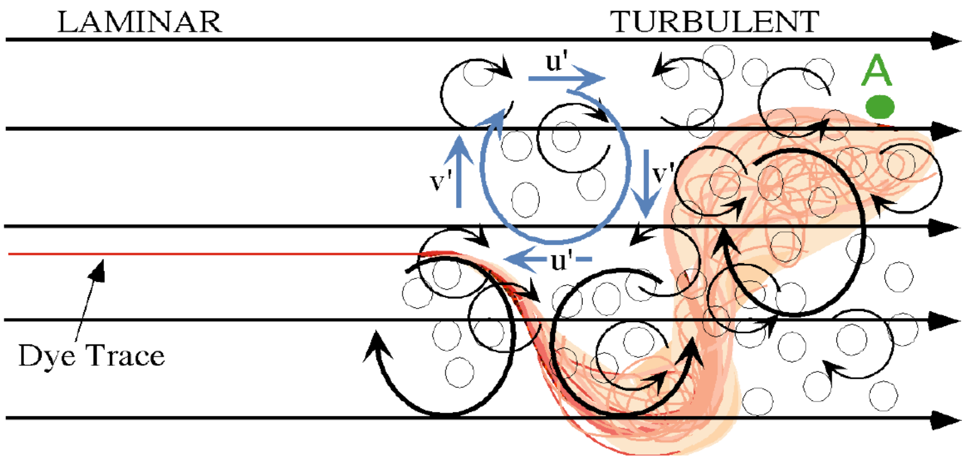
(*b*) Turbulent flow

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;

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

- 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

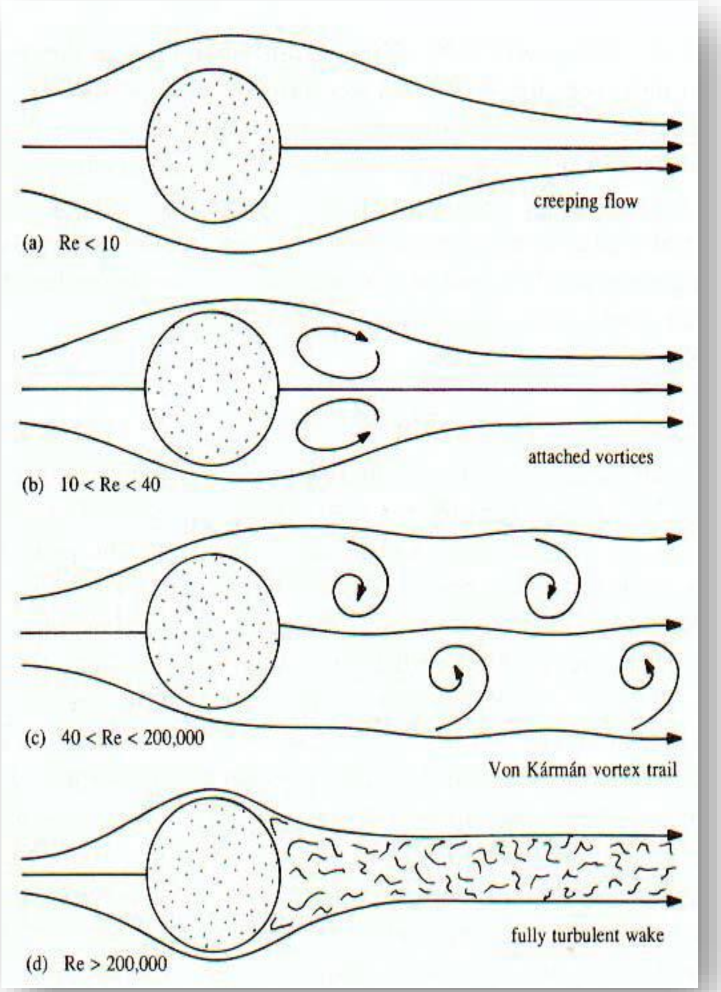
✓ The flow pattern around some an obstruction in the flow depends on the Reynolds Number, *Re*, and on the shape of an object. For a cylindrical obstruction, the following patterns are observed.

– 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”.

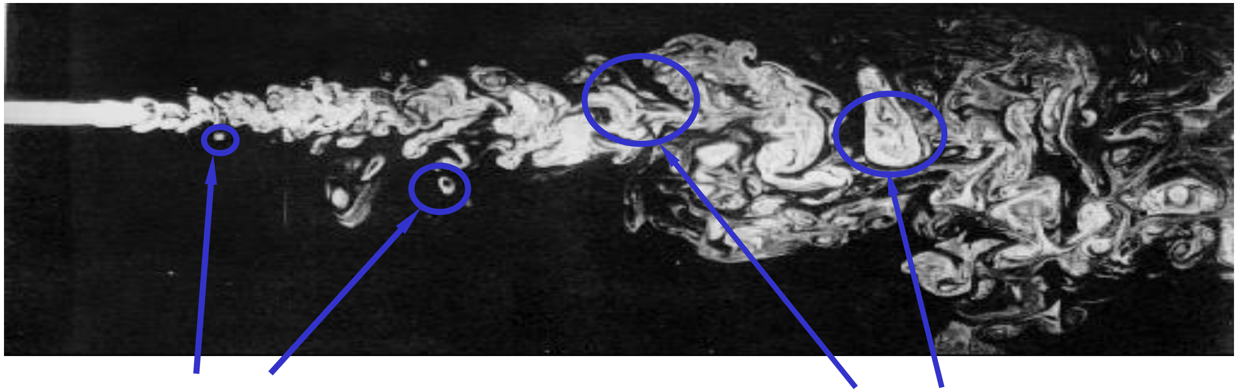
– Turbulence starts to develop at around *Re* ~ 1000, and the flow in the wake of the cylinder becomes more and more chaotic.



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)

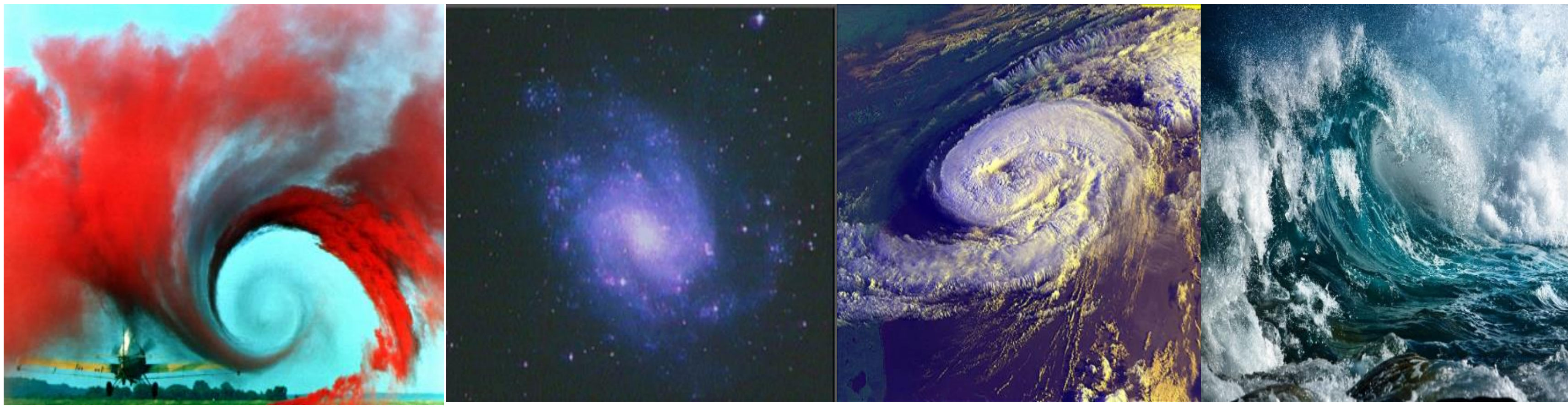


Small
Structure

Large
Structure

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.

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

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

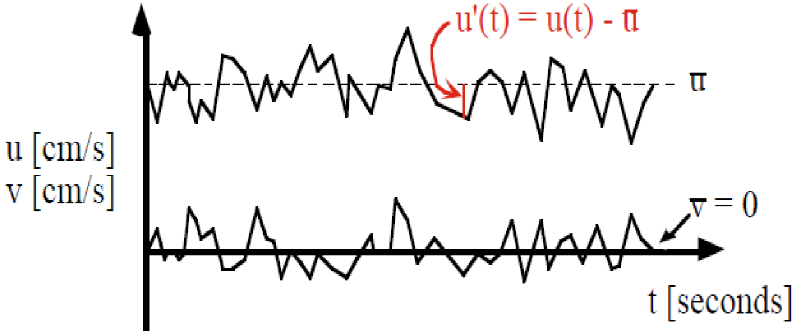
Ensemble averaging $\bar{u}(\vec{x},t) = \sum_{n=1}^{M} \bar{u}_n(\vec{x},t)$

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.



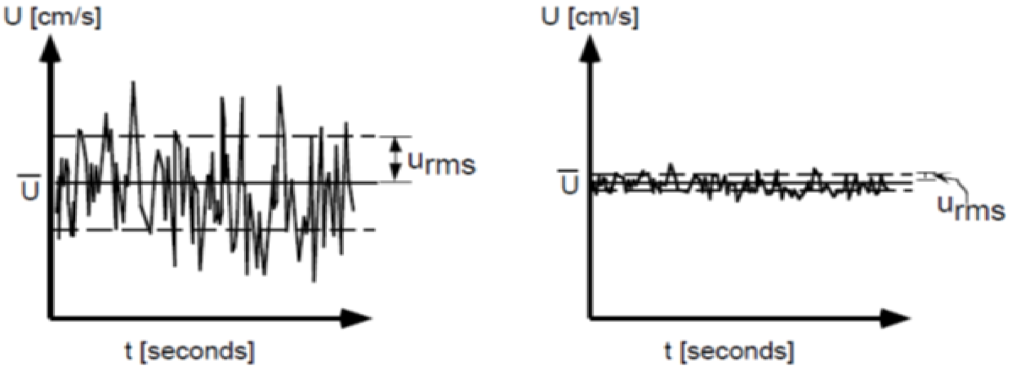
Turbulent Fluctuation: $u'(t) = u(t) - \bar{u}$: continuous record

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

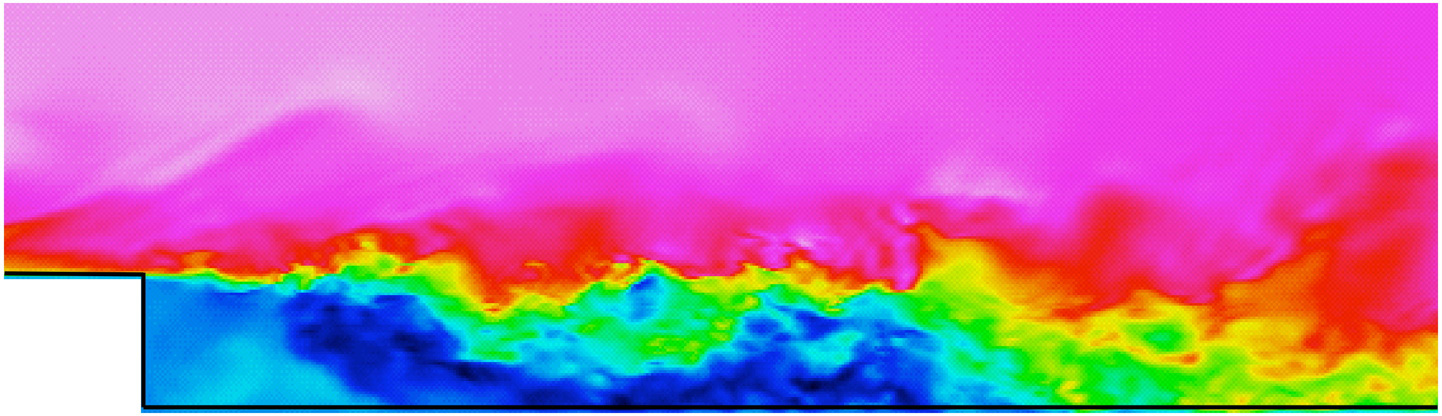
Turbulence Strength: $u_{rms} = \sqrt{\overline{u'(t)^2}} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(u'_i)^2}$

continuous record — discrete, equi-spaced

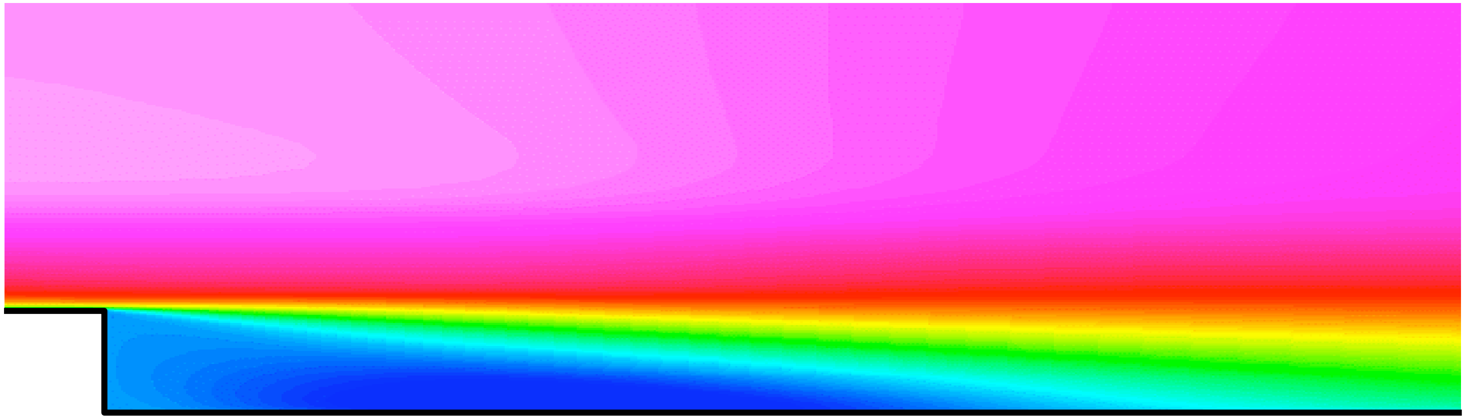
Turbulence Intensity: $u_{rms}/\bar{u}$



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 :

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

Velocity decomposition

- Velocity and pressure decomposition:

$$\text{Velocity}: \ \mathbf{u} = \mathbf{U} + \mathbf{u}'$$

$$\text{Pressure}: \ p = P + p'$$

- Turbulent kinetic energy k (per unit mass) is defined as:

$$k = \frac{1}{2}\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right)$$

$$\text{Turbulence intensity}: \ T_i = \frac{\left(\frac{2}{3}k\right)^{1/2}}{U_{ref}}$$

- Continuity equation:

$$div\,\mathbf{u} = 0; \ Time\ average: \overline{div\,\mathbf{u}} = div\,\mathbf{U} = 0$$

$$\Rightarrow \text{continuity equation for the mean flow}: \ div\,\mathbf{U} = 0$$

- Next step, time average the momentum equation. This results in the Reynolds equations.

Turbulent flow - Reynolds equations

$$x-momentum: \quad \frac{\partial(\rho U)}{\partial t} + div(\rho U \mathbf{U}) = -\frac{\partial P}{\partial x} + div(\mu \; grad \; U) + S_{Mx}$$

$$+\left[-\frac{\partial(\rho \overline{u'^2})}{\partial x} - \frac{\partial(\rho \overline{u'v'})}{\partial y} - \frac{\partial(\rho \overline{u'w'})}{\partial z} \right]$$

$$y-momentum: \quad \frac{\partial(\rho V)}{\partial t} + div(\rho V \mathbf{U}) = -\frac{\partial P}{\partial y} + div(\mu \; grad \; V) + S_{My}$$

$$+\left[-\frac{\partial(\rho \overline{u'v'})}{\partial x} - \frac{\partial(\rho \overline{v'^2})}{\partial y} - \frac{\partial(\rho \overline{v'w'})}{\partial z} \right]$$

$$z-momentum: \quad \frac{\partial(\rho W)}{\partial t} + div(\rho W \mathbf{U}) = -\frac{\partial P}{\partial z} + div(\mu \; grad \; W) + S_{Mz}$$

$$+\left[-\frac{\partial(\rho \overline{u'w'})}{\partial x} - \frac{\partial(\rho \overline{v'w'})}{\partial y} - \frac{\partial(\rho \overline{w'^2})}{\partial z} \right]$$

Turbulent flow - continuity and scalars

- Continuity: $$\frac{\partial \rho}{\partial t} + div(\rho\ \mathbf{U}) = 0$$

- Scalar transport equation:

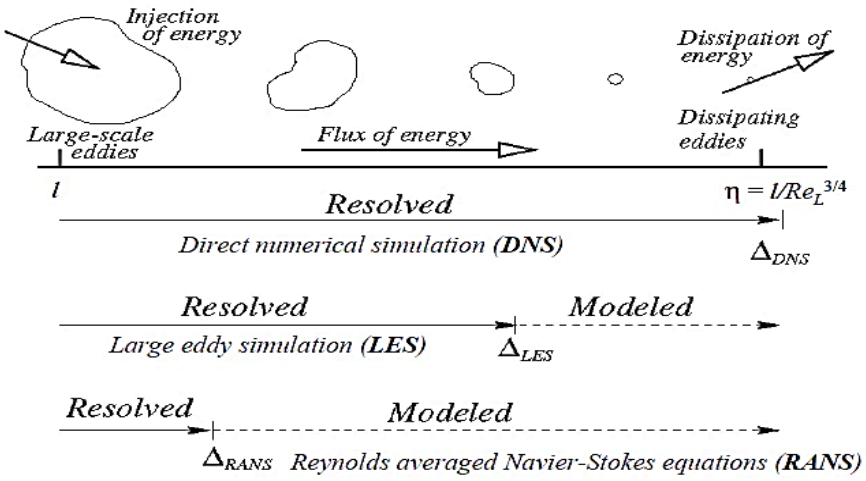
$$\frac{\partial (\rho \Phi)}{\partial t} + div(\rho \Phi \mathbf{U}) = div(\Gamma_{\Phi}\ grad\ \Phi) + S_{\Phi}$$

$$+ \left[-\frac{\partial (\rho \overline{u'\varphi'})}{\partial x} - \frac{\partial (\rho \overline{v'\varphi'})}{\partial y} - \frac{\partial (\rho \overline{w'\varphi'})}{\partial z} \right]$$

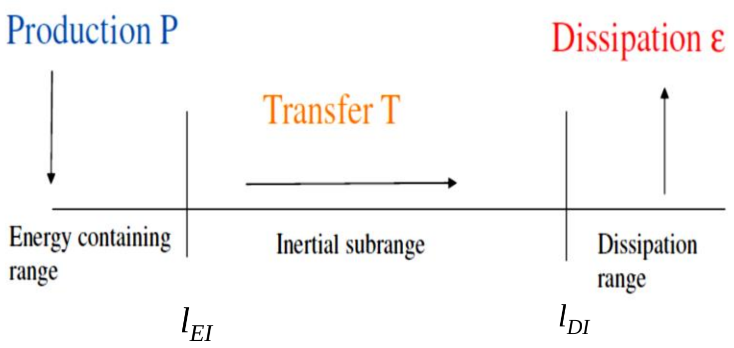
- Notes on density:
  - Here r is the mean density.
  - This form of the equations is suitable for flows where changes in the mean density are important, but the effect of density fluctuations on the mean flow is negligible.
  - For flows with T_i<5% this is up to Mach 5 and with T_i<20% this is valid up to around Mach 1.

Energy Transfer/Turbulent scales

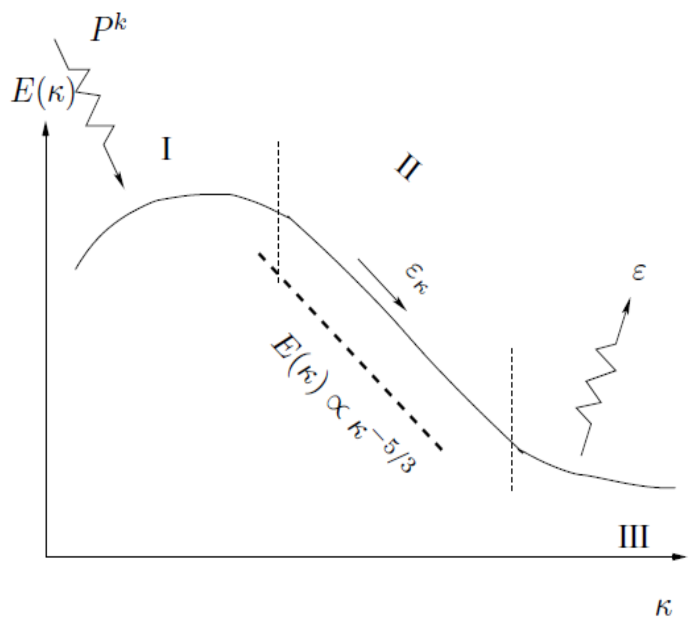
- The large eddies are unstable and break up, transferring their energy to somewhat smaller eddies.
- These smaller eddies undergo a similar break-up process and transfer their energy to yet smaller eddies.
- This ***energy cascade*** – in which energy is transferred to successively smaller and smaller 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.



Kolmogorov’s hypothesis of local isotropy states that *at sufficiently high Reynolds numbers, the small-scale turbulent motions are statistically isotropic*



Here, the term local isotropy means isotropy at small scales. Large scale turbulence may still be anisotropic. l_{EI} is the length scale that forms the demarcation between the large scale anisotropic eddies ($l>l_{\mathrm{EI}}$) and the small scale isotropic eddies ($l<l_{\mathrm{EI}}$). For many high Reynolds number flows l_{EI} can be estimated as $l_{\mathrm{EI}} \approx l_0/6$.



Energy Spectrum

Dimensional analysis gives:

$$\boxed{E(\kappa) = C\varepsilon^{2/3}\kappa^{-5/3}}$$

This is the famous Kolmogorov “–5/3” spectrum and C is the universal Kolmogorov constant, which experimentally was determined to be C = 1.5. (K. R. Sreenivasa (1995))

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

Thermal convection

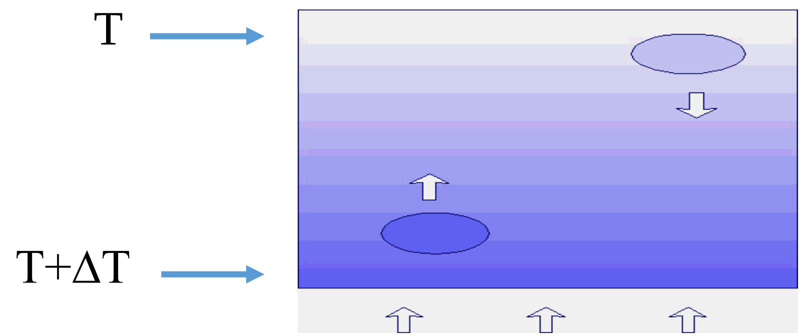
Buoyancy-driven flows

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

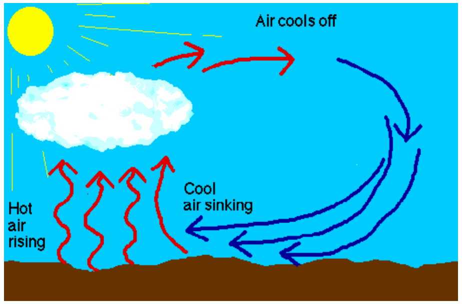
α: Fluid thermal expansion coefficient

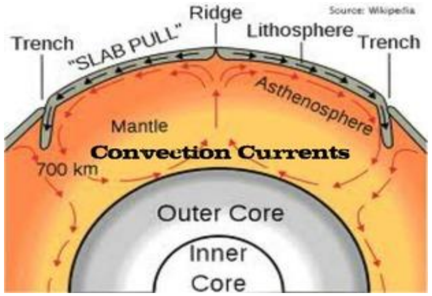
υ: Fluid kinematic viscosity

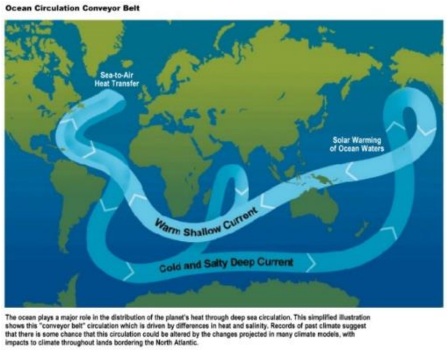
κ: Fluid thermal diffusivity



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





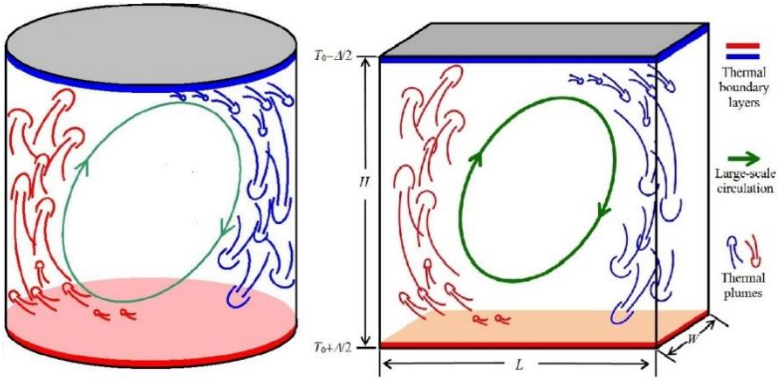


Rayleigh-Bénard convection

- ✓ 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.

RBC system

- <u>Rayleigh-Bénard (RB)</u> 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 $Nu = \frac{QH}{\kappa\Delta T}$

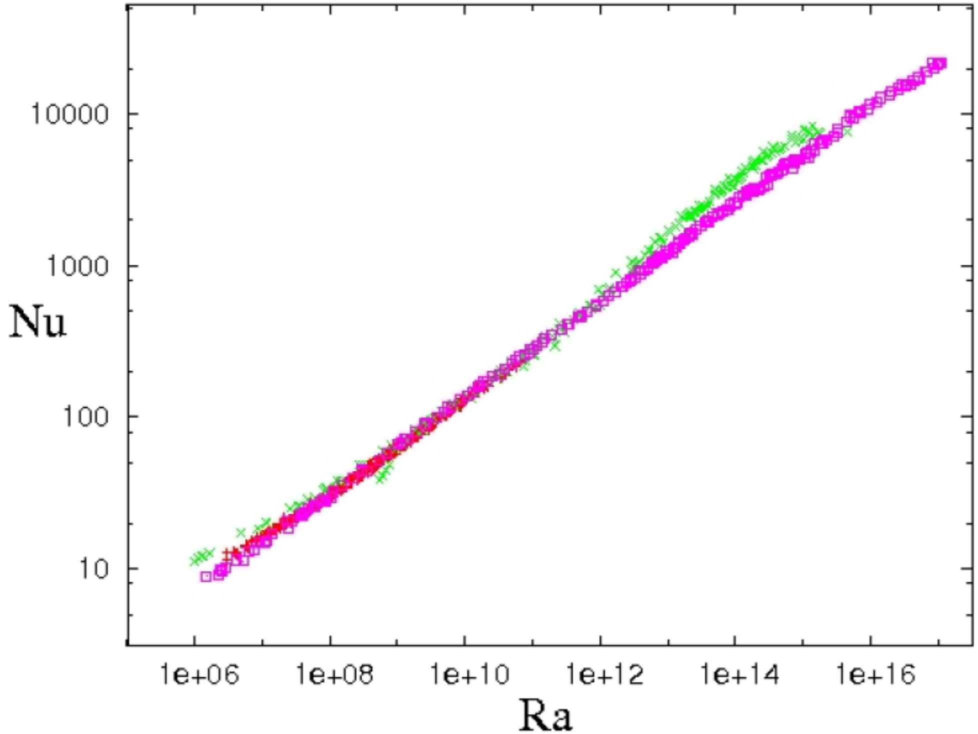
Reynold number $Re = \frac{UH}{\nu}$

Ra=f(Nu, Pr, Γ, shape)

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)

Equations of motion

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

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

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;

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

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

- DAY 2 morning

Computational methods for Fluid Dynamics (CFD)

Recall

- Equations of motion for an incompressible flow:

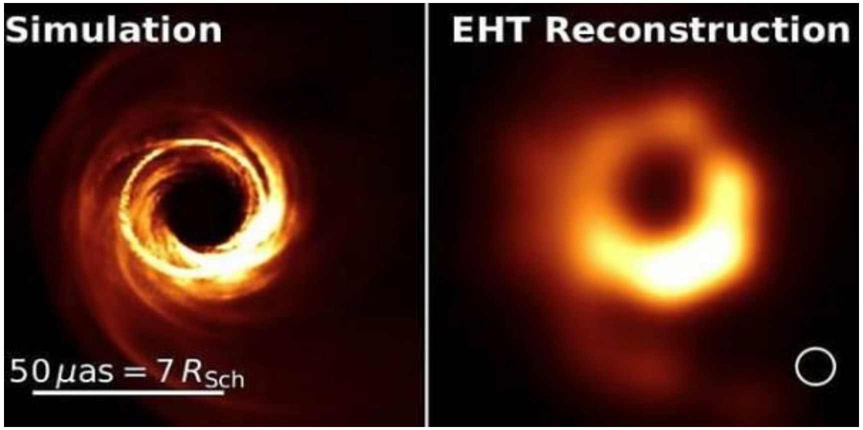
$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0$$

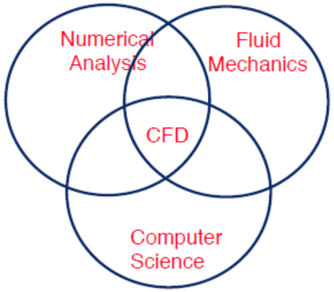
$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial P}{\partial x}+\rho g_x+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)$$

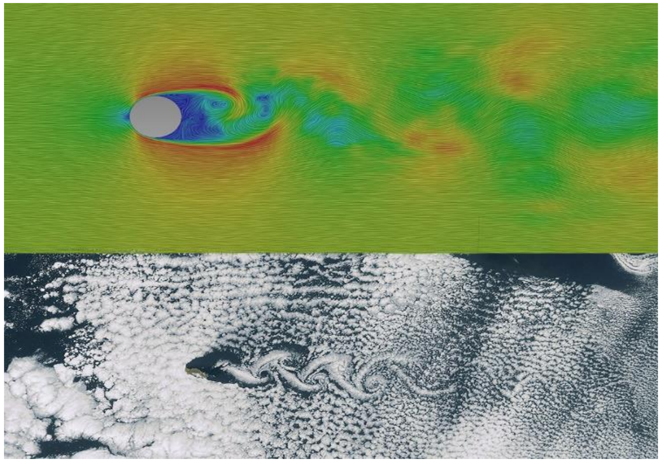
$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{\partial P}{\partial y}+\rho g_y+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)$$

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial P}{\partial z}+\rho g_z+\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)$$

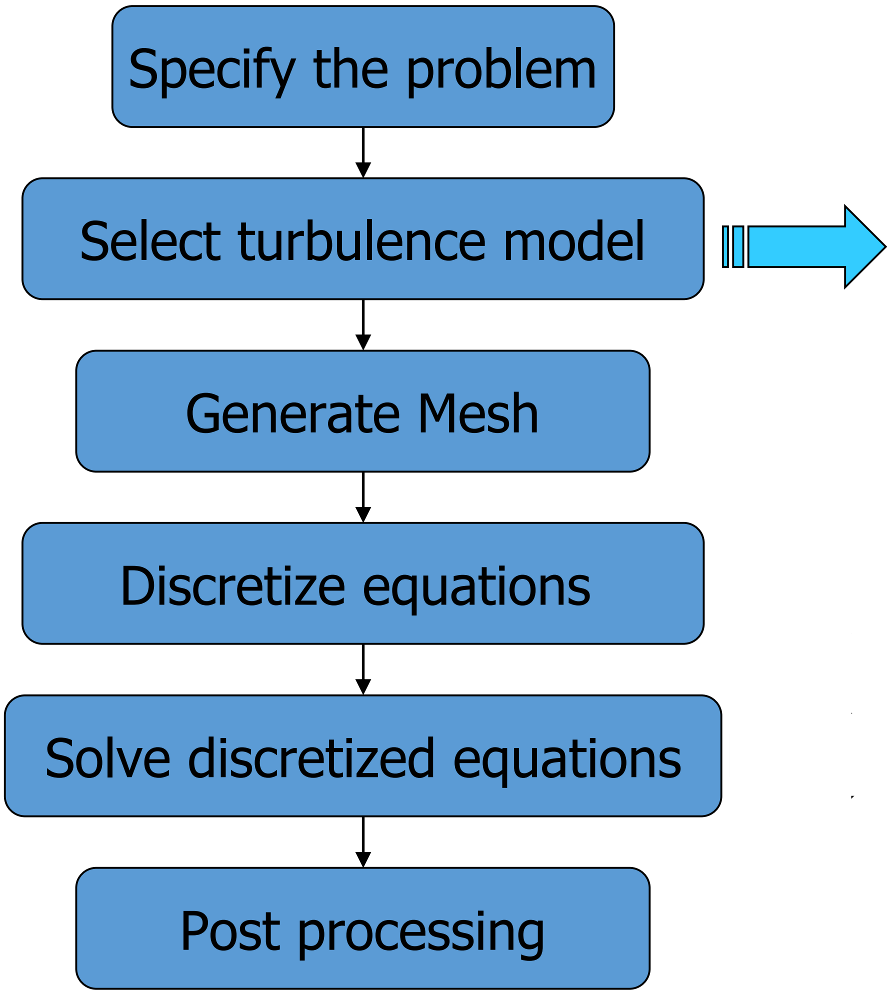
Simulation or?







CFD road map



Turbulence models

- These are semi-empirical mathematical models introduced to CFD to describe the turbulence in the flow

Main topics

- Three levels of CFD simulations
- Classification of turbulence models
- Examples of popular models
- Special considerations
- General remarks about turbulence modelling

Finite difference (FD)

Starting from the <u>differential form of the equations</u>
The computational domain is covered by a grid
At each grid point, the differential equations (partial derivatives) are approximated
Only used in structured grids and normally straightforward
Disadvantage: conservation is not always guaranteed
Disadvantage: Restricted to simple geometries.

Finite Volume (FV)

Starting from the <u>integral form of the equations</u>
The solution domain is covered by control volumes (CV)
The conservation equations are applied to each CV
The FV can accommodate any type of grid and suitable for complex geometries
The method is conservative (as long as surface integrals are the same for CVs sharing the boundary) *Most widely used method in CFD*
Disadvantage: more difficult to implement higher than 2nd order methods in 3D.

Finite element (FE)

The domain is broken into a set of discrete volumes: finite elements

The equations are multiplied by a weight function before they are integrated over the entire domain.

The solution is to search a set of non-linear algebraic equations for the computational domain.

Advantage: FE can easily deal with complex geometries.

Disadvantage: since unstructured in nature, the resultant matrices of linearized equations are difficult to find efficient solution methods. Not often used in CFD

Geometry

- The starting point for all problems is a “geometry.”
- The geometry describes the shape of the problem to be analyzed.
- Can consist of volumes, faces (surfaces), edges (curves) and vertices (points).
- Many different cell/element and grid types are available.

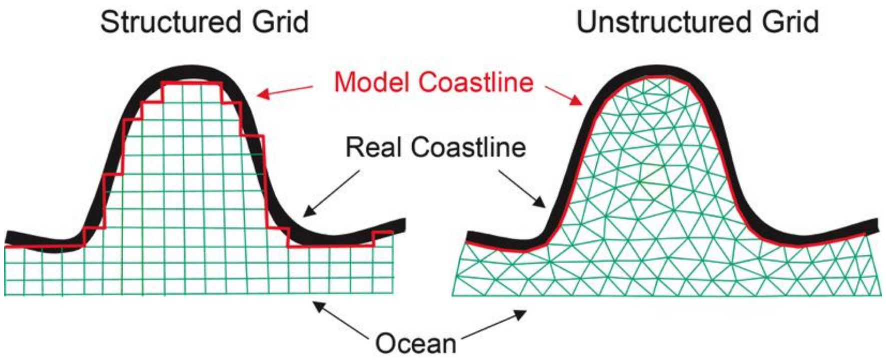
Choice depends on the problem and the solver capabilities.

Grids:

- Structured grid

  - all nodes have the same number of elements around it

  - only for simple domains
- Unstructured grid
  - for all geometries
  - irregular data structure



Structure/unstructured mesh

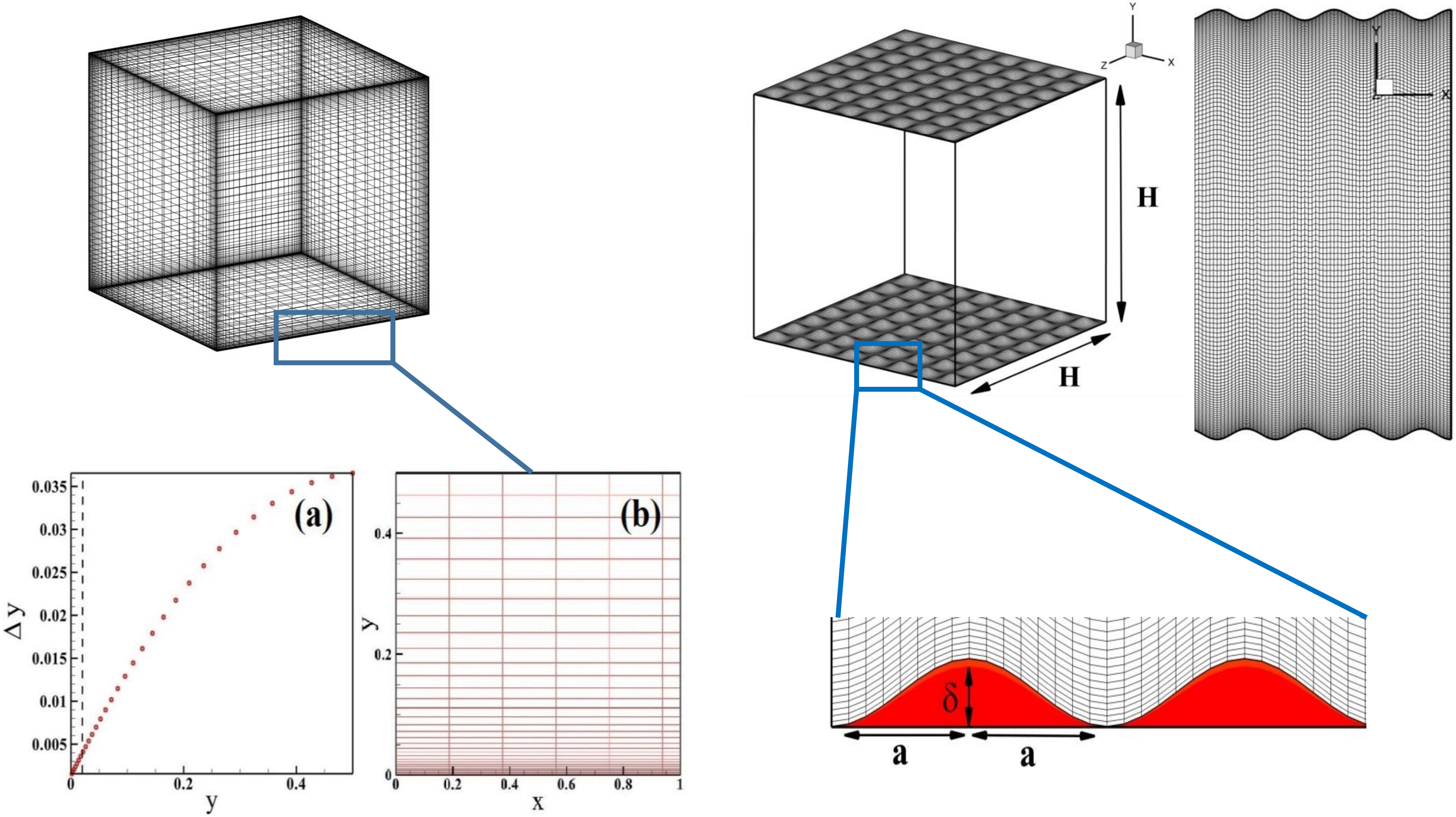
- Structured grid

  Advantages:
  - Economical in terms of both memory & computing time
  - Easy to code/more efficient solvers available
  - The user has full control in grid generation
  - Easy in post processing

  Disadvantages
  - Difficult to deal with complex geometries

- Unstructured grid
  - Advantages/disadvantages: opposite to above points!!

Structure/unstructured mesh



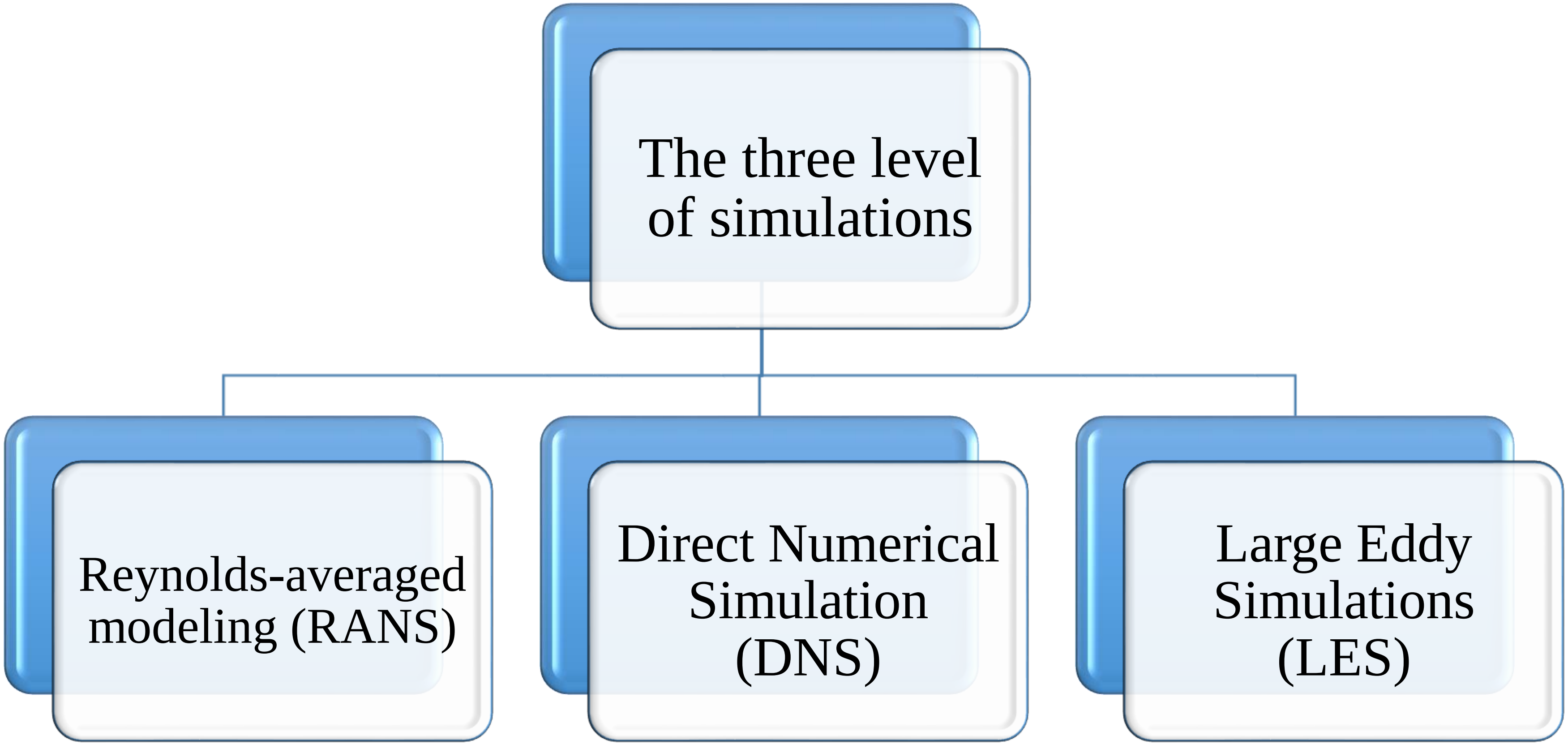
Stretched grid points within the thermal boundary layer (close to the solid wall)

Errors involved in CFD results

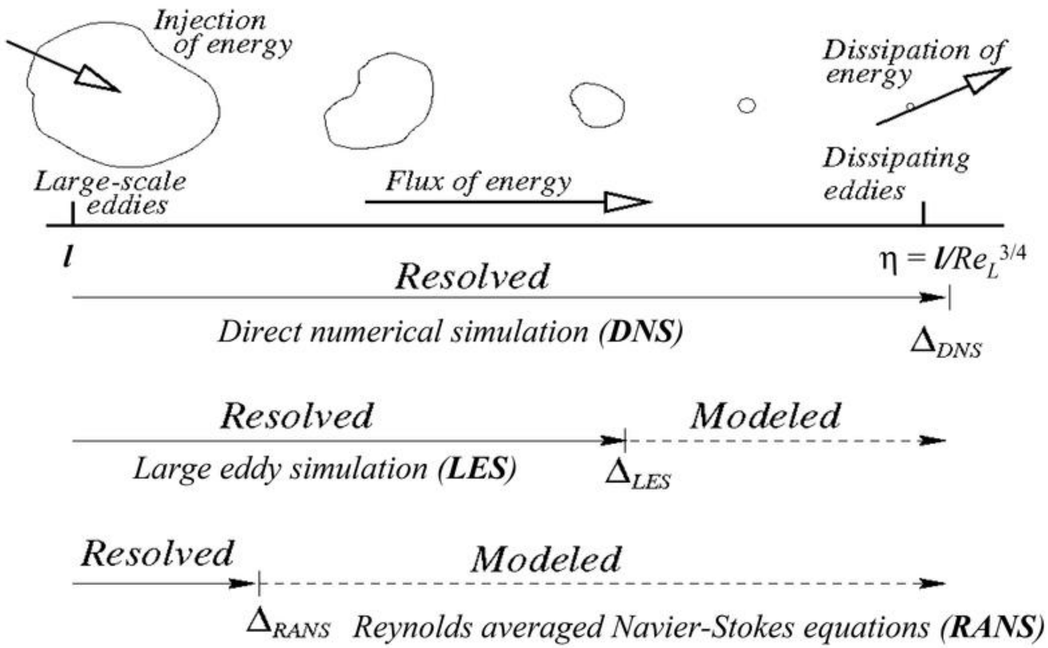
- Discretization errors
  - Depending on ‘schemes’ used. Use of higher order schemes will normally help to reduce such errors
  - Also depending on mesh size – reducing mesh size will normally help to reduce such errors. (skewness)
- Iteration errors
  - For converged solutions, such errors are relatively small.

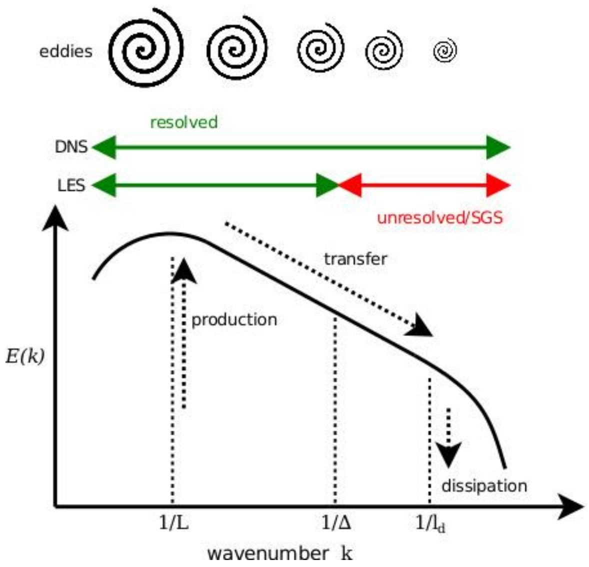
- Turbulence modelling
  - Some turbulence models are proved to produce good results for certain flows
  - Some models are better than others under certain conditions
  - But no turbulence model can claim to work well for all flows
- Physical problem *vs* mathematical model
  - Approximation in boundary conditions
  - Use of a 2D model to simplify calculation
  - Simplification in the treatment of properties

Introduction



Energy cascade





Reynolds-Averaged NS equations (RANS)

A more sophisticated method involves the use of Reynolds averaging: the long term average of a quantity f is defined as

$$\bar{f} = \frac{1}{T}\int_{t}^{t+T} f(\tau)d\tau$$

where T is a time interval much longer than all the time scales of the turbulent flow.

By averaging the Navier-Stokes equations, we obtain the Reynolds averaged Navier-Stokes (RANS) equations;

$$\frac{\partial u_i}{\partial x_i} = 0, \qquad \rho\frac{\partial u_i}{\partial t} + \rho\frac{\partial}{\partial x_j}\left(u_j u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{x_j}(2\mu S_{ij})$$

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \qquad \rho\frac{\partial \bar{u}_i}{\partial t} + \rho\frac{\partial}{\partial x_j}\left(\bar{u}_j \bar{u}_i\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{x_j}(2\mu S_{ij} - \rho\overline{u_i' u_j'})$$

$$R_{ij} = -\rho\begin{bmatrix} \overline{u'u'} & \overline{u'v'} & \overline{u'w'} \\ \overline{v'u'} & \overline{v'v'} & \overline{v'w'} \\ \overline{w'u'} & \overline{w'v'} & \overline{w'w'} \end{bmatrix}$$

In order to close the RANS equations, the Reynolds stress tensor must be modeled.

How can we close the RANS equations?

The objective of the turbulence models for the RANS equations is to compute the Reynolds stresses, which can be done by three main categories of RANS-based turbulence models:

- Linear eddy viscosity models
- Nonlinear eddy viscosity models
- Reynolds stress model (RSM)

Direct Numerical Simulation (DNS)

- **Direct numerical simulation (DNS)** is a simulation in CFD in which the NS-equations are numerically solved without any turbulence model. This means that the whole range of spatial and temporal scales of the turbulence must be resolved. All the spatial scales of the turbulence must be resolved in the computational mesh, from the smallest dissipative scales (Kolmogorov microscales), up to the integral scale L, associated with the motions containing most of the kinetic energy.

- Given the current processing speed and memory of the largest computers, only very modest Reynolds number flows with simple geometries are possible. i.e., The cost of a simulation increases as Re^3

- **Advantages:** DNS can be used as numerical flow visualization and can provide more information than experimental measurements; DNS can be used to understand the mechanisms of turbulent production and dissipation.

- **Disadvantages:** Requires supercomputers; limited to simple geometries.

- **Is DNS a useful tool?**

Large Eddy Simulation (LES)

- KEY IDEA is to directly solve the unsteady and 3D large-scale energy-carrying structures and to parametrize the more isotropic and dissipative small structures (subgrid-scales, SGS)
- Separation of the scales: application of a low-pass **filter** to the NS equations

$$\overline{f}(x) = \int_D f(x')G(x,x')dx'$$

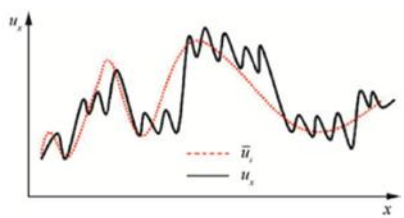
$G(x,x')$ is the filter function

FIRST NEED TO SEPARATE THE FLOW FIELD

Large eddies, most energy and fluxes, explicitly calculated, must be resolved.

Small eddies, little energy and fluxes, **parameterized**

- LES is a three dimensional, time dependent and computationally expensive simulation, though less expensive than DNS.

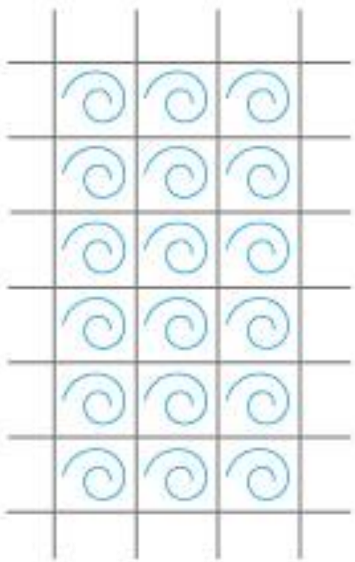


LES *vs* RANS

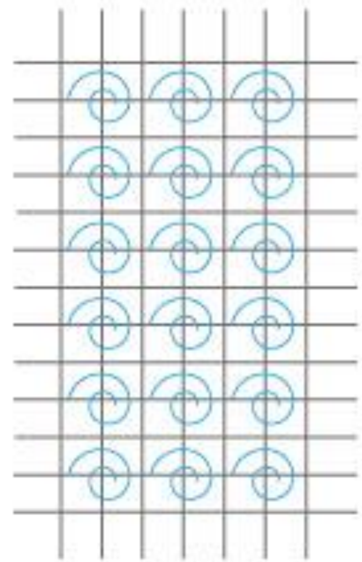
- LES can handle many flows which RANS (Reynolds Averaged Navier Stokes) cannot; the reason is that in LES more, turbulent scales are resolved. Here are some examples that could be studied by LES only:

- ❑ Flows with large separation
- ❑ Bluff-body flows (e.g. flow around a car); the wake often includes large, unsteady, turbulent structures
- ❑ Transition

- In RANS all turbulent scales are modeled⇒ inaccurate
- In LES only small, isotropic turbulent scales are modeled⇒accurate
- LES is *very* much more expensive than RANS.

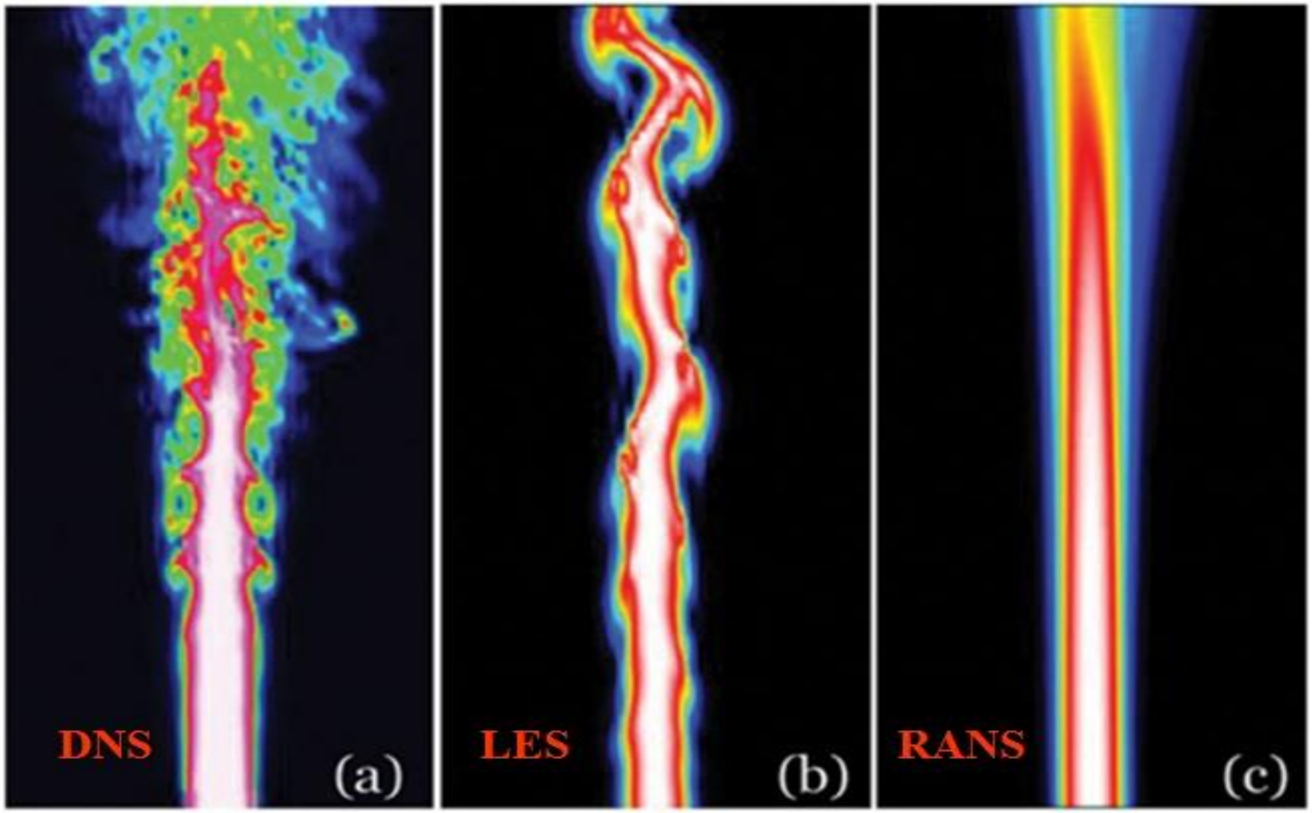


Mesh is coarse for eddies
→ RANS calculation



Mesh is fine for eddies
→ LES calculation

DNS, LES and RANS



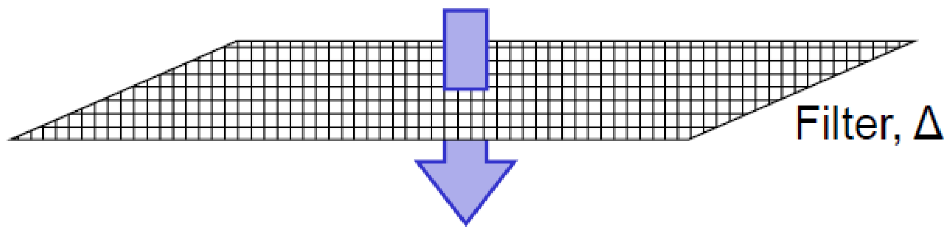
DNS (left), LES (middle) and RANS (right) predictions of a turbulent jet. LES requires less computational effort than DNS, while delivering more detail than the inexpensive RANS. (A. Maries, University of Pittsburgh)

LES

$$u_i(\mathbf{x},t) = \overline{u}_i(\mathbf{x},t) + u_i'(\mathbf{x},t)$$

Instantaneous component — Resolved Scale — Subgrid Scale

$$\frac{\partial u_i}{\partial t} + \frac{\partial \left(u_i u_j\right)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial u_i}{\partial x_j}\right)$$



Filtered N-S equation

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \left(\overline{u}_i \overline{u}_j\right)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial \overline{u}_i}{\partial x_j}\right) - \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\tau_{ij} = \rho\left(\overline{u_i u_j} - \overline{u}_i \overline{u}_j\right)$$

(Subgrid scale Turbulent stress)

- Spectrum of turbulent eddies in the Navier-Stokes equations is filtered:
  - The filter is a function of grid size
  - Eddies smaller than the grid size are removed and modeled by a subgrid scale (SGS) model.
  - Larger eddies are directly solved numerically by the filtered transient NS equation

Filtered momentum equation

- Filter the momentum eq. with an arbitrary homogenous filter of width $\bar{\Delta}$
- homogeneity of filter allows commutation with differentiation:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\overline{u_i u_j})}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \bar{u}_i}{\partial x_j^2}$$

- $\overline{u_i u_j} = \overline{u_i u_j} + \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j$ leads to

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$$

- τ_{ij} is an unknown stress accounting for the effect of the filtered-out small scales on the large scales governed by the filtered equation

Residual (subgrid-scale (SGS)) stress

- Note that in general: $A_{ij}^{d} \equiv A_{ij} - (1/3)\delta_{ij} A_{kk}$

Decompose the SGS stress as $\tau_{ij} = \tau_{ij}^{d} + \tau_{ij}^{iso}$

$$\tau_{ij}^{d} = (\underbrace{\overline{u_i u_j} - \overline{u}_i \overline{u}_j}_{\tau_{ij}}) - \frac{1}{3}\delta_{ij}(\underbrace{\overline{u_k u_k} - \overline{u}_k \overline{u}_k}_{\tau_{kk}}) \qquad \tau_{ij}^{iso} = \frac{1}{3}\delta_{ij}(\underbrace{\overline{u_k u_k} - \overline{u}_k \overline{u}_k}_{\tau_{kk}})$$

deviatoric (trace-free) component

isotropic component

- This decomposition leads to

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial(\overline{u}_i \overline{u}_j)}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial^2 \overline{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}^{d}}{\partial x_j}$$

- The modified filtered pressure contains the isotropic part of the SGS stress

Filtered equations

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

SGS stress

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}^d}{\partial x_j} + Ri(\bar{\rho} - \bar{\rho}_b)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \bar{u}_i \frac{\partial \bar{\rho}}{\partial x_i} = \kappa \frac{\partial^2 \bar{\rho}}{\partial x_i^2} - \frac{\partial \lambda_i}{\partial x_i}$$

SGS density flux

SGS stress: $\tau_{ij}^d = (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)^d \equiv (\overline{u_i u_j} - \bar{u}_i \bar{u}_j) - \frac{1}{3}\delta_{ij}(\overline{u_k u_k} - \bar{u}_k \bar{u}_k)$

SGS density flux: $\lambda_i \equiv \overline{\rho u_i} - \bar{\rho}\bar{u}_i$

(obtained in same way as the SGS stress)

Comments on the filtered equations

- The filtered equations are numerically solved for the filtered $(\overline{u_i}, \bar{\rho}, \bar{P})$ variables describing the large scales

- The SGS stress and SGS density flux present closure problems and must be modeled or approximated in terms of filtered variables only

- In theory, the filter used to obtain the filtered equations is arbitrary

- In practice, the filter is inherently assumed by the discretization (i.e. the numerical method used to solve the filtered equations and the SGS models)

- The discretization can only represent (resolve) down to scales on the order of 1,2, or 3 times the grid cell size, *h*, thereby “filtering-out” smaller scales.

Smagorinsky SGS model

- Recall that the SGS stress and density buoyancy flux must be modeled or approximated

Both are trace-free

Smagorinsky (1967) model:

$$\tau_{ij}^{d} \equiv (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)^{d} \approx -2\nu_T \bar{S}_{ij}$$

$$\nu_T = (C_S \bar{\Delta})^2 \,|\bar{S}|$$

Smagorinsky coefficient

$$|\bar{S}| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$$

$$\bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)$$

Analogously:

$$\lambda_i \equiv \overline{\rho u_i} - \bar{\rho}\bar{u}_i \approx -\kappa_T (\partial \bar{\rho} / \partial x_i)$$

$$\kappa_T = (C_\rho \bar{\Delta})^2 \,|\bar{S}|$$

The eddy (turbulent) viscosity

The turbulent viscosity has units L^2/T. Because we are working with the smallest resolved scales, we can set $L=\overline{\Delta}$

- And we may have $T=(\overline{\Delta}^2/\varepsilon)^{1/3}\Rightarrow \nu_T = C\varepsilon^{1/3}\overline{\Delta}^{4/3}$

- In a global sense, the rate of energy transfer within the inertial range is roughly equal to the SGS dissipation. Here we assume it locally:

$$\varepsilon \approx \overbrace{-\tau_{ij}^d \overline{S}_{ij}} = \nu_T\,|\,\overline{S}\,|^2 \Rightarrow \nu_T = \underbrace{C}_{C_S^2}{}^{3/2}\,\overline{\Delta}^2\,|\,\overline{S}\,|$$

Difficulties with the Smagorinsky model

Smagorinsky model: $$\tau_{ij}^{d} \equiv (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)^d \approx -2\nu_T \bar{S}_{ij}$$

$$\nu_T = (C_S \bar{\Delta})^2 |\bar{S}|$$

- For isotropic turbulence, Lilly (1967) showed that $C_S = 0.16$

Major difficulty:

- The constant coefficient allows for a non-vanishing turbulent viscosity at boundaries and in the presence of relaminarization

- The Smagorinsky coefficient should be a function of **space and time**

- In 1991, Germano and collaborators derived a dynamic expression for the Smagorinsky coefficient

Dynamic Smagorinsky model

- Recall filtering the N-S equations with an homogeneous filter of width

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}^d}{\partial x_j} \qquad \tau_{ij}^d \equiv (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)^d \approx -2(C_S \bar{\Delta})^2 |\bar{S}| \bar{S}_{ij}$$

Consider a new filter made up from successive applications of the 1st filter (above) and a new "test" filter. This "double" filter has width $\hat{\bar{\Delta}}$

Application of this "double" filter is denoted by a "bar-hat" in the form of $\hat{\bar{f}}$

With this new filter, the filtered momentum equation becomes:

$$\frac{\partial \hat{\bar{u}}_i}{\partial t} + \hat{\bar{u}}_j \frac{\partial \hat{\bar{u}}_i}{\partial x_j} = -\frac{\partial \hat{\bar{P}}}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \hat{\bar{u}}_i}{\partial x_j^2} - \frac{\partial T_{ij}^d}{\partial x_j} \qquad T_{ij}^d \equiv (\overline{u_i u_j} - \hat{\bar{u}}_i \hat{\bar{u}}_j)^d \approx -2(C_S' \hat{\bar{\Delta}})^2 |\hat{\bar{S}}| \hat{\bar{S}}_{ij}$$

- Scale invariance: Both $\hat{\bar{\Delta}}$ and $\bar{\Delta}$ are in the inertial range, thus $C_S' = C_S$

Dynamic Smagorinsky model

- Consider the following tensor proposed by Germano (GI) : $L_{ij}^{d} \equiv T_{ij}^{d} - \tau_{ij}^{d}$

$$L_{ij}^{d} = (\widehat{\overline{u_i u_j}} - \hat{\bar{u}}_i \hat{\bar{u}}_j)^d - (\widehat{\overline{u_i u_j}} - \widehat{\bar{u}_i \bar{u}_j})^d = (\widehat{\bar{u}_i \bar{u}_j} - \hat{\bar{u}}_i \hat{\bar{u}}_j)^d \longleftarrow \text{(resolved)}$$

$$L_{ij}^{d} = -2(C_S \hat{\bar{\Delta}})^2 |\hat{\bar{S}}| \hat{\bar{S}}_{ij} + 2(C_S \bar{\Delta})^2 \widehat{|\bar{S}| \bar{S}_{ij}} \longleftarrow \text{(modeled)}$$

- Minimization of the difference between these two with respect to Cs leads to:

$$(C_S \bar{\Delta})^2 = \frac{< L_{ij} M_{ij} >}{< 2 M_{kl} M_{kl} >} \qquad M_{ij} = |\bar{S}| \bar{S}_{ij} - \alpha |\hat{\bar{S}}| \hat{\bar{S}}_{ij}$$

$< \cdot >$ - Averaging in statistically homogenous direction(s)

$$L_{ij} = \widehat{\bar{u}_i \bar{u}_j} - \hat{\bar{u}}_i \hat{\bar{u}}_j \qquad \alpha = \left(\hat{\Delta} / \Delta \right)^2$$

- Explicit application of test filter (denoted by a “hat”) is required, unlike 1st filter

LES methodology used in computations

$$
\begin{cases}
\dfrac{\partial \bar{u}_i}{\partial x_i} = 0 \\[2ex]
\dfrac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \dfrac{\partial \bar{u}_i}{\partial x_j} = -\dfrac{\partial \bar{P}}{\partial x_i} + \dfrac{1}{\mathrm{Re}} \dfrac{\partial^2 \bar{u}_i}{\partial x_j^2} - \dfrac{\partial \tau_{ij}^d}{\partial x_j} + F\delta_{i1} + Ri(\bar{\rho} - \bar{\rho}_b) \\[2ex]
\dfrac{\partial \bar{\rho}}{\partial t} + \bar{u}_i \dfrac{\partial \bar{\rho}}{\partial x_i} = \kappa \dfrac{\partial^2 \bar{\rho}}{\partial x_i^2} - \dfrac{\partial \lambda_i}{\partial x_i}
\end{cases}
$$

SGS stress

SGS density flux

SGS stress model: $\tau_{ij}^d \approx -2\underbrace{(C_s \bar{\Delta})^2 |\bar{S}|}_{\nu_T} \bar{S}_{ij}$

SGS density flux model: $\lambda_i \approx -\underbrace{(C_s \bar{\Delta})^2 |\bar{S}|}_{\kappa_T} \partial \bar{\rho} / \partial x_i$

- Model coefficients in SGS models are computed **dynamically** as described

The Dynamic Lagrangian SGS model (Meneveau et al., 1996)

This model tries to improve the performance of the dynamic Smagorinsky model for non-homogeneous flows.

Rationale

- Dynamic model not reliable without averaging
  - Numerical instability
- So some averaging necessary
  - Global averaging successful but requires homogeneous direction
  - Local averaging possible but results depend on volume chosen
- Need an averaging procedure that works in complex flows.

Meneveau *et al*. (1996)* developed a Lagrangian version of DSM where C_s is averaged along fluid-paricle trajectories (back in time). The objective function to be minimized is given by

$$E = \int_{pathline} \epsilon_{ij}(z)\epsilon_{ij}(z)dz = \int_{-\infty} \epsilon_{ij}(z(t'),t')\epsilon_{ij}(z(t'),t')W(t-t')dt'$$

Time weighting function: $W(t-t') = T^{-1}e^{-(t-t')/T}$

$$\frac{D\Im_{LM}}{Dt} \equiv \frac{\partial \Im_{LM}}{\partial t} + \bar{u}_i \frac{\partial \Im_{LM}}{\partial x_i} = \frac{1}{T}\left(L_{ij}M_{ij} - \Im_{LM}\right)$$

$$\frac{D\Im_{MM}}{Dt} \equiv \frac{\partial \Im_{MM}}{\partial t} + \bar{u}_i \frac{\partial \Im_{MM}}{\partial x_i} = \frac{1}{T}\left(M_{ij}M_{ij} - \Im_{MM}\right)$$

$$(C_s\Delta)^2 = \frac{\Im_{LM}}{\Im_{MM}}$$

Time scale $T = \theta\Delta(\Im_{LM}\Im_{MM})^{-1/8}$; $\theta = 1.5$

* SGS density flux computed as (Armenio and Sarkar 2002 JFM):

$$\lambda_j = -C_\rho \Delta^2 |\bar{S}| \frac{\partial \bar{\rho}}{\partial x_j} \qquad C_\rho = -\frac{1}{2}\frac{\Im_i \mathcal{M}_i}{\mathcal{M}_k \mathcal{M}_k}$$

$$\mathcal{M}_i = \hat{\Delta}^2 |\hat{\bar{S}}| \widehat{\frac{\partial \bar{\rho}}{\partial x_i}} - \Delta^2 \widehat{|\bar{S}| \frac{\partial \bar{\rho}}{\partial x_i}} \qquad \Im_i = \widehat{\bar{\rho}\bar{u}_i} - \hat{\bar{\rho}}\hat{\bar{u}}_i$$

In summary….

DNS , LES, RANS require solving the unsteady form of the NS or RANS equations.

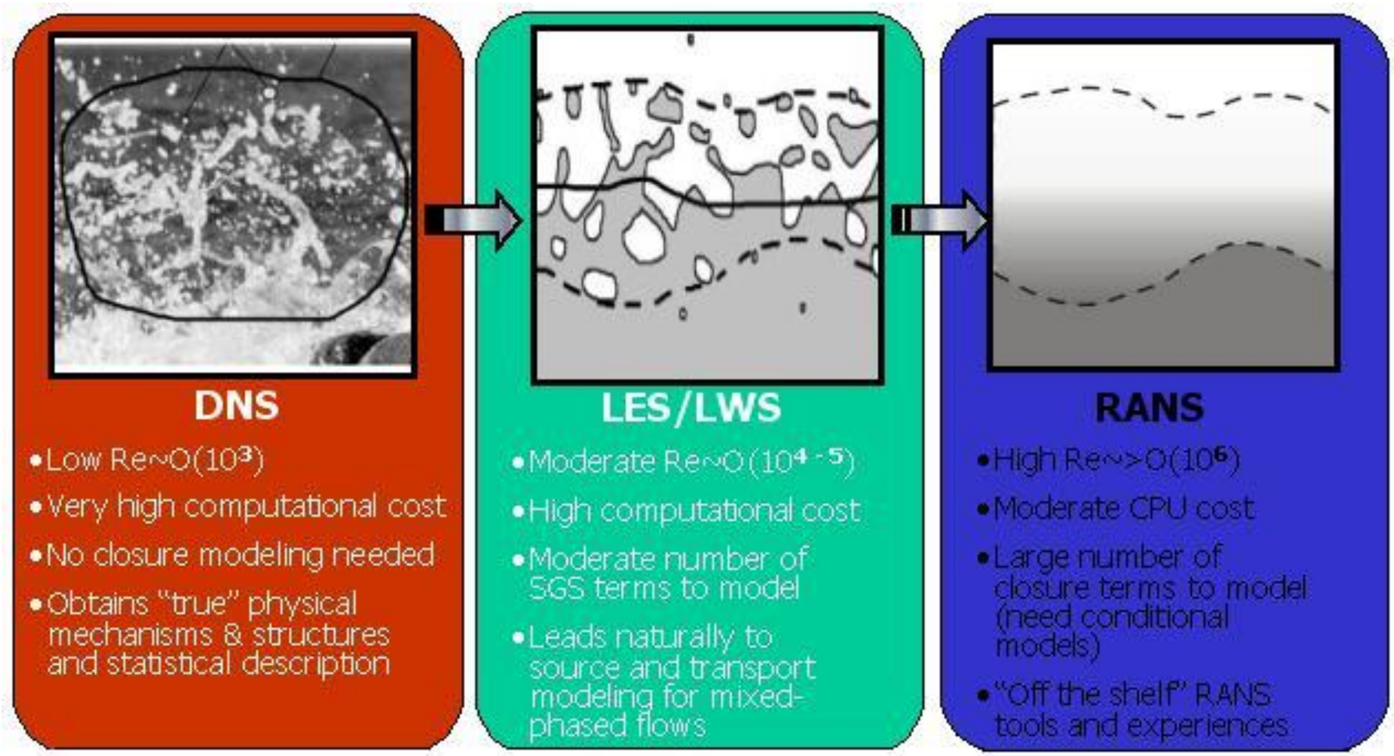
Main differences between steady-flow and unsteady-flow solvers are:

In steady –flow algorithms, typically continuity equation is not satisfied during the time-advancement of the solution and conservation laws are fulfilled at the convergent state of the solution

In unsteady-flow solvers conservation laws are satisfied at each time step

This makes a strong difference in CPU time request.

Typically projection methods are employed


DNS
•Low Re~O(10³)
•Very high computational cost
•No closure modeling needed
•Obtains "true" physical mechanisms & structures and statistical description
LES/LWS
•Moderate Re~O(10⁴⁻⁵)
•High computational cost
•Moderate number of SGS terms to model
•Leads naturally to source and transport modeling for mixed-phased flows
RANS
•High Re~>O(10⁶)
•Moderate CPU cost
•Large number of closure terms to model (need conditional models)
•"Off the shelf" RANS tools and experiences

General remarks on turbulence models

- There are no generically best models.
- Near wall treatment is generally a very important issue.
- A good mesh is important to get good accurate results.
- Different models may have different requirement on the mesh.
- Expertise/validation are of great importance to CFD.

Motivation of the Study

VOLUME 87, NUMBER 18 PHYSICAL REVIEW LETTERS 29 OCTOBER 2001

Does Turbulent Convection Feel the Shape of the Container?

Z. A. Daya and R. E. Ecke

PHYSICAL REVIEW E **90**, 063003 (2014)

Influence of container shape on scaling of turbulent fluctuations in convection

N. Foroozani,[1,2] J. J. Niemela,[1] V. Armenio,[2] and K. R. Sreenivasan[3]

Formulation of the problem

$$\frac{\partial \overline{u}_j}{\partial x_j} = 0,$$

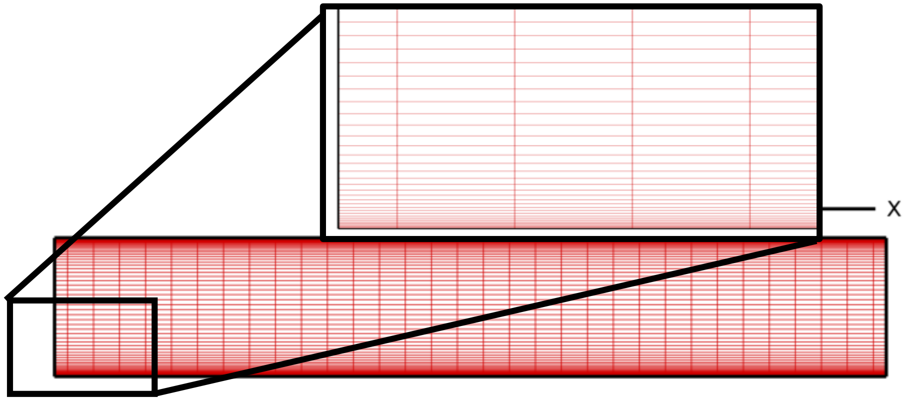
$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_j \overline{u}_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial \overline{P}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j} - \frac{\overline{\rho}}{\rho_0} g \delta_{i2} - \frac{\partial \tau_{ij}}{\partial x_j},$$

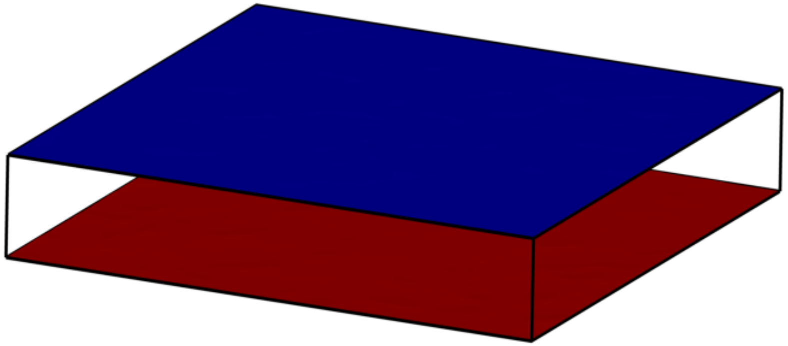
$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{u}_j \overline{\rho}}{\partial x_j} = k \frac{\partial^2 \overline{\rho}}{\partial x_j \partial x_j} - \frac{\partial \lambda_j}{\partial x_j},$$

RBC with periodic walls, but why?

- First we need to find a proper numerical method in terms of definite geometry therefore we performed LES and DNS in an unbounded, homogeneous, domain.

- Our geometry is a 3D rectangular box (6,1,6) ($\Gamma = 6$), note in our study "*y*" is in vertical direction, with periodic boundary conditions over horizontal domain (*x*-*z*), no-slip velocity on the top and bottom surface, $\frac{d\rho}{\rho_0} = 1$ is applied in wall normal directions
- Molecular Prandtl number Pr=1 and *Ra* number vary $6.3 \times 10^5 \leq Ra \leq 10^8$.
- The vertical resolution in all LES was chosen such that the thermal boundary layer λ_θ is properly resolved.





Introduction

The number of nodes required in thermal and viscous boundary layers computed as:

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

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

Shishkina *et al.*, 2010.

We performed two tests for LES:

1) $\kappa_{sgs} = \dfrac{\upsilon_{sgs}}{Pr_{sgs}}$ with Pr_{sgs} set *a priori* test (static)

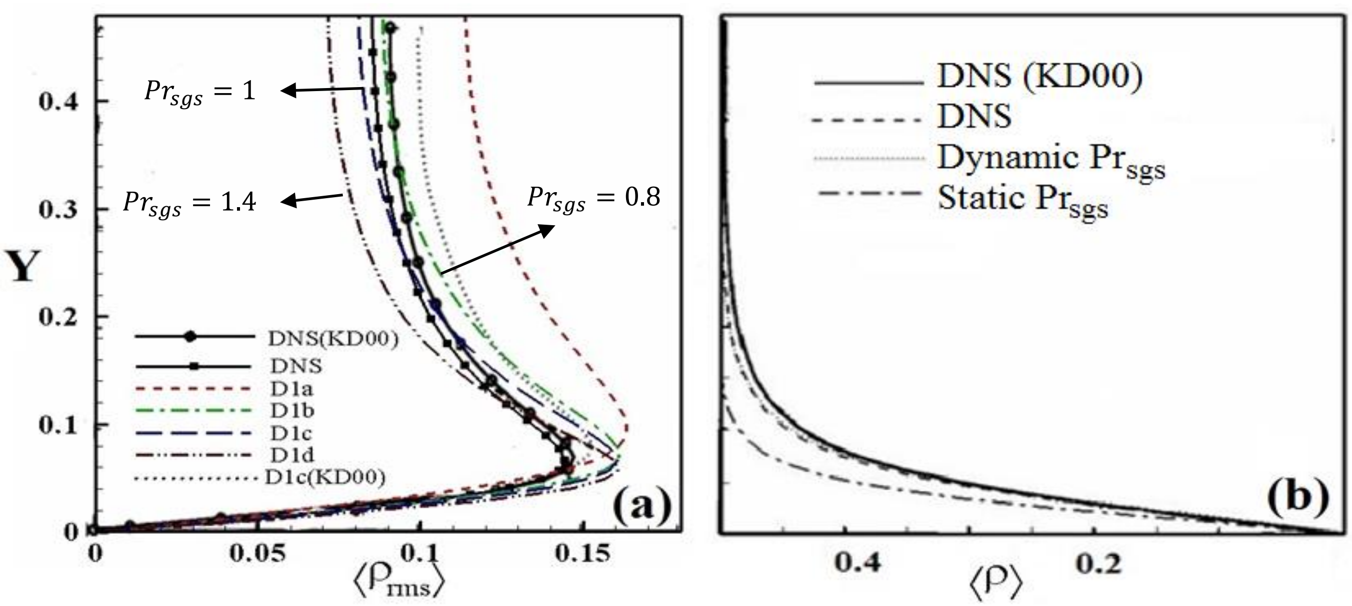
2) Both υ_{sgs} and κ_{sgs} calculated dynamically

Introduction

Total turbulent fluctuations = Resolved + SGS

The resolved root-mean-square of density fluctuations computed as:

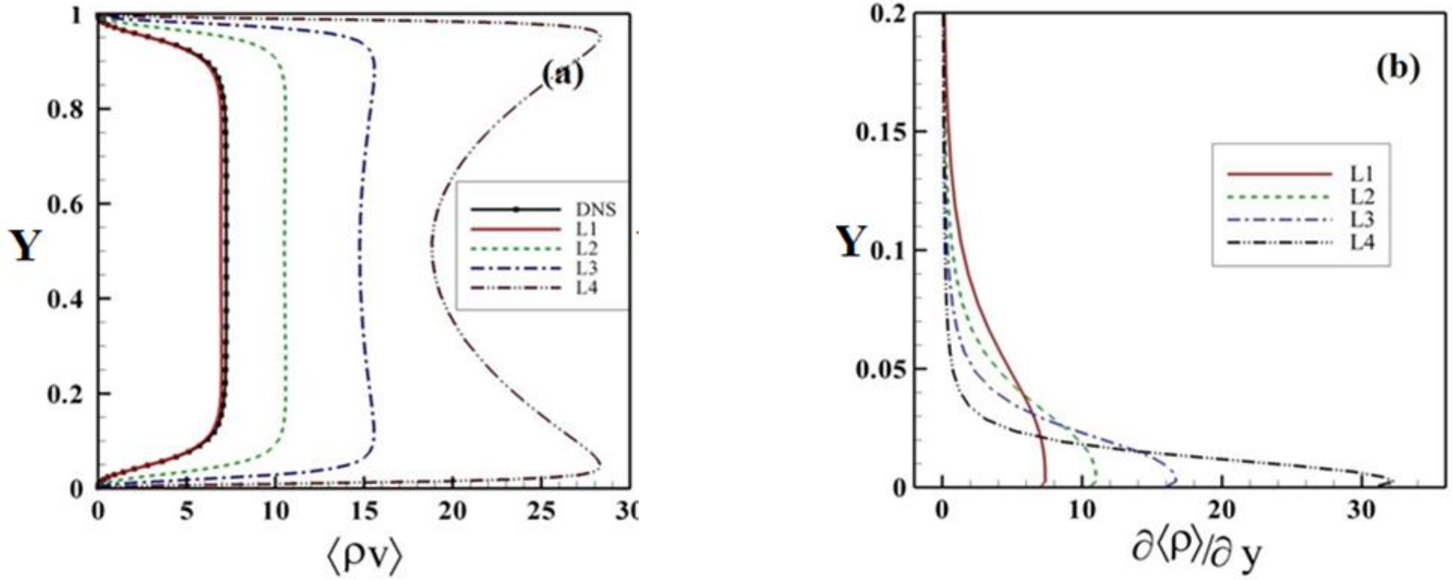
$$\rho_{rms} = [\langle\rho(x)\rho(x)\rangle_t - \langle\rho(x)\rangle_t\langle\rho(x)\rangle_t]^{1/2}$$



(a) The resolved *rms* density fluctuations computed with the dynamic model at $\mathrm{Ra} = 6.3 \times 10^5$ *on the* $32 \times 64 \times 32$ grids (b) Mean density profiles for $\mathrm{Ra} = 6.3 \times 10^5$ with dynamic (L0) and static (D1c) Pr_{sgs}. Data are compared with Kimmel and Domaradzki (2000).

The key response of the system to the imposed parameters is the heat flux from bottom to top (Nu).

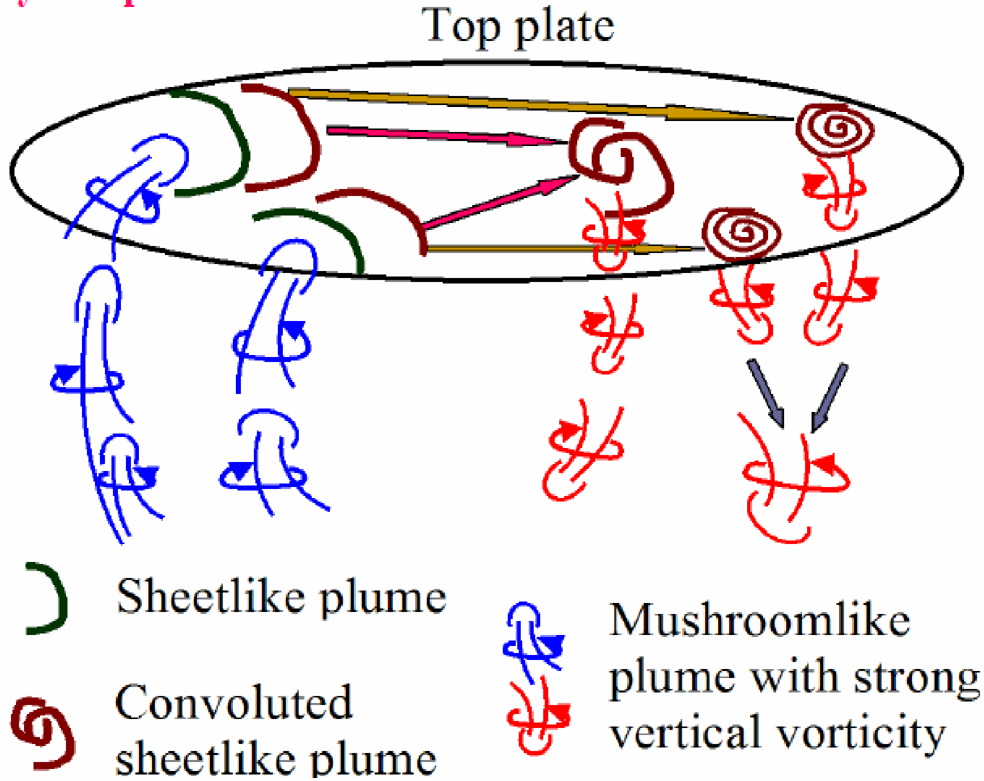
Global Nusselt number: $$Nu = \frac{\langle \rho v \rangle_{A,t} - \kappa \frac{\partial \langle \rho \rangle_{A,t}}{\partial y}}{\kappa \Delta \rho / H}$$ $\Rightarrow$ $\boldsymbol{Nu = 0.14 Ra^{0.29}}$

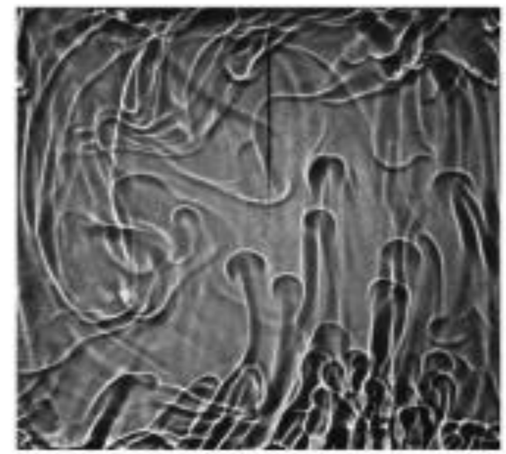


Comparison of the Nusselt number , Nu, components using dynamic Pr_{sgs} as a function of Ra numbers; (a) resolved vertical density flux and (b) resolved density gradient along vertical direction. The letters represent L1 (6.3×10^5), L2 (2.5×10^6), L3 (10^7), L4 (10^8)

Flow topology in convection

Physical picture

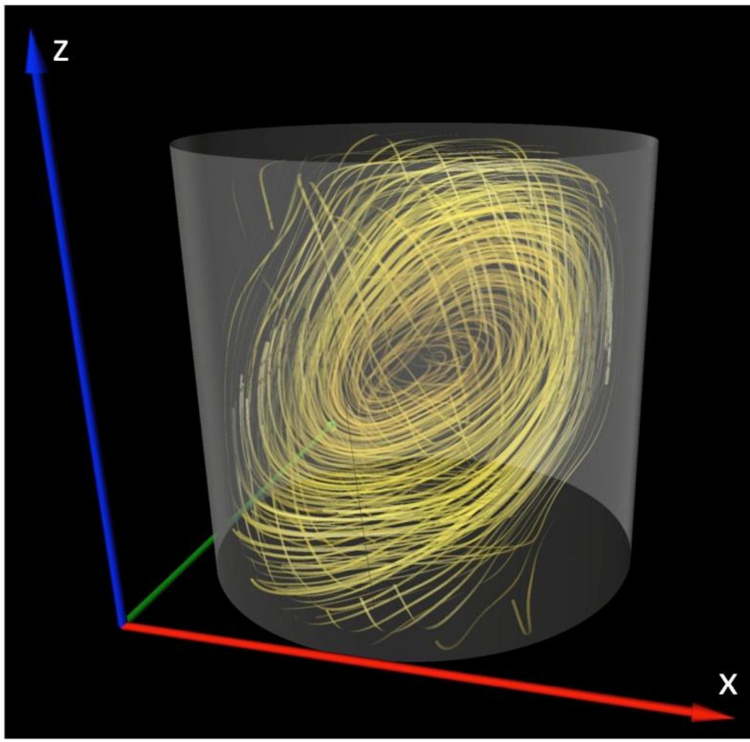




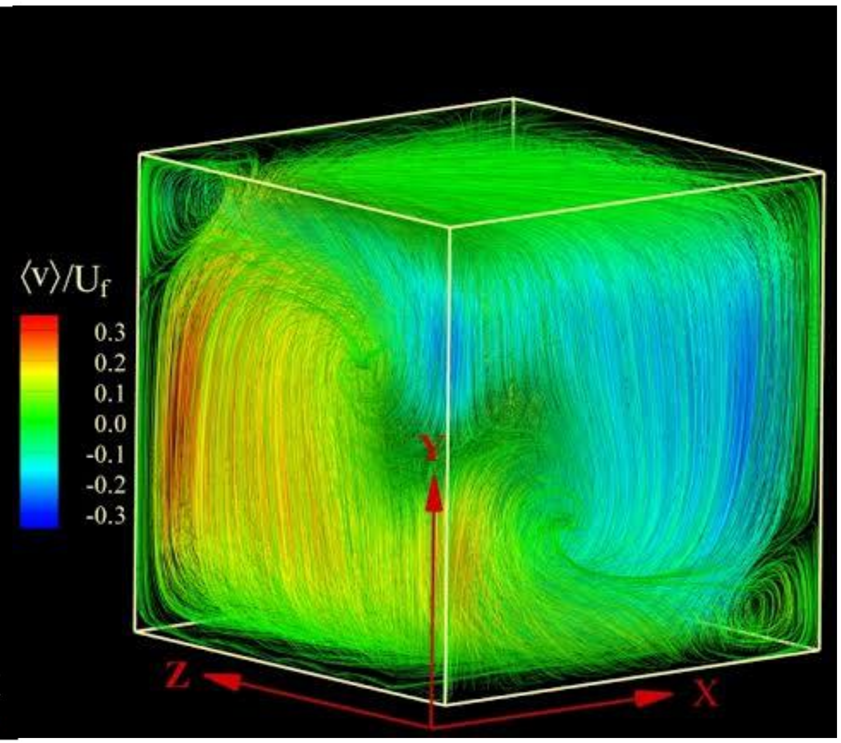
Mushroom-like plumes (side view)

Zhang et al, PoF 2007

The mean wind



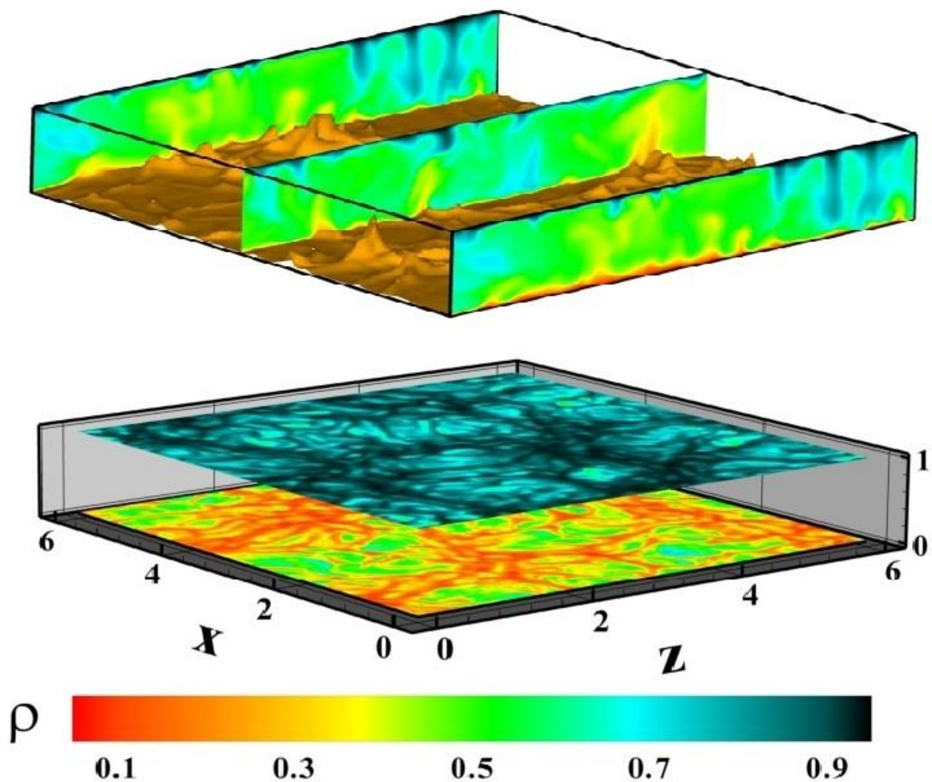
For convection in a round cylinder, the mean wind precesses freely.



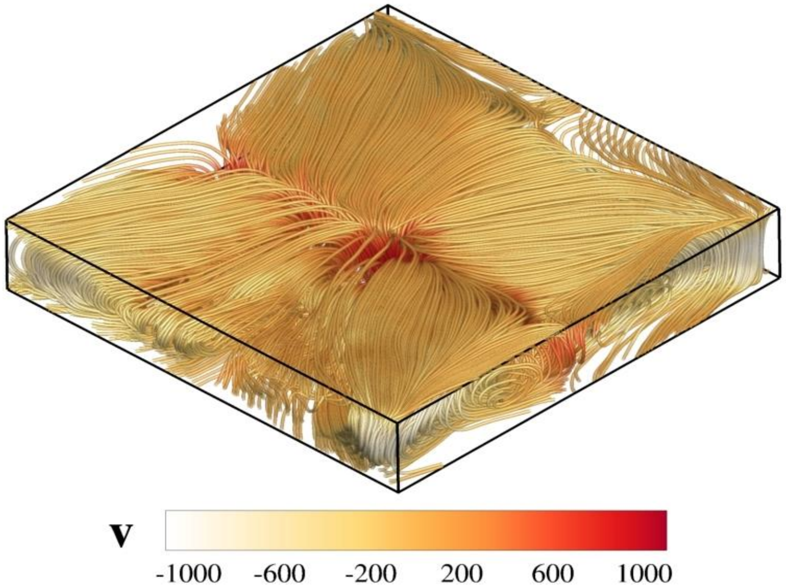
For convection in a cubic box, the mean wind is constrained along a diagonal.

From my simulation…

Instantaneous field



Time averaged field



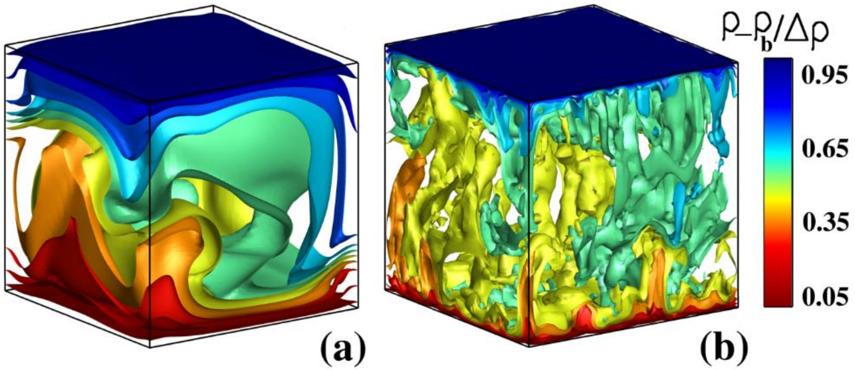
Influence of the geometry

- We perform LES in a closed cubic cell Γ=1, for $10^6 < Ra < 10^{10}$, molecular Prandtl number set to Pr =0.7
- Vertical walls are adiabatic ($\partial\rho/\partial\vec{n}$=0),
- We applied no-slip BCs at the walls,
- Finer grid close to the walls (Verzicco and Camussi JFM 2003),
- We use coarse grid at low Ra numbers, and finer resolution at high Ra. Hyperbolic tangent function is used to stretch the mesh.

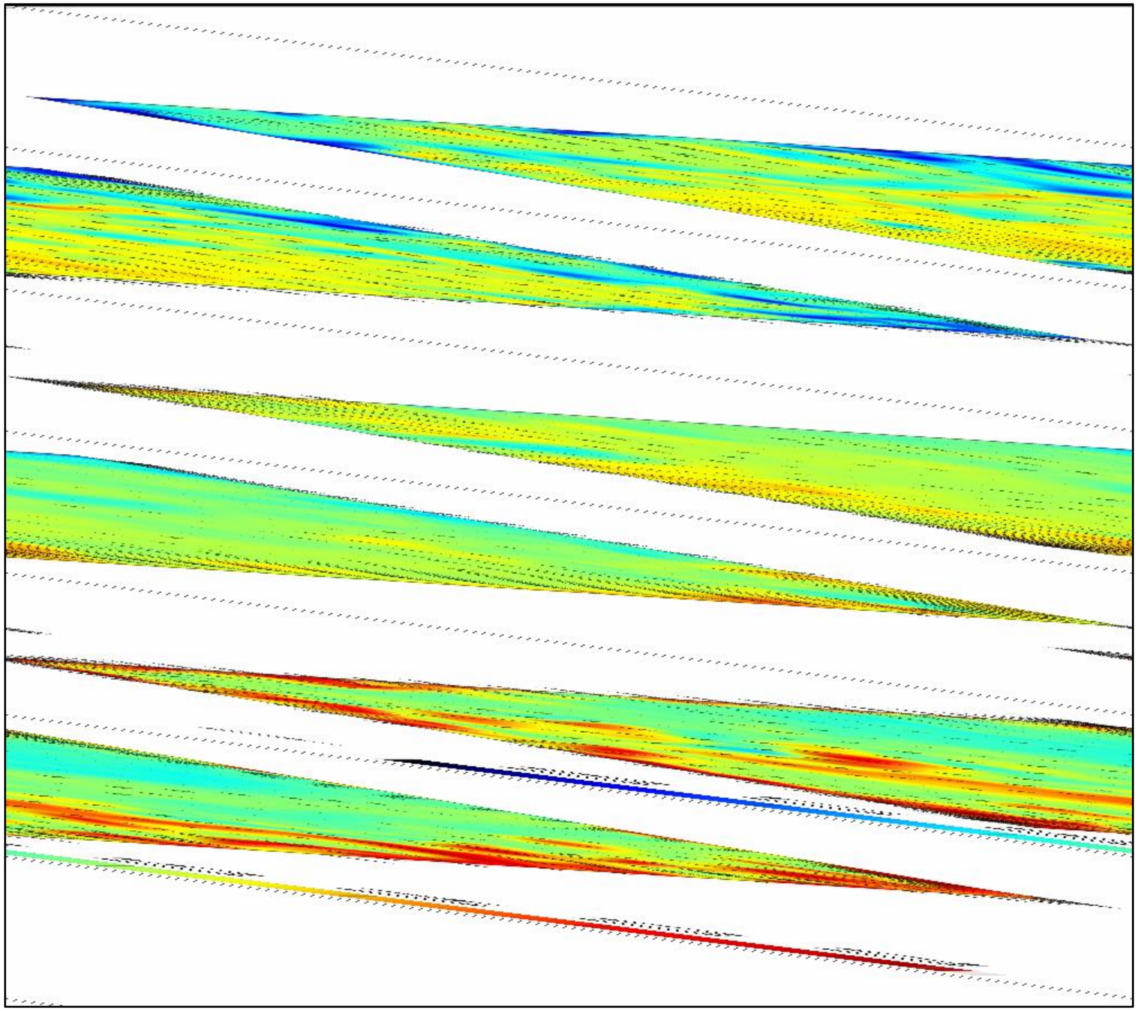
✓ We compute global Nusselt number: $$Nu = \frac{\kappa\partial_y<\rho>_{A,t} - <u_y\rho>_{A,t}}{\kappa\Delta\rho H^{-1}}$$

✓ Scaling of Nu(Ra) is in good agreement with both the laboratory experiment [Qiu & Xia 1998], and DNS of Kaczorowski & Xia 2013 (JFM 722,569)

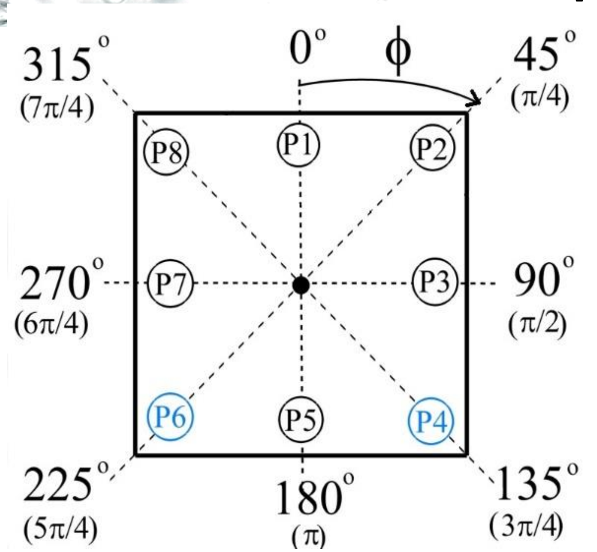
Ra	$N_x \times N_y \times N_z$	N_{BL}	Nu	Nu_{Ref}
1×10^6	32 × 64 × 32	14	8.31	8.32
3×10^6	32 × 64 × 32	11	11.4	11.5
1×10^7	32 × 64 × 32	10	16.4	16.3
3×10^7	32 × 64 × 32	8	22.4	22.0
1×10^8	32 × 64 × 32	6	31.6	31.3
1×10^9	64 × 96 × 64	5	63.4	
1×10^{10}	64 × 96 × 64	5	116.2	



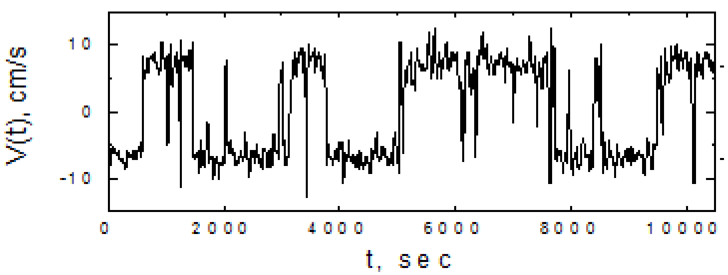
Structures of the mean flow

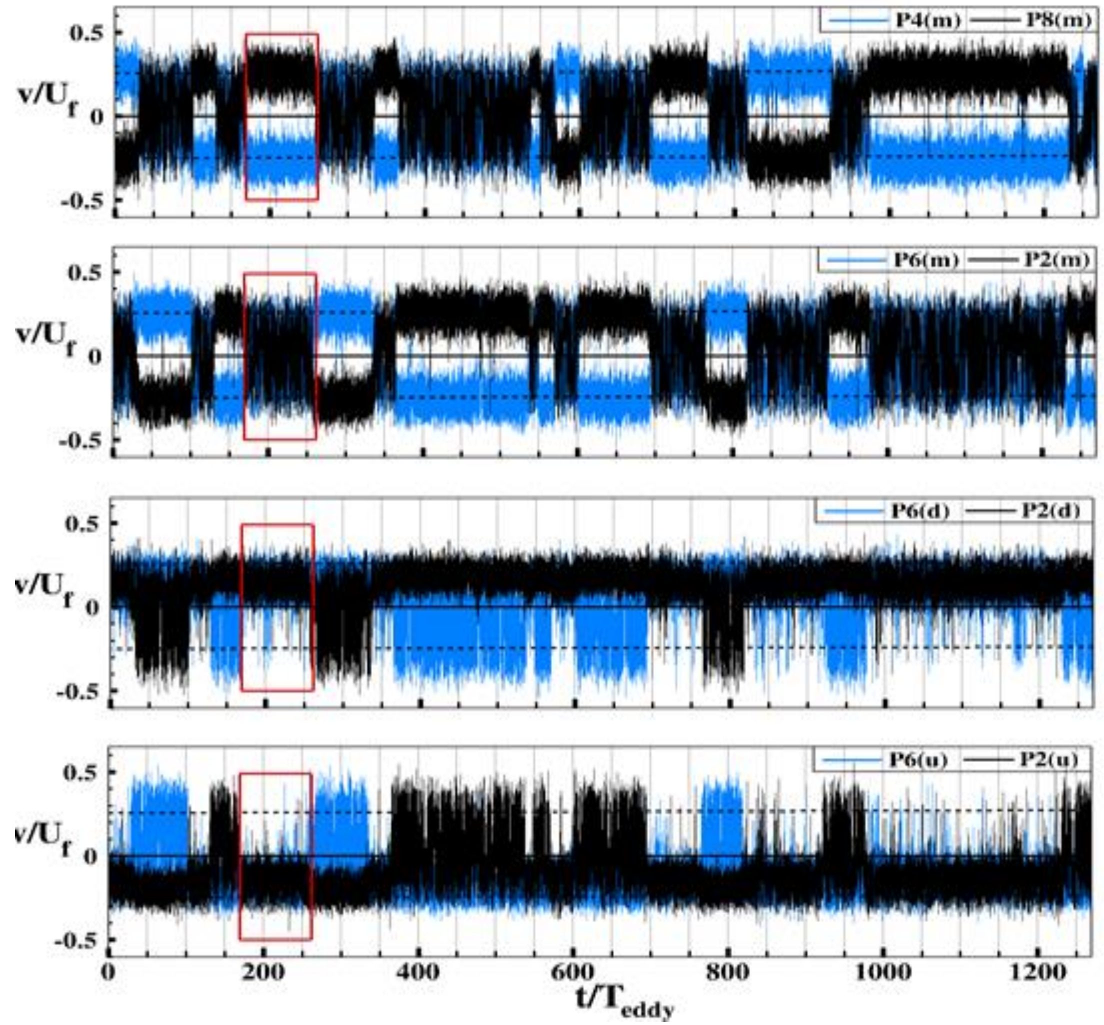


Velocity statistics



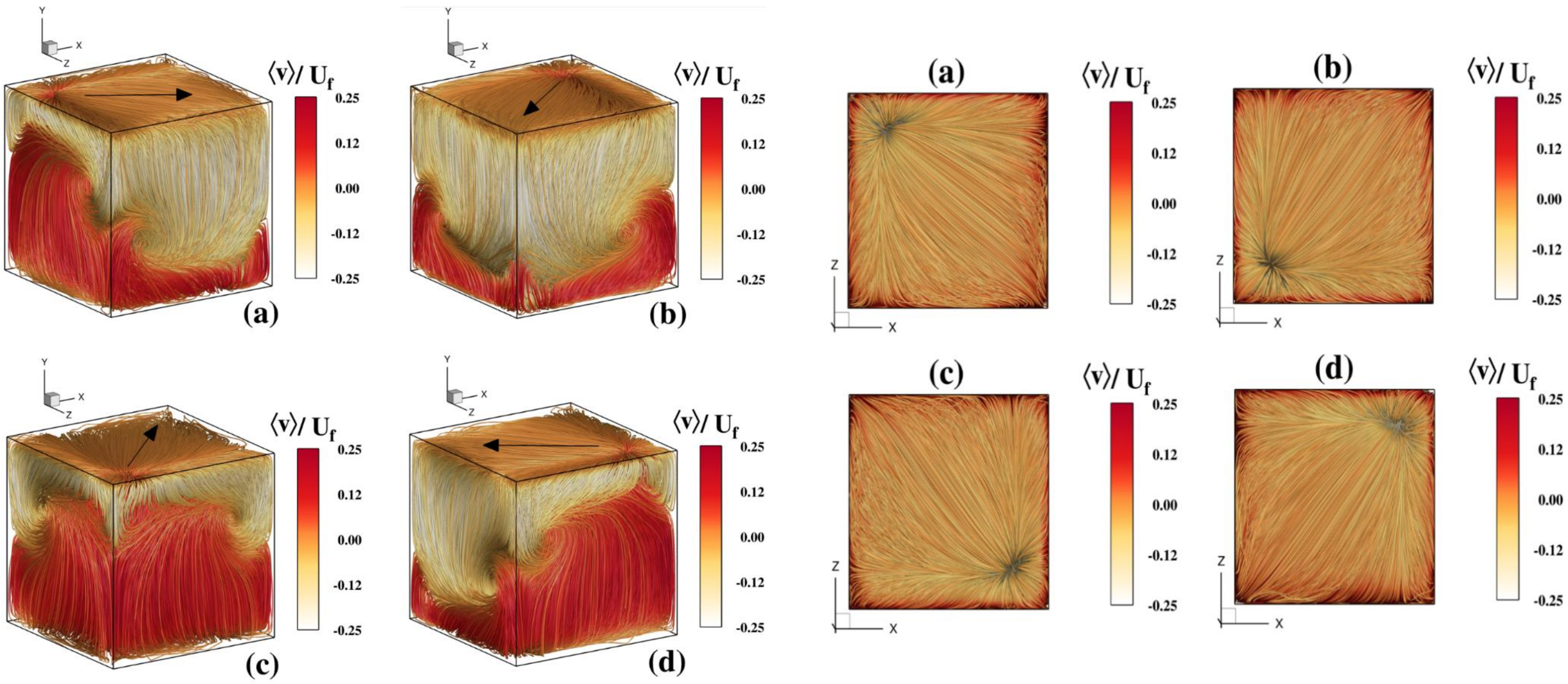
Schematic of an arbitrary horizontal plane showing the azimuthal positions for probes, placed at azimuthal angles $\varphi_i = (i\pi)/4$, i=1,…,8 . The distance from the vertical walls are 0.1H for all cases.





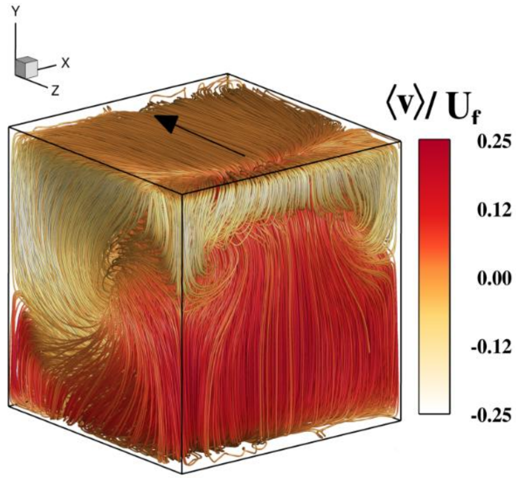
Niemela and Sreenivasan, *Nature* (2000).

Mean flow structure at $Ra = 10^8$

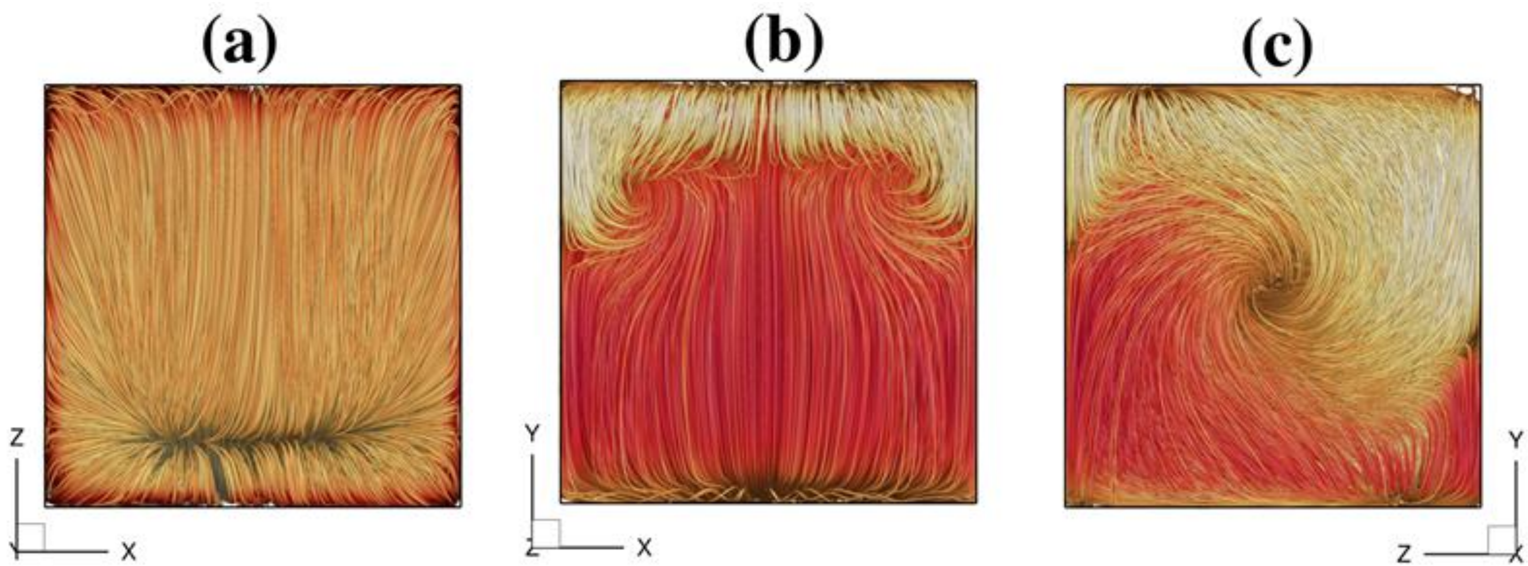


Time averaged of velocity streamlines. The color coding depicts the magnitude of the vertical velocity normalized by free fall velocity. The large arrow shows the direction of the LSC.

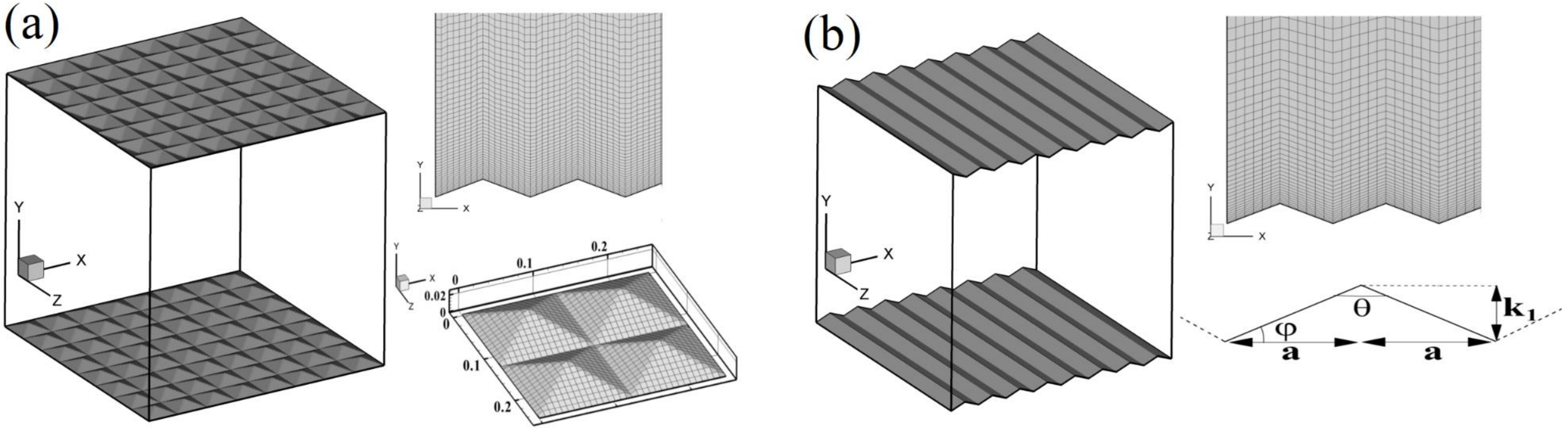
Transient state during the re-orientation of the LSC

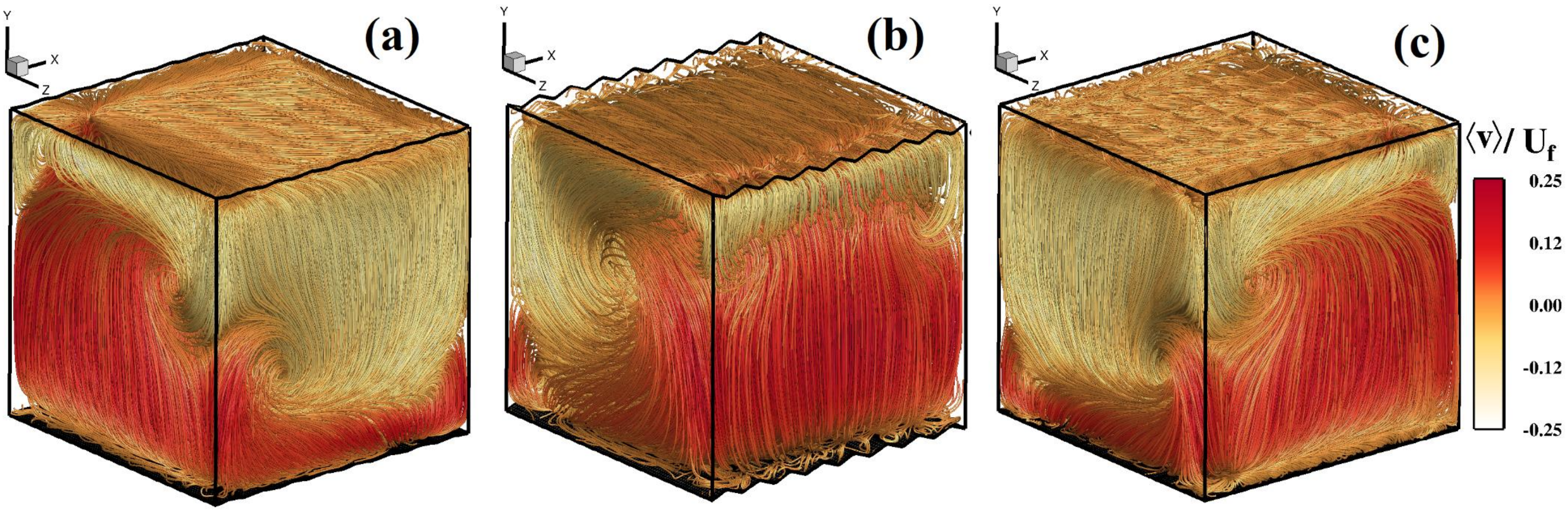


The 3D perspective of the transition state of the global ow structure during a reorientation of the LSC from one stable diagonal plane to the other.



Thermal Convection in the presence of rough surfaces





Introduction

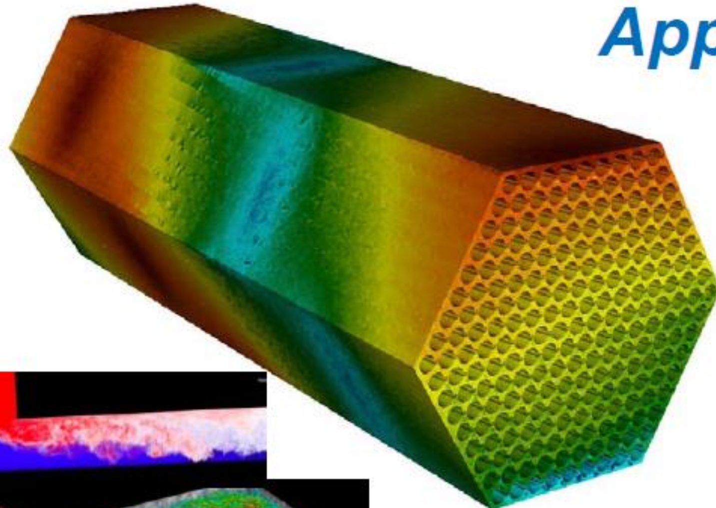
Nek5000 and Spectral Element

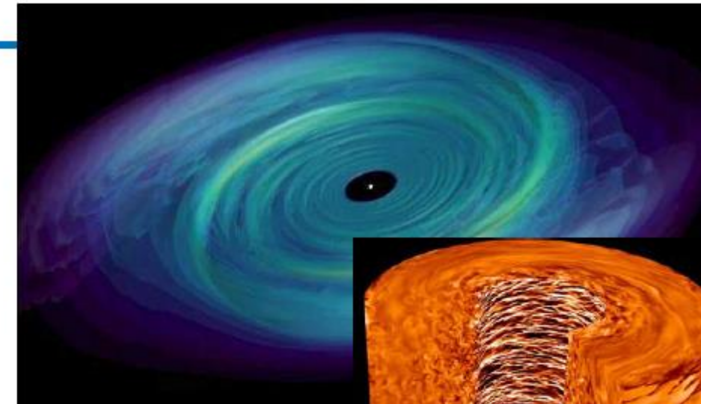
Paul Fischer
Mathematics and Computer Science Division
Argonne National Laboratory

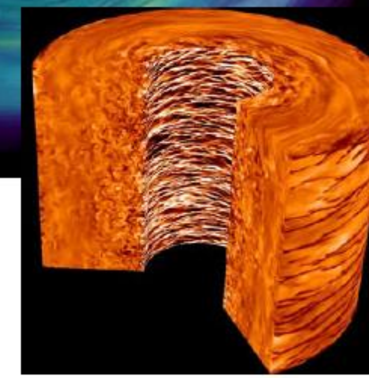
NEK5000

- ❑ Nek5000: Scalable Open Source Spectral Element Code
- ❑ Developed at MIT in mid-80s (Patera, F., Ho, Ronquist)
- ❑ Spectral Element Discretization: High accuracy at low cost
- ❑ Tailored to LES and DNS of turbulent heat transfer, but also supports
  - ✓ Low-Mach combustion, MHD, conjugate heat transfer, moving meshes
  - ✓ New features in progress: compressible flow (Duggleby), adjoints, immersed boundaries (KTH)
- ❑ Current Verification and validation.

Applications

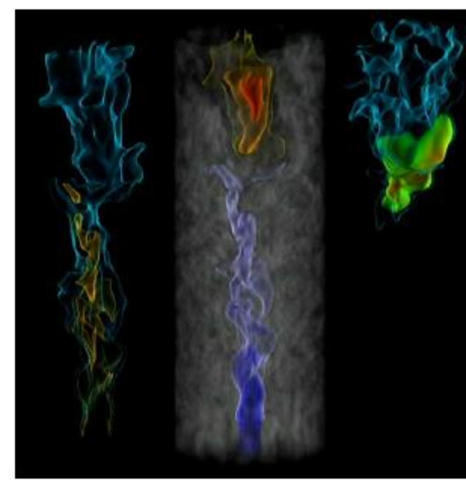


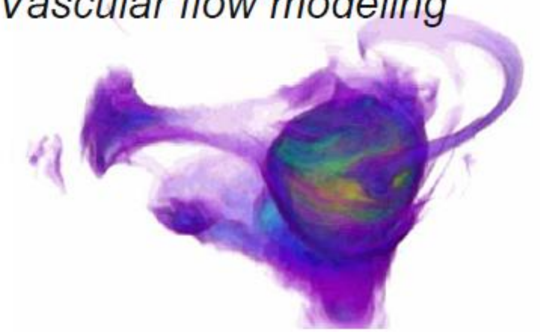


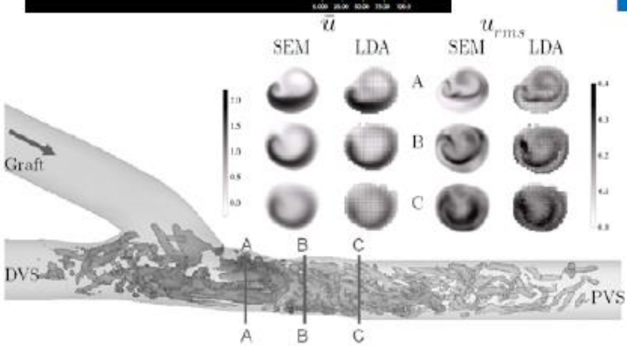


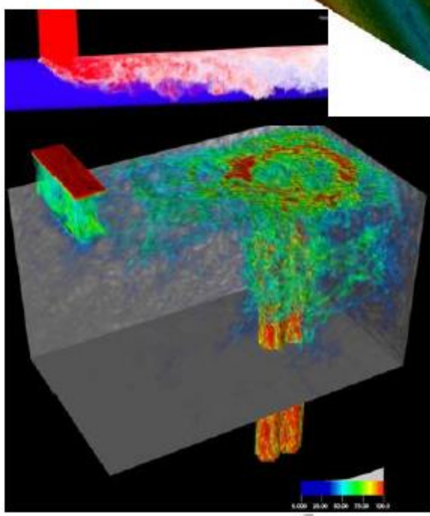
Clockwise from upper left:

- Reactor thermal-hydraulics
- Astrophysics
- Combustion
- Oceanography
- Vascular flow modeling









Strengths of Nek5000

- *High-order accuracy at low cost Extremely rapid (exponential) convergence in space*
- *3rd-order accuracy in time*

- *Highly scalable Fast scalable multigrid solvers*
- *Scales to > 290,000 processors with ~104 pts/proc on BGP*

- *Extensively tested*
- *> 10s of platforms over 25 years*
- *> 150 journal articles & > 60 users worldwide*
- *> 400 tests after each build to ensure verified source*
- *(more tests to be added)*

Nek5_svn repository

- **nek5_svn**

```
|-- 3rd_party
|-- branches
|-- examples
|   |-- axi
|   |-- benard
|   |-- conj_ht
|   |-- eddy
|   |-- fs_2
|   |-- fs_hydro
|   |-- kovasznay
|   |-- lowMach_test
|   |-- moab
|   |-- peris
|   |-- pipe
|   |-- rayleigh
|   |-- shear4
|   |-- timing
|   |-- turbChannel
|   |-- turbJet
|   `-- vortex
|-- tags
|-- tests
`-- trunk
```

- **nek5_svn**

```
|--   :
|--   :
`-- trunk
    |-- nek
    |   |       :
    |   |-- source files….
    |   |       :
    `-- tools
        |-- amg_matlab
        |-- avg
        |-- genbox
        |-- genmap
        |-- makefile
        |-- maketools
        |-- n2to3
        |-- nekmerge
        |-- postnek
        |-- prenek
        |-- reatore2
        `-- scripts
```

Base NEK5000 case files

- **SIZE** – an f77 include file that determines
  - spatial dimension (ldim =2 or 3)
  - approximation order (lx1,lx2,lx3,lxd) - N := lx1-1
  - upper bound on number of elements per processor: lelt
  - upper bound on total number of elements, lelg

- <case>**.rea** – a file specifying
  - job control parameters (viscosity, dt, Nsteps, integrator, etc.)
  - geometry – element vertex and curvature information
  - boundary condition types
  - restart conditions

- <case>**.usr** – f77 source file specifying
  - initial and boundary conditions
  - variable properties
  - forcing and volumetric heating
  - geometry morphing
  - data analysis options: min/max, runtime average, rms, etc.

Snapshots of SIZE

```
      parameter (ldim=2)
      parameter (lx1=14,ly1=lx1,lz1=1,lelt=80,lelv=lelt)
      parameter (lxd=20,lyd=lxd,lzd=1)
      parameter (lelx=1,lely=1,lelz=1)
c
c     NOTE: for IBM BLUE GENE LX1,LXD has to be an even number (double hummer)

      parameter (ldimt= 1)         ! upper limit for passive scalars + T

      parameter (lp =      64)     ! upper limit for number of CPUs
      parameter (lelg = 5000)      ! upper limit for total number of elements

C
C    ******************************************************************
C
      parameter (lzl=3 + 2*(ldim-3))

      parameter (lx2=lx1-0)
      parameter (ly2=ly1-0)
      parameter (lz2=lz1)

      parameter (lx3=lx2)
      parameter (ly3=ly2)
      parameter (lz3=lz2)
```

Snapshots of .rea file

- Parameters section

```
        2 DIMENSIONAL RUN
      118 PARAMETERS FOLLOW
   1.00000      P001: DENSITY
  -40.0000      P002: VISCOS
  0.000000E+00 P003:
  0.000000E+00 P004:
  0.000000E+00 P005:
  0.000000E+00 P006:
   1.00000      P007: RHOCP
   1.00000      P008: CONDUCT
  0.000000E+00 P009:
  0.000000E+00 P010: FINTIME
   2000.00      P011: NSTEPS
 -0.100000E-02 P012: DT
  0.000000E+00 P013: IOCOMM
  0.000000E+00 P014: IOTIME
  0.000000E+00 P015: IOSTEP
  0.000000E+00 P016: PSSOLVER: 0=default
   1.00000      P017:
  0.500000E-01 P018: GRID < 0 --> # cells
  -1.00000      P019: INTYPE
   4.00000      P020: NORDER
  0.100000E-05 P021: DIVERGENCE
  0.100000E-09 P022: HELMHOLTZ
  0.000000E+00 P023: NPSCAL
  0.000000E+00 P024: TOLREL
  0.000000E+00 P025: TOLABS
   2.00000      P026: COURANT/NTAU
   3.00000      P027: TORDER
```

- Geometry and boundary conditions

```
     ELEMENT            5 [    1 ]    GROUP     0
-0.5000000       0.0000000E+00  0.0000000E+00 -0.5000000
 0.5000000       0.5000000       1.000000       1.000000
     ELEMENT            6 [    1 ]    GROUP     0
 0.0000000E+00    1.000000       1.000000      0.0000000E+00
 0.5000000       0.5000000       1.000000       1.000000
     ELEMENT            7 [    1 ]    GROUP     0
-0.5000000       0.0000000E+00  0.0000000E+00 -0.5000000
  1.000000        1.000000       1.500000       1.500000
     ELEMENT            8 [    1 ]    GROUP     0
 0.0000000E+00    1.000000       1.000000      0.0000000E+00
  1.000000        1.000000       1.500000       1.500000
 ***** CURVED SIDE DATA *****
       0 Curved sides follow IEDGE,IEL,CURVE(I),I=1,5, CCURVE
 ***** BOUNDARY CONDITIONS *****
 ***** FLUID   BOUNDARY CONDITIONS *****
P    1  1   7.00000      3.00000      0.000000E+00  0.000000E+00
E    1  2   2.00000      4.00000      0.000000E+00  0.000000E+00
E    1  3   3.00000      1.00000      0.000000E+00  0.000000E+00
v    1  4  0.000000E+00 0.000000E+00  0.000000E+00  0.000000E+00
P    2  1   8.00000      3.00000      0.000000E+00  0.000000E+00
v    2  2  0.000000E+00 0.000000E+00  0.000000E+00  0.000000E+00
E    2  3   4.00000      1.00000      0.000000E+00  0.000000E+00
E    2  4   1.00000      2.00000      0.000000E+00  0.000000E+00
E    3  1   1.00000      3.00000      0.000000E+00  0.000000E+00
E    3  2   4.00000      4.00000      0.000000E+00  0.000000E+00
E    3  3   5.00000      1.00000      0.000000E+00  0.000000E+00
v    3  4  0.000000E+00 0.000000E+00  0.000000E+00  0.000000E+00
E    4  1   2.00000      3.00000      0.000000E+00  0.000000E+00
v    4  2  0.000000E+00 0.000000E+00  0.000000E+00  0.000000E+00
E    4  3   6.00000      1.00000      0.000000E+00  0.000000E+00
```

Snapshot of .usr file

```
c-----------------------------------------------------------------------
      subroutine userf  (ix,iy,iz,eg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'

      integer e,f,eg
c     e = gllel(eg)

c     Note: this is an acceleration term, NOT a force!
c     Thus, ffx will subsequently be multiplied by rho(x,t)

      ffx = 0.0
      ffy = 0.0
      ffz = 0.0

      return
      end
c-----------------------------------------------------------------------
      subroutine userchk
      include 'SIZE'
      include 'TOTAL'
      return
      end
c-----------------------------------------------------------------------
      subroutine userbc (ix,iy,iz,iside,ieg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
      ux=0.0
      uy=0.0
      uz=0.0
      temp=0.0
      return
      end
c-----------------------------------------------------------------------
      subroutine useric (ix,iy,iz,ieg)
```

Derived Nek5000 Case Files

- <case>**.re2** – binary file specifying
  - geometry – element vertex and curvature information
  - boundary condition types

  This file is not requisite for small problems but important for element counts E > ~10,000

- <case>**.map** – ascii file derived from .rea/.re2 files specifying
  - mesh interconnect topology
  - element-to-processor map

  This file is needed for each run and is generated by running the "genmap" tool (once, for a given .rea file).

- **amg…dat** – binary files derived from .rea/.re2 files specifying
  - algebraic multigrid coarse-grid solver parameters

  These files are needed only for large processor counts (P > 10,000) and element counts (E > 50,000).

Equation Sets (2D/3D)

- Incompressible Navier-Stokes plus energy equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot\mu\left(\nabla\mathbf{u} + \nabla^T\mathbf{u}\right) + \mathbf{f}$$

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

$$\rho C_p\left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) = \nabla\cdot k\nabla T + q'''$$

plus additional passive scalars:

$$\rho C_{p_i}\left(\frac{\partial T_i}{\partial t} + \mathbf{u}\cdot\nabla T_i\right) = \nabla\cdot k_i\nabla T_i + q_i''', \quad i = 3, \ldots, n_{flds}$$

Navier-Stokes Boundary Conditions

- A few key boundary conditions are listed below.

cbc	name	condition
v	velocity	specified in .usr
V	velocity	specified in .rea
W	wall	$\mathbf{u} = 0$
O	outflow	$\frac{\partial \mathbf{u}}{\partial \mathbf{n}} = 0,\ p = 0$
SYM	symmetry	$\frac{\partial u_t}{\partial \mathbf{n}} = 0,\ u_n = 0$
P	periodic	$\mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x} + \mathbf{L})$

- There are many more, particularly for moving walls, free surface, etc.

- Special conditions include:
  - Recycling boundary conditions (special form of “v”)
  - Accelerated outflow to avoid incoming characteristics

Thermal Boundary Conditions

- A few key boundary conditions are listed below.

cbc	name	condition
t	temperature	specified in .usr
T	temperature	specified in .rea
I	insulated	$\frac{\partial T}{\partial \mathbf{n}} = 0$
f	flux	$k\frac{\partial T}{\partial \mathbf{n}} = f$
c	Newton cooling	$k\frac{\partial T}{\partial \mathbf{n}} = h(T - T_\infty)$
O	outflow	$\frac{\partial T}{\partial \mathbf{n}} = 0$
P	periodic	$T(\mathbf{x}) = T(\mathbf{x} + \mathbf{L})$