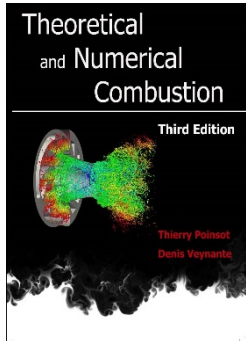**POLITECNICO**
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Iran First International Combustion School (ICS2019)
Tehran, 24-26 August 2019

Combustion modeling
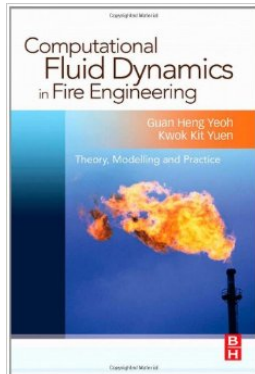## 5. Introduction to numerical modeling of turbulent reacting flows

Alberto Cuoci

References

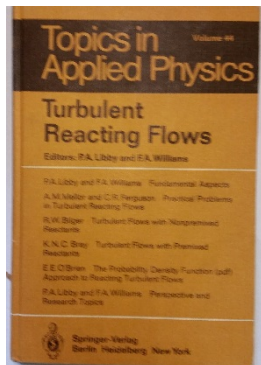**Poinsot T., Veynante D.**

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Princeton Combustion Summer School 2018
https://cefrc.princeton.edu/combustion-summer-school/archived-programs/2018-session/lecture-notes

Outline

1. **Introduction to turbulent flows**

2. **Statistical description of turbulent flows**
   a) Reynolds and Favre average
   b) 2-point correlations
   c) Turbulent eddies and energy cascade

3. **Kolmogorov's Theory**
   a) Kolmogorov's similarity hypotheses
   b) Kolmogorov's scales
   c) Energy spectrum

4. **Transport equations for mean variables**
   a) Need of mean/filtered equations
   b) Favre's averaged transport equations for continuity and momentum
   c) Closure models for turbulent flows: $\kappa - \varepsilon$ model
   d) Favre's averaged transport equations for passive scalars and species
   e) Large Eddy Simulation (LES)

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- **Turbulence is random**

The properties of the fluid $(\rho, P, \boldsymbol{u}, T, \dots)$ at any given point $(\boldsymbol{x}, t)$ cannot be predicted. But statistical properties (time and space averages, correlation functions, and probability density functions) show regular behavior. The fluid motion is stochastic.

- **Turbulence decays without energy input**

Turbulence must be driven or else it decays, returning the fluid to a laminar state.

- **Turbulence displays scale-free behavior**

On all length scales larger than the viscous dissipation scale but smaller than the scale on which the turbulence is being driven, the appearance of a fully developed turbulent flow is the same.
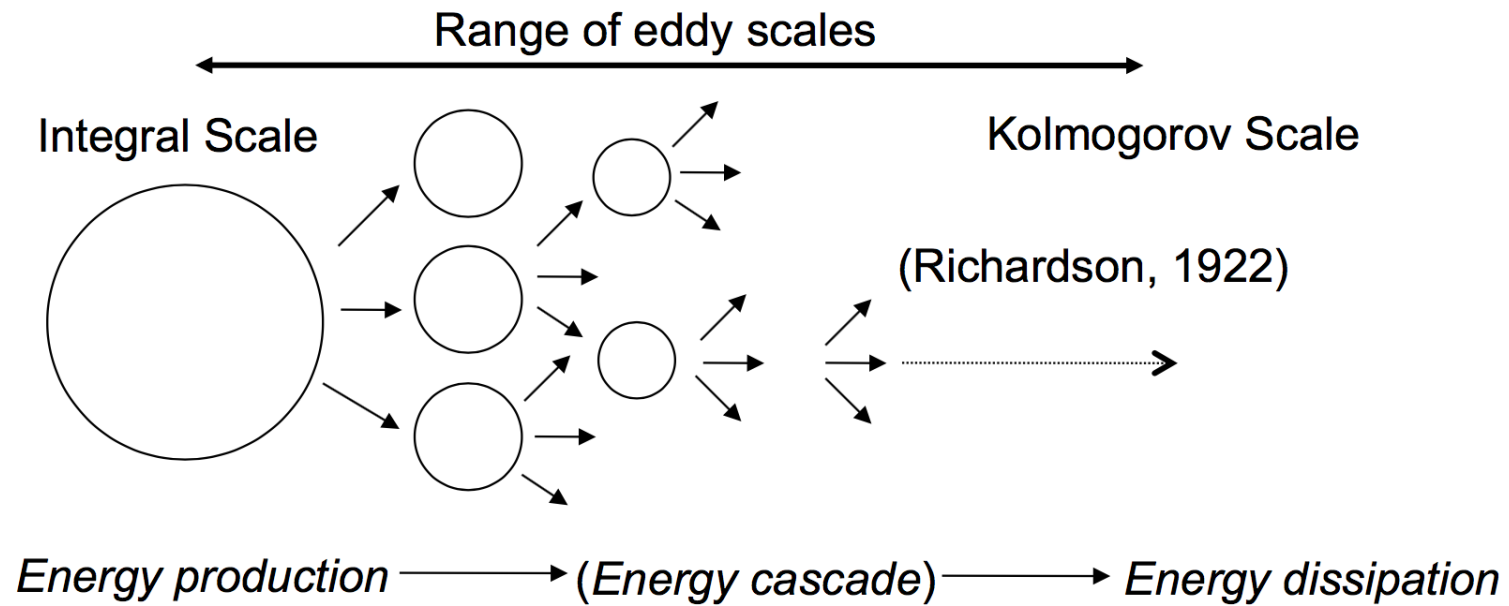
- **Turbulence displays intermittency**

"Outlier" fluctuations occur more often than chance would predict.

- **Mixing effect**

Turbulence mixes quantities (e.g., pollutants, chemicals, velocity components, etc.), which acts reduce gradients. This lowers the concentration of harmful scalars, but increases drag.
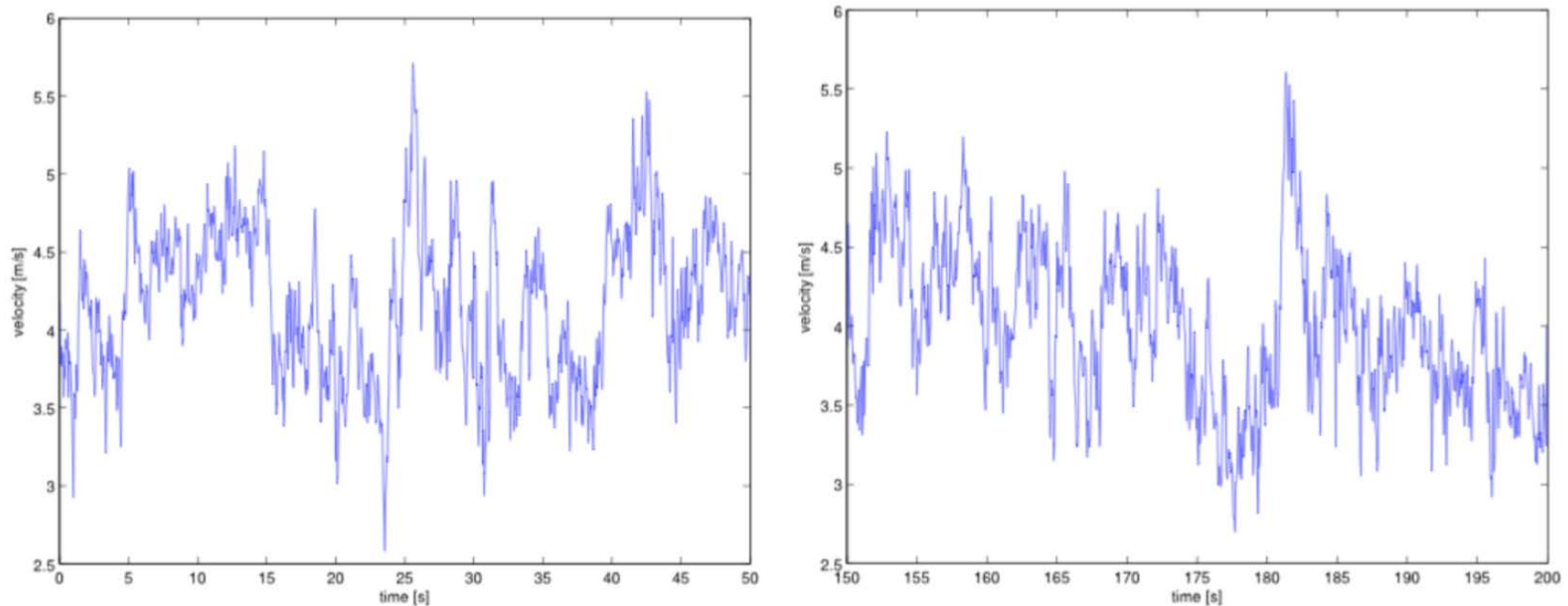
- **A continuous spectrum (range) of scales**

Range of eddy scales

Integral Scale

Kolmogorov Scale

(Richardson, 1922)

Energy production ⟶ *(Energy cascade)* ⟶ *Energy dissipation*

Mean features of turbulent flows

• turbulent flows are intrinsically unsteady: velocity (and any other relevant quantities, such as temperature, pressure, composition etc.) show a chaotic, non reproducible and unpredictable behavior

• turbulent flows are intrinsically tri-dimensional: mean quantities can exhibit in particular circumstances spatial symmetries, but this is not true for local quantities, which are alway function of the three spatial coordinates

• turbulence strongly increases mixing of chemical species and more in general every diffusion process (stirring)

• turbulent flows are characterized by a very wide range of characteristic times and lengths
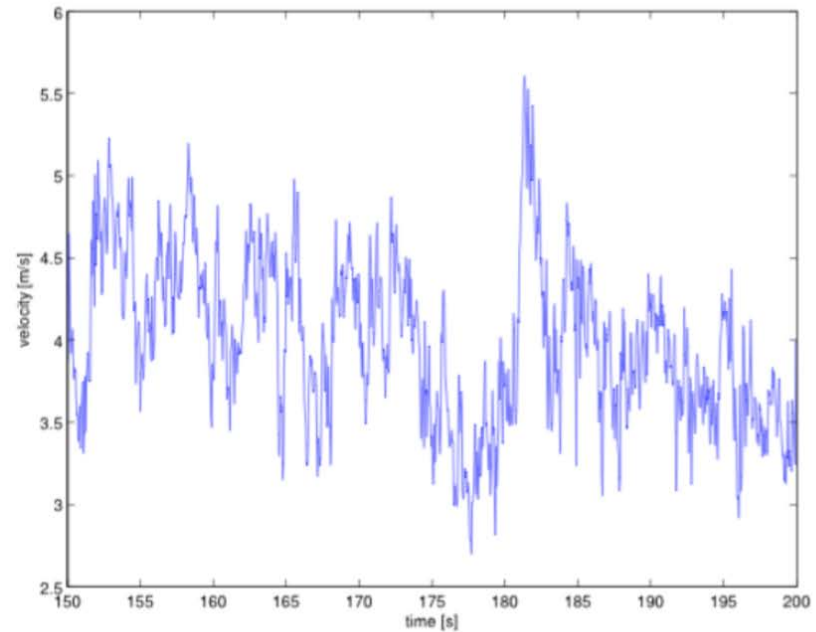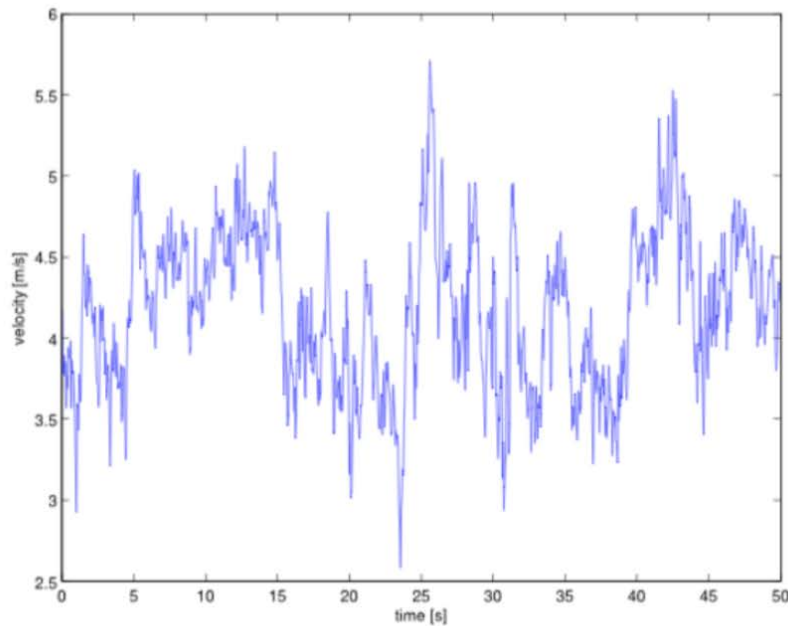
Sonic anemometer data at 20Hz taken in the ABL (Atmospheric Boundary Layer).

The above figure is an example of the **random nature of turbulent flows**. Pope (2000) notes that using the term "random" means nothing more than that an event may or may not occur (it says nothing about the nature of the event)

- The signal is highly disorganized and has structure on a wide range of scales (that is also disorganized).

- Notice the small (fast) changes verse the longer timescale changes that appear in no certain order.

The signal appears unpredictable.

Compare the left plot with that on the right (100 s later). Basic aspects are the same but the details are completely different. From looking at the left signal, it is impossible to predict the right signal.

Some of the properties of the signal appear to be reproducible.

The reproducible property isn't as obvious from the signal. Instead we need to look at the histogram.

$\mu = 4.17$
$\sigma = 0.48$

$\mu = 4.00$
$\sigma = 0.50$

Notice that the histograms are similar with similar means μ and standard deviations σ.

An example: turbulent jet

concentration in a turbulent jet
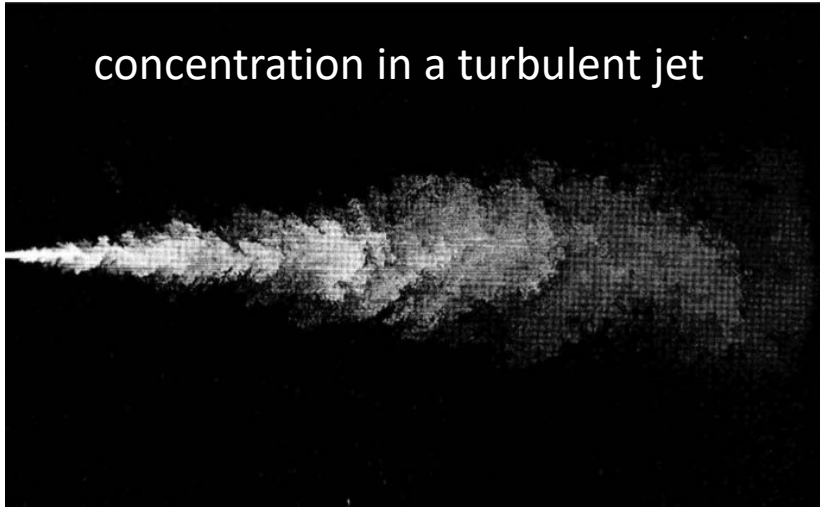
the time history along the centerline
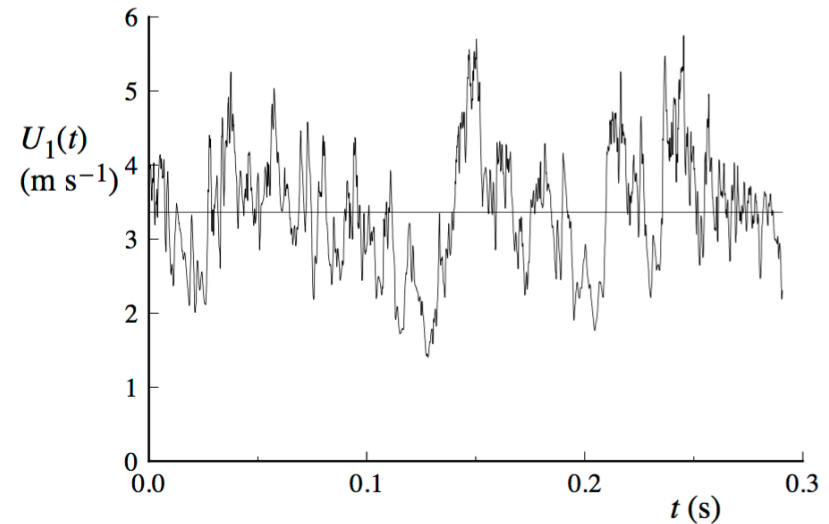
Normalized mean axial velocity in a turbulent jet
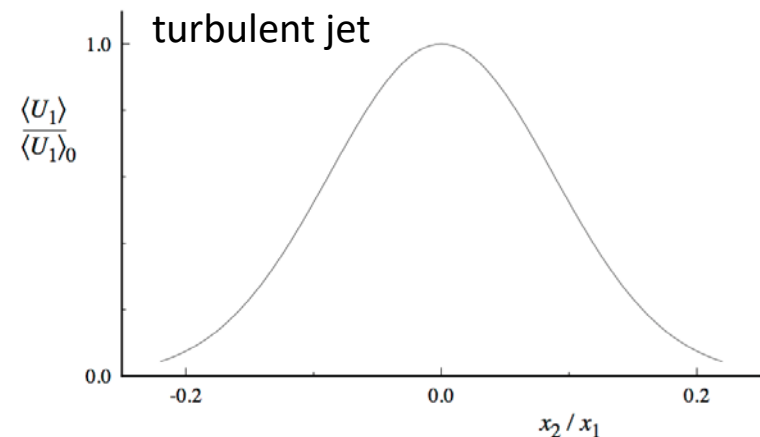
Some of the properties of the signal appear to be reproducible.
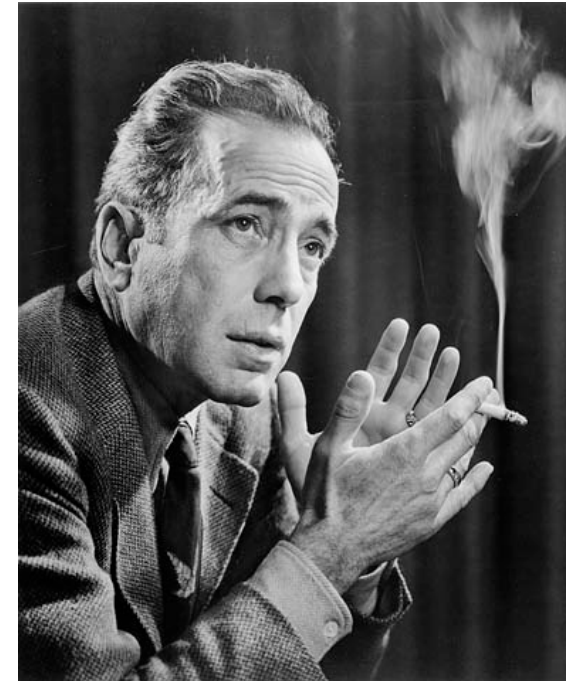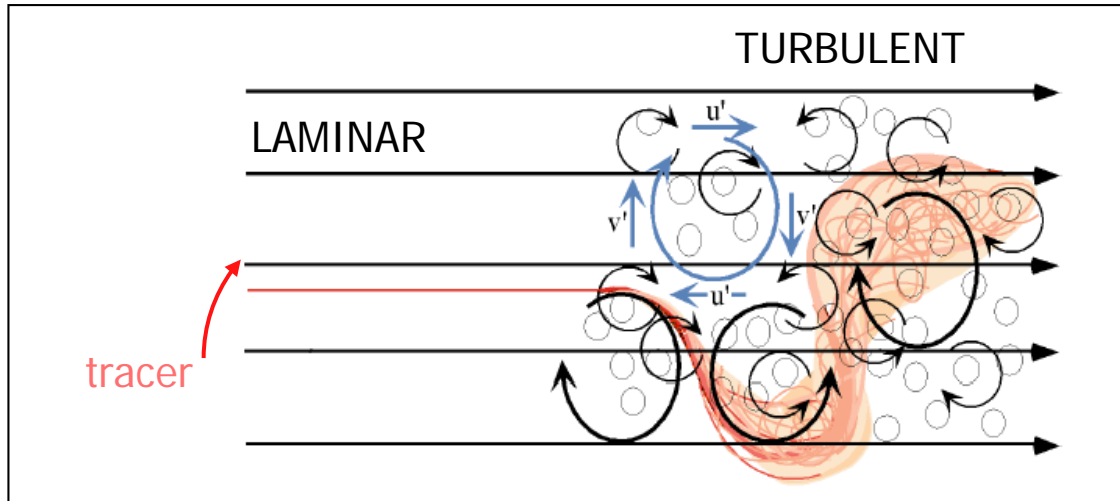
O. Reynolds (1883): if Re>4000, after an initial length in which oscillations can be observed with increasing amplitude, the ink signal strongly diffuses along the whole pipe section. This regime is defined turbulent flow ad it is characterized by a disordered movement, fully tridimensional and unsteady, with velocity fluctuations with non deterministic features.

Turbulent flows arise according to the stability of the laminar configuration, which becomes unstable when the ratio between inertial forces and viscous forces increases

Reynolds' number   **Re=inertial forces / viscous forces**

For increasing Reynolds' number, the flows are not able to maintain the ordered features and become turbulent. We can observe the formation of vortices which moves completely disordered.

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Statistical description of turbulence

- We have seen that turbulent flows are random, but their histograms are apparently reproducible.

- As a consequence, turbulence is usually studied from a **statistical viewpoint**.

- Consider the velocity field u. Since u is a random variable, its value is unpredictable for a turbulent flow.

- Thus, any theory used to predict a particular value for u will likely fail.

- Instead, theories should aim at determining the probability of events

- We need statistical tools to characterize random variables.

Statistical description of turbulent flows

Conventional Averaging/Reynolds Decomposition

Ensemble average

$$\bar{u}_i(x, y, z, t) = \frac{1}{N} \sum_{k=1}^{N} u_i^{(k)}(x, y, z, t)$$

N sufficiently large

Time average

$$\bar{u}_i(x, y, z) = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} u_i(x, y, z, t) \, dt$$

Δt sufficiently large

For constant density flows
Reynolds' decomposition: mean and fluctuation, e.g. for the flow velocity u_i

$$u_i = \bar{u}_i + u_i'$$

Mean of the fluctuation is zero (applies for all quantities):

$$\overline{u_i'} = 0$$

Mean of the squared fluctuation is not zero:

$$\sqrt{\overline{u_i' u_i'}} = \sqrt{\overline{u_i'^2}} = \sqrt{\overline{u_1'^2} + \overline{u_2'^2} + \overline{u_3'^2}} \neq 0$$

$$\sqrt{\overline{p'^2}} = \neq 0$$

These averages are called **RMS-values (root mean square)**

Combustion: change in density → correlation of density and other quantities

Reynolds' decomposition (for non constant density):

$$\overline{\rho u_i} = \overline{(\bar{\rho} + \rho')(\bar{u}_i + u_i')} = \bar{\rho}\bar{u}_i + \overline{\rho' u_i'} \neq \bar{\rho}\bar{u}_i$$

Favre decomposition:

$$u_i = \tilde{u}_i + u_i''$$

By definition: mean of density weighted fluctuation equal to zero

$$\overline{\rho u_i''} = 0$$

Density weighted mean velocity:

$$\overline{\rho u_i} = \overline{\rho(\tilde{u}_i + u_i'')} = \bar{\rho}\tilde{u}_i + \overline{\rho u_i''} = \bar{\rho}\tilde{u}_i \qquad\qquad \tilde{u}_i = \frac{\overline{\rho u_i}}{\bar{\rho}}$$

Favre averaging as a function of conventional mean and fluctuation:

$$\tilde{u}_i = \frac{\overline{\rho u_i}}{\bar{\rho}} = \frac{\overline{(\bar{\rho} + \rho')(\bar{u}_i + u'_i)}}{\bar{\rho}} = \frac{\bar{\rho}\bar{u}_i + \overline{\rho' u'_i}}{\bar{\rho}} = \bar{u}_i + \frac{\overline{\rho' u'_i}}{\bar{\rho}}$$

And for the fluctuating quantity:

$$u''_i = u'_i - \frac{\overline{\rho' u'_i}}{\bar{\rho}}$$

$$\overline{u''_i} = -\frac{\overline{\rho' u'_i}}{\bar{\rho}} \neq 0$$

For non-constant density: Favre average leads to much simpler expression

Types of turbulence: statistically homogeneous

All statistics of fluctuating quantities are invariant under translation of the coordinate system:

$$\overline{u'_i(x_k)u'_j(x_k)} = \overline{u'_i(x_k + \Delta x_k)u'_j(x_k + \Delta x_k)} \qquad i, j, k = 1,2,3$$

Constant gradients of the mean velocity are allowed:

$$\frac{\partial}{\partial x_l}\bar{u}_i(x_k) = \frac{\partial}{\partial x_l}\bar{u}_i(x_k + \Delta x_k) \qquad i, j, k = 1,2,3$$
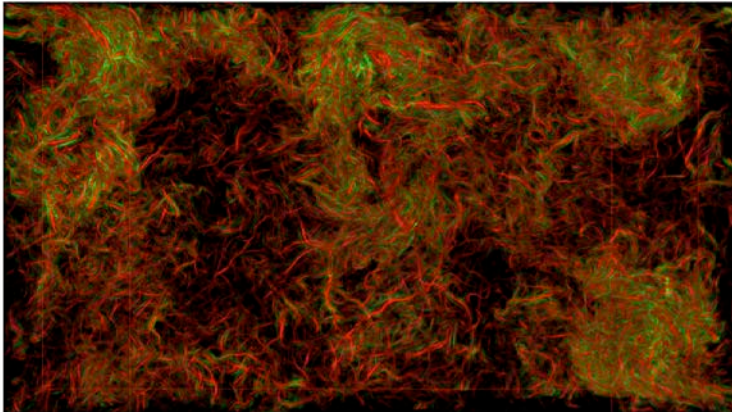
Vorticity in a statistically homogeneous turbulent flow
http://turbulence.pha.jhu.edu/

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Types of turbulence: isotropic homogeneous

All statistics are invariant under translation, rotation, and reflection of the coordinate system:

$$\overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2} = 0$$

$$\overline{u_i' u_j'} \neq 0 \quad if \ i \neq j$$

Mean velocities are equal to zero:

$$\overline{u_i'} = 0$$

Isotropy requires homogeneity

Relevance:
- Theoretical studies (because of the strong simplifications)
- Turbulent motions on small scales are typically assumed to be isotropic (Kolmogorov hypotheses)

Example of isotropic homogeneous turbulent flow
http://turbulence.pha.jhu.edu/

Types of turbulence: shear flows

Relevant flow cases in technical systems
- Round jet
- Flow around airfoil
- Flows in combustion chamber

Due to the complexity of these turbulent flows they cannot be described theoretically
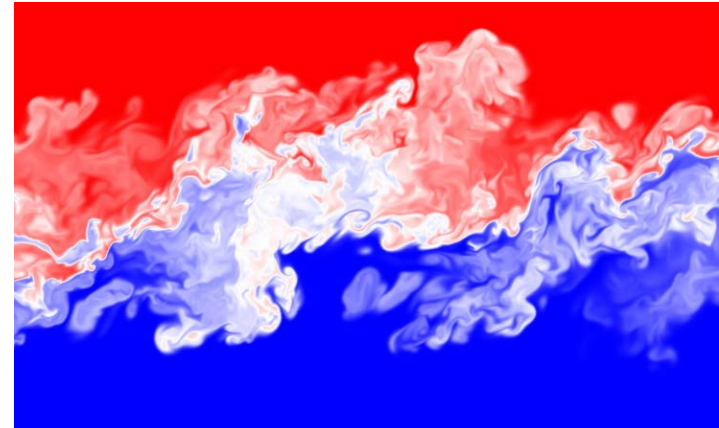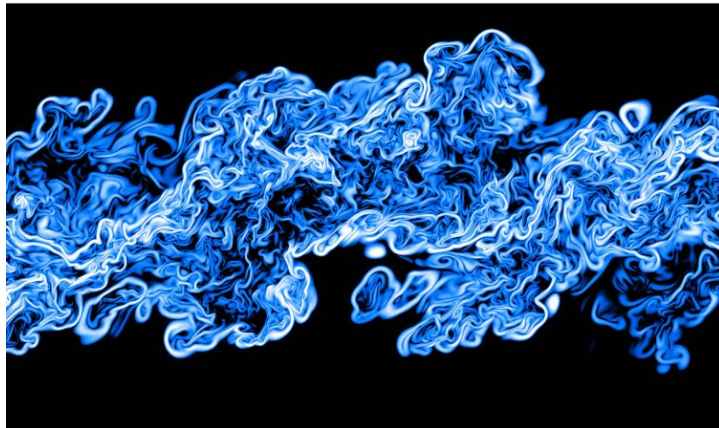
Temporally evolving shear layer: Scalar dissipation rate χ (left), mixture fraction Z (right) from [Pitsch2018]

- Kolmogorov's theory describes how energy is transferred from larger to smaller eddies; how much energy is contained by eddies of a given size; and how much energy is dissipated by eddies of each size.

- We will derive three main turbulent length scales (and corresponding Reynolds numbers):
  - the integral scale
  - the Kolmogorov scale

- We will also discuss the concept of energy and dissipation spectra.

Relatively low Reynolds number
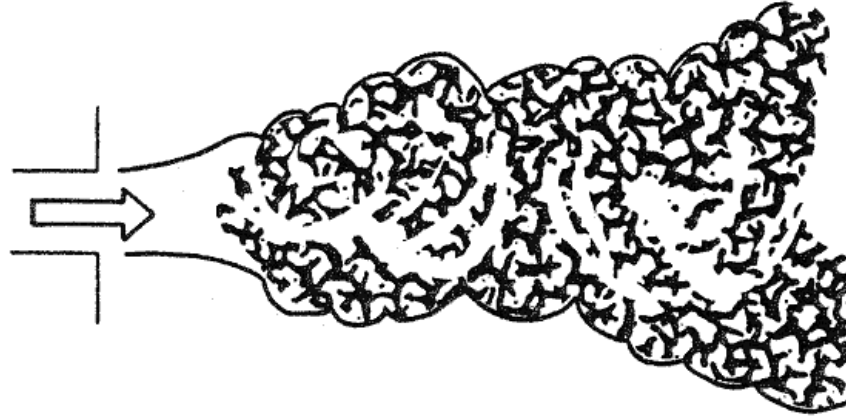
Relatively high Reynolds number

Source: Tennekes & Lumley. Page 22.

Turbulent eddies

- Consider fully turbulent flow at **high Reynolds number** $Re = UL/v$

- Turbulence can be considered to consist of **eddies of different sizes**

- An 'eddy' preludes precise definition, but it is conceived to be a turbulent motion, localized over a region of size l, that is at least moderately coherent over this region

- The region occupied by a larger eddy can also contain smaller eddies.

- Eddies of size l have a characteristic velocity $u(l)$ and timescale $t(l) = \dfrac{l}{u(l)}$

- Eddies in the largest size range are characterized by the integral length scale $l0$ which is comparable to the flow length scale L

Richardson's Theory

Big whorls have little whorls
That feed on their velocity
And little whorls have lesser whorls
And so on to viscosity.

Mean life time $\qquad t_\lambda \approx \dfrac{\lambda}{u'_\lambda}$

Rotation velocity $\qquad \omega_\lambda \approx \dfrac{u'_\lambda}{\lambda}$

Vortices density $\qquad N_\lambda \approx \dfrac{1}{\lambda^3}$

Macro vortices

Scale l_0
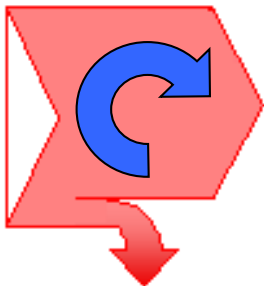
Intermediate vortices
Scale λ
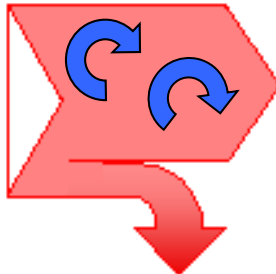
Micro vortices

Scale η
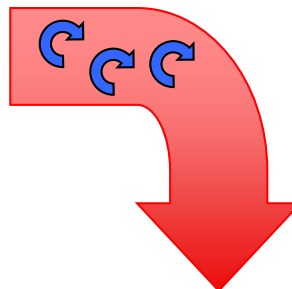
Turbulent kinetic energy dissipation rate

$$\varepsilon \approx \frac{u_0^2}{l_0/u_0} = \frac{u_0^3}{l_0}$$

Characteristic feature of turbulent flows: eddies exist at different length scales
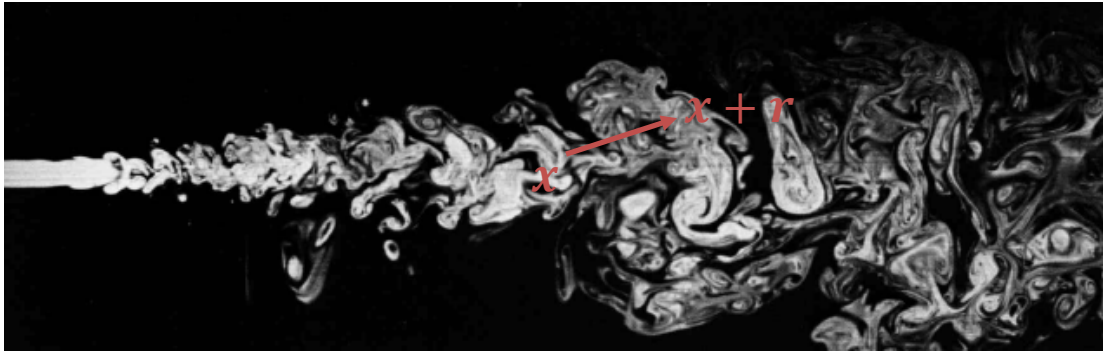
Turbulent round jet: Reynolds number Re ≈ 2300 [Pitsch2018]

Determination of the **distribution of eddy size** at a single point:
- Measurement of velocity fluctuation $u_i'(\boldsymbol{x}, t)$ and $u_i'(\boldsymbol{x} + \boldsymbol{r}, t)$
- Two-point correlation:

$$R_{ij}(\boldsymbol{x}, \boldsymbol{r}, t) = \overline{u_i'(\boldsymbol{x}, t) u_i'(\boldsymbol{x} + \boldsymbol{r}, t)}$$

Homogeneous isotropic turbulence:

$$\boldsymbol{r} \rightarrow r \qquad and \qquad \overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2}$$

Two-point correlation normalized by its variance:

$$f(r,t) = \frac{R(r,t)}{u_{rms}^2(t)}$$

Degree of correlation of stochastic signals:
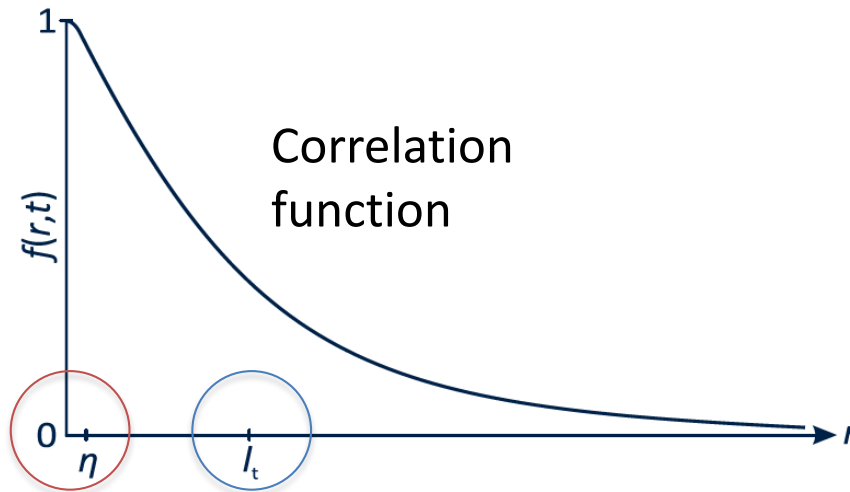
Correlation function

Pitsch H.
"Combustion Theory and Applications in CFD"
Princeton Combustion Summer School 2018

Largest scales: physical scale of the problem
- Integral length scale l_0 (largest eddies)
- Integral velocity scale

$$u' \sim \sqrt{\frac{2}{3}\bar{k}}$$

$$l_0 \stackrel{\text{def}}{=} \int_0^\infty f(r,t)\,dr$$

Integral time scale:

$$\tau \stackrel{\text{def}}{=} \frac{l_0}{u'}$$
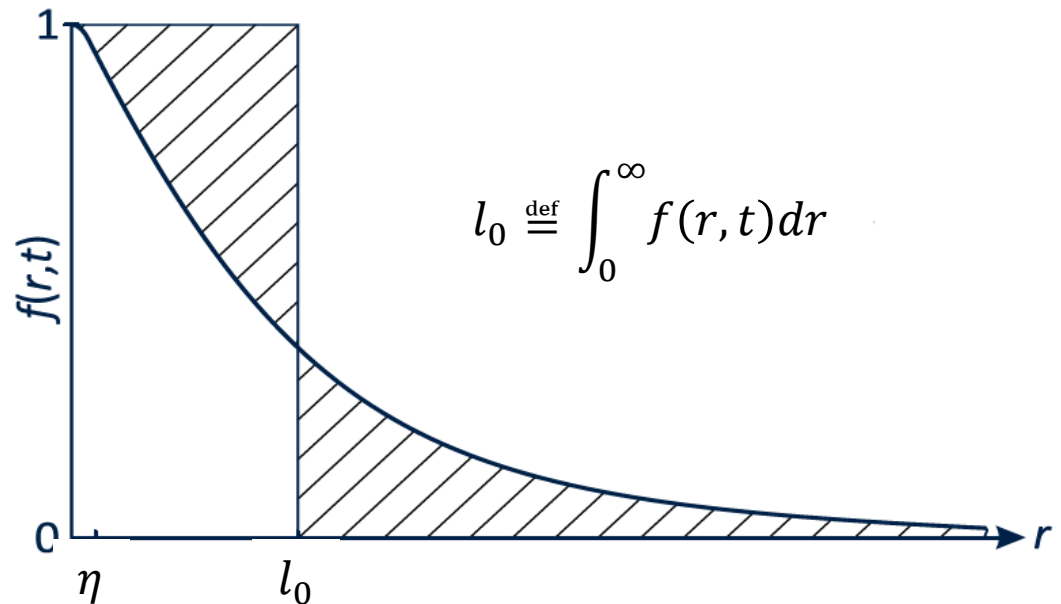
Pitsch H.
"Combustion Theory and Applications in CFD"
Princeton Combustion Summer School 2018

- Thus, the integral scale is:

$$l_0 \propto \frac{k^{3/2}}{\varepsilon}$$

- The Reynolds number associated with these large eddies is referred to as the turbulence Reynolds number Re_{l_0}, which is defined as:

$$Re_{l_0} = \frac{k^{1/2} l_0}{\nu} = \cdots = \frac{k^2}{\varepsilon \nu}$$

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Kolmogorov's Theory

- Many questions remain unanswered.
  - What is the size of the smallest eddies that are responsible for dissipating the energy?
  - As l decreases, do the characteristic velocity and timescales $u'(l)$ and $\tau(l)$ increase, decrease, or stay the same? The assumed decrease of the Reynolds number $u_0 l_0/\nu$ by itself is not sufficient to determine these trends.

- These and others are answered by Kolmogorov's theory of turbulence (1941).

- Kolmogorov's theory is based on three important hypotheses combined with dimensional arguments and experimental observations.

Kolmogorov's hypothesis of local isotropy

- For **homogenous turbulence**, the turbulent kinetic energy k is the same everywhere. For **isotropic turbulence** the eddies also behave the same in all directions: $\overline{u_x'^2} = \overline{u'^2_y} = \overline{u'^2_z}$

- Kolmogorov argued that the directional biases of the large scales are lost in the chaotic scale-reduction process as energy is transferred to smaller eddies.

- Hence Kolmogorov's hypothesis of local isotropy states that:
  at sufficiently high Reynolds numbers, the small-scale turbulent motions $(l \ll l_0)$ 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 $(l > l_{EI})$ and the small scale isotropic eddies $(l < l_{EI})$. For many high Reynolds number flows l_{EI} can be estimated as $l_{EI} \approx l_0/6$

Kolmogorov's first similarity hypothesis

- Kolmogorov also argued that not only does the directional information get lost as the energy passes down the cascade, but that all information about the geometry of the eddies gets lost also.

- As a result, the statistics of the small-scale motions are universal: they are *similar* in every high Reynolds number turbulent flow, independent of the mean flow field and the boundary conditions.

- These small scale eddies depend on the rate T_{EI} at which they receive energy from the larger scales (which is approximately equal to the dissipation rate ε) and the viscous dissipation, which is related to the kinematic viscosity ν.

- Kolmogorov's first similarity hypothesis states that:
  in every turbulent flow at sufficiently high Reynolds number, the statistics of the small scale motions $(l < l_{EI})$ have a universal form that is uniquely determined by ε and ν.

Given the two parameters ε and ν we can form the following unique length, velocity, and time scales:

- Length scale: $\eta = \left(\dfrac{\nu^3}{\varepsilon}\right)^{1/4}$

- Velocity scale: $u_\eta = (\varepsilon\nu)^{1/4}$

- Time scale: $\tau_\eta = \left(\dfrac{\nu}{\varepsilon}\right)^{1/2}$

The corresponding Reynolds' number is:

$$Re_\eta = \frac{\eta u_\eta}{\nu} = 1$$

- These scales are indicative of the smallest eddies present in the flow, the scale at which the energy is dissipated.

- Note that the fact that the Kolmogorov Reynolds number Re_η of the small eddies is 1, is consistent with the notion that the cascade proceeds to smaller and smaller scales until the Reynolds number is small enough for dissipation to be effective.

- The size range ($l < l_{EI}$) is referred to as the **universal equilibrium range**

- In this range, the timescales $l/u(l)$ are small compared to l_0/u_0 so that the small eddies can adapt quickly to maintain dynamic equilibrium with the energy transfer rate T_{EI} imposed by the large eddies

- On these scales all high Reynolds number flow fields are statistically identical if the flow fields are scaled by the Kolmogorov scales

- When we use the relationship $l_0 \sim k^{3/2}/\varepsilon$ and substitute it in the equations for the Kolmogorov scales, we can calculate the ratios between the small scale and large scale eddies.

  - $\dfrac{\eta}{l_0} \sim Re_{l_0}^{-3/4}$

  - $\dfrac{u_\eta}{u_0} \sim Re_{l_0}^{-1/4}$

  - $\dfrac{\tau_\eta}{\tau_0} \sim Re_{l_0}^{-1/2}$

- As expected, at high Reynolds numbers, the velocity and timescales of the smallest eddies are small compared to those of the largest eddies.

- Since η/l_0 decreases with increasing Reynolds number, at high Reynolds number there will be a range of intermediate scales l which is small compared to l_0 and large compared with η.

Kolmogorov's second similarity hypothesis

- Because the Reynolds number of the intermediate scales l is relatively large, they will not be affected by the viscosity ν

- Based on that, Kolmogorov's second similarity hypothesis states that: *in every turbulent flow at sufficiently high Reynolds number, the statistics of the motions of scale l in the range $l_0 >> l >> \eta$ have a universal form that is uniquely determined by ε independent of ν.*

- We introduce a new length scale l_{DI}, (with $l_{DI} \approx 60\eta$ for many turbulent high Reynolds number flows) so that this range can be written as $l_{EI} > l > l_{DI}$

- This length scale splits the universal equilibrium range in 2 subranges:
  - The **inertial subrange** $(l_{EI} > l > l_{DI})$ where motions are determined by inertial effects and viscous effects are negligible.
  - The **dissipation range** $(l < l_{DI})$ where motions experience viscous effects.

- The bulk of the energy is contained in the larger eddies in the size range $l_{EI} = l_0/6 < l < 6l_0$, which is therefore called the energy-containing range.

- The suffixes EI and DI indicate that l_{EI} is the demarcation line between energy (E) and inertial (I) ranges, as l_{DI} is that between the dissipation (D) and inertial (I) ranges.

Universal Equilibrium Range   **Energy containing Range**

Dissipation range   Inertial sub-range

η l_{DI} l_{EI} l_0 L
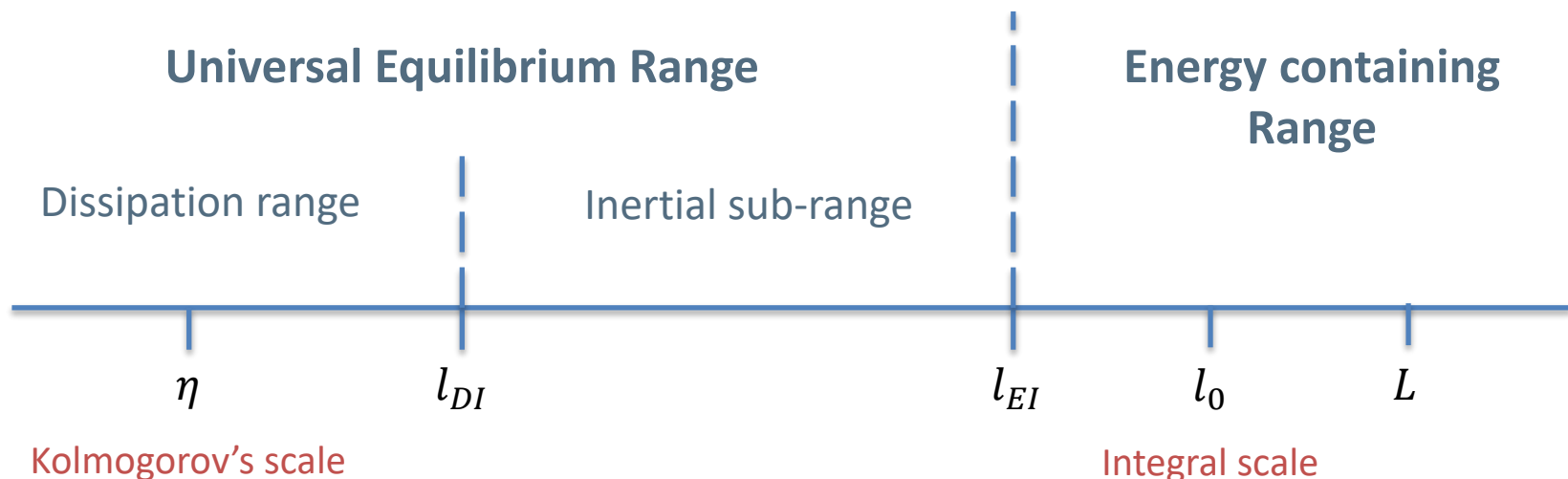
Kolmogorov's scale   Integral scale

- The rate at which energy is transferred from the larger scales to the smaller scales is $T(l)$.

- Under the equilibrium conditions in the inertial subrange this is equal to the dissipation rate ε.
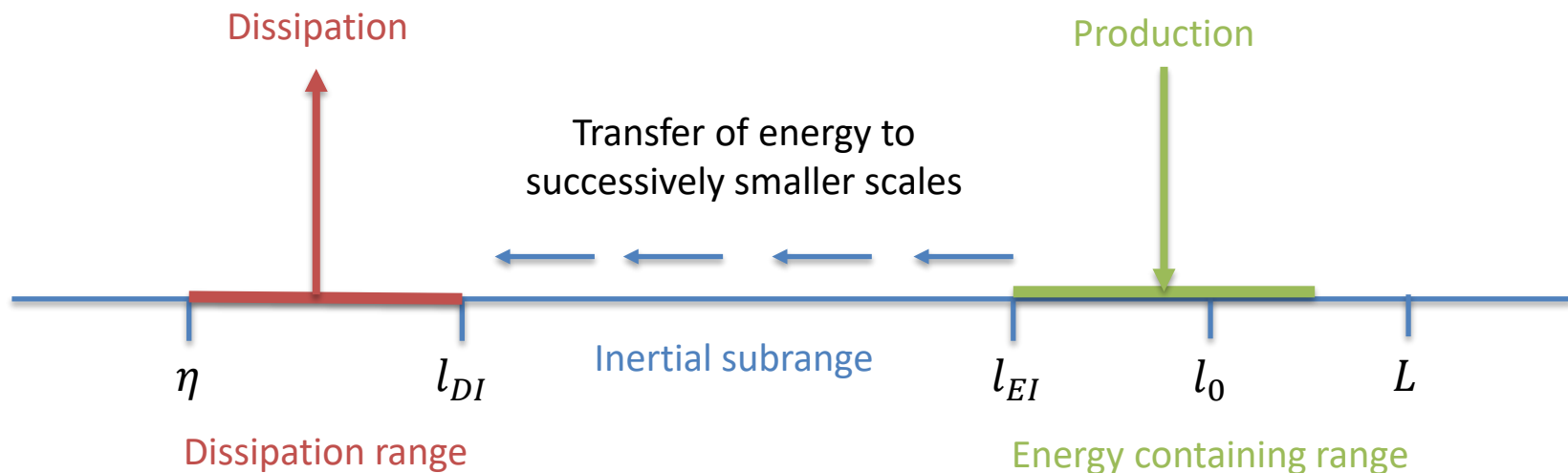
Wavenumbers

- The wavenumber κ is defined as $\kappa = 2\pi/l$

- The different ranges can be shown as a function of wavenumber

- The wavenumber can also be made non-dimensional by multiplying it with the Kolmogorov length scale η to result in the commonly used dimensionless group (

- The turbulent kinetic energy k is given by:

$$k = \frac{1}{2}\overline{u_i' u_i'} = \frac{1}{2}\left(\overline{u_1'^2} + \overline{u_2'^2} + \overline{u_3'^2}\right)$$

- It remains to be determined how the turbulent kinetic energy is distributed among the eddies of different sizes.

- This is usually done by considering the energy spectrum $E(\kappa)$

- Here $E(\kappa)$ is the energy contained in eddies of size l and wavenumber κ, defined as $\kappa = 2\pi/l$

- By definition k is the integral of $E(\kappa)$ over all wavenumbers:

$$k = \int_0^\infty E(\kappa)\,d\kappa$$

- The energy contained in eddies with wavenumbers between κ_A and κ_B is then:

$$k_{\kappa_A,\kappa_B} = \int_{\kappa_A}^{\kappa_B} E(\kappa)\,d\kappa$$

- We will develop an equation for $E(\kappa)$ in the inertial sub-range.

- According to the second similarity hypothesis $E(\kappa)$ will solely depend on κ and ε.

- On the basis of a dimensional analysis, we can demonstrate that:

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

- The last equation describes the famous **Kolmogorov –5/3 spectrum**. C is the universal Kolmogorov constant, which experimentally was determined to be $C = 1.5$.

- Model equations for E(κ) in the production range and dissipation range have been developed. We will not discuss the theory behind them here.

- The full spectrum is:

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

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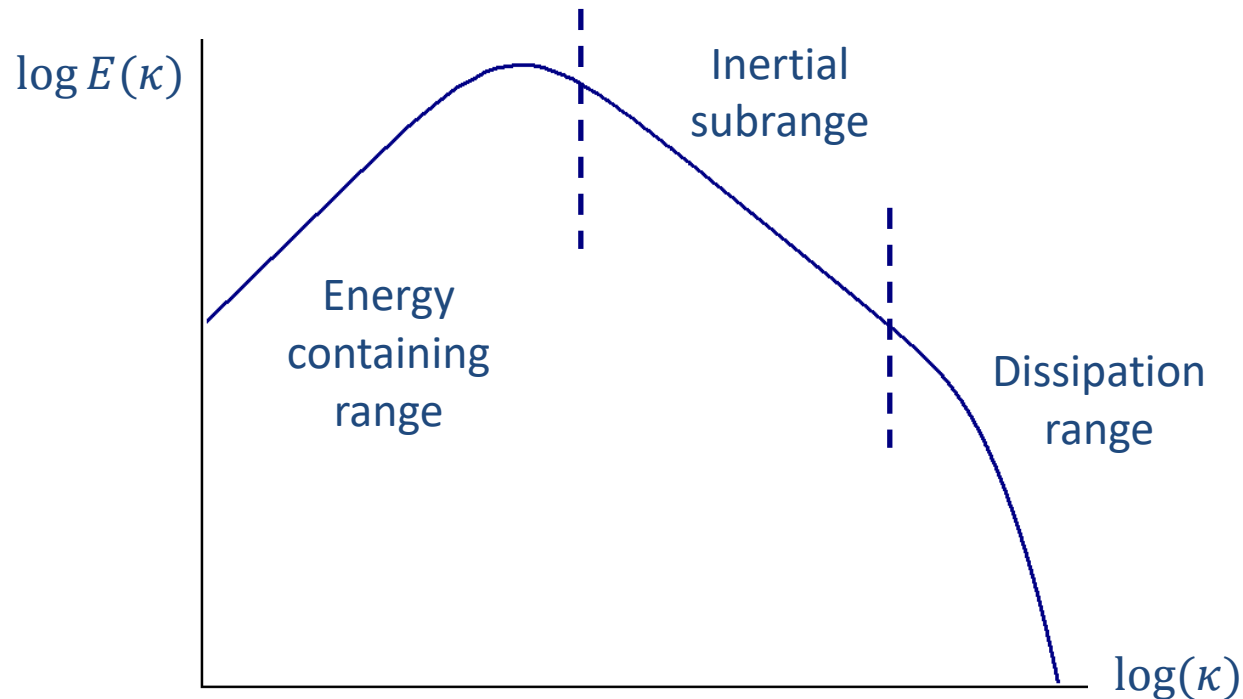
- The production range is governed by f_L (which goes to unity for large (κl_0):

$$f_L = \left(\frac{\kappa l_0}{[(\kappa l_0)^2 + c_L]^{1/2}} \right)^{p_0 + 5/3}$$

- The dissipation range is governed by f_η (which goes to unity for small (

- For given values of ε, ν, and k the full spectrum can now be calculated based on these equations.

- It is, however common to normalize the spectrum in one of two ways: based on the Kolmogorov scales or based on the integral length scale.

- Based on Kolmogorov scale:
  - Measure of length scale becomes (
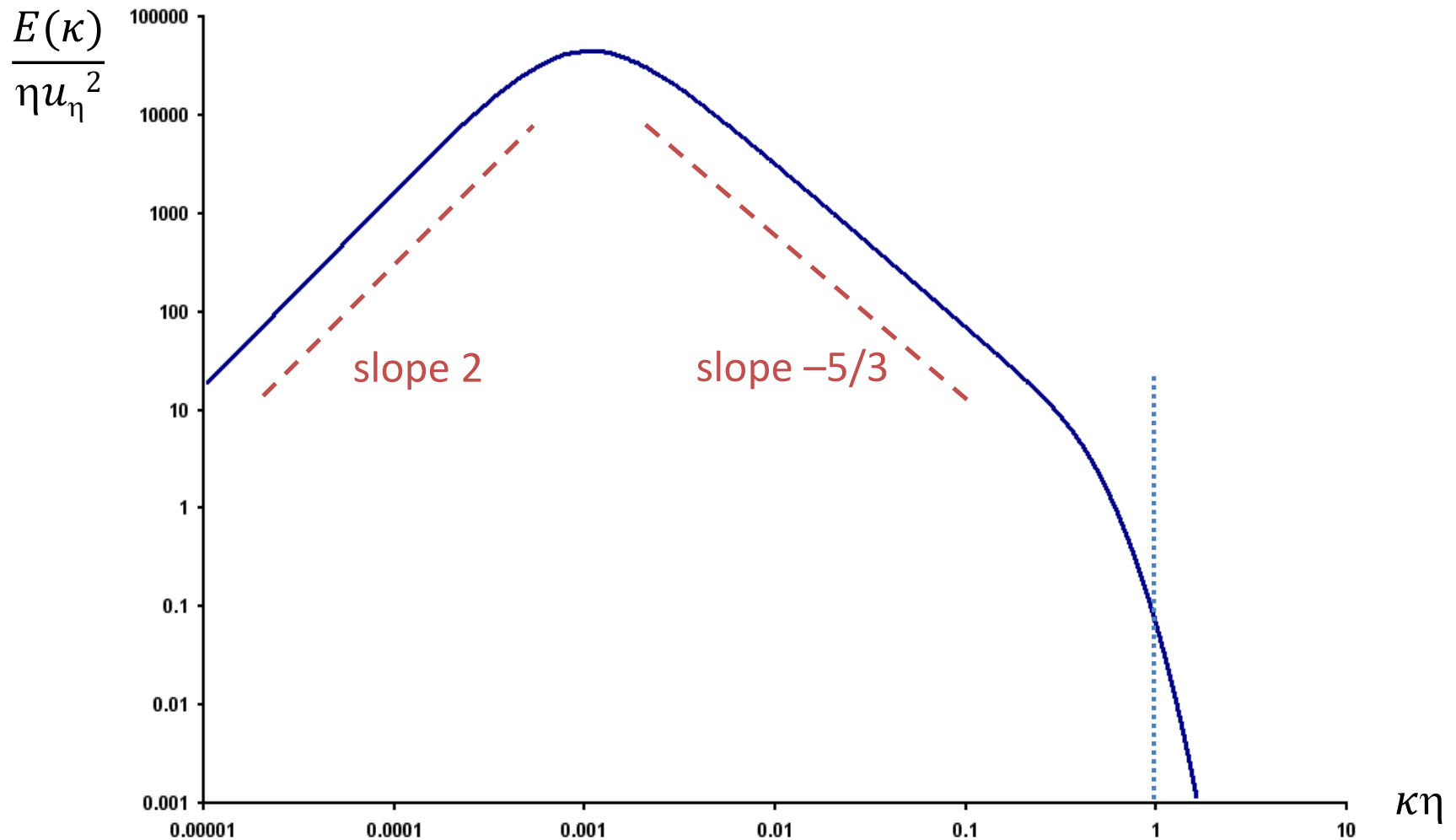
$$\frac{E(\kappa)}{\eta u_\eta{}^2}$$

Re$_\lambda$ = 1000

Re$_\lambda$ = 300

Re$_\lambda$ = 100

Re$_\lambda$ = 30

$\kappa\eta$
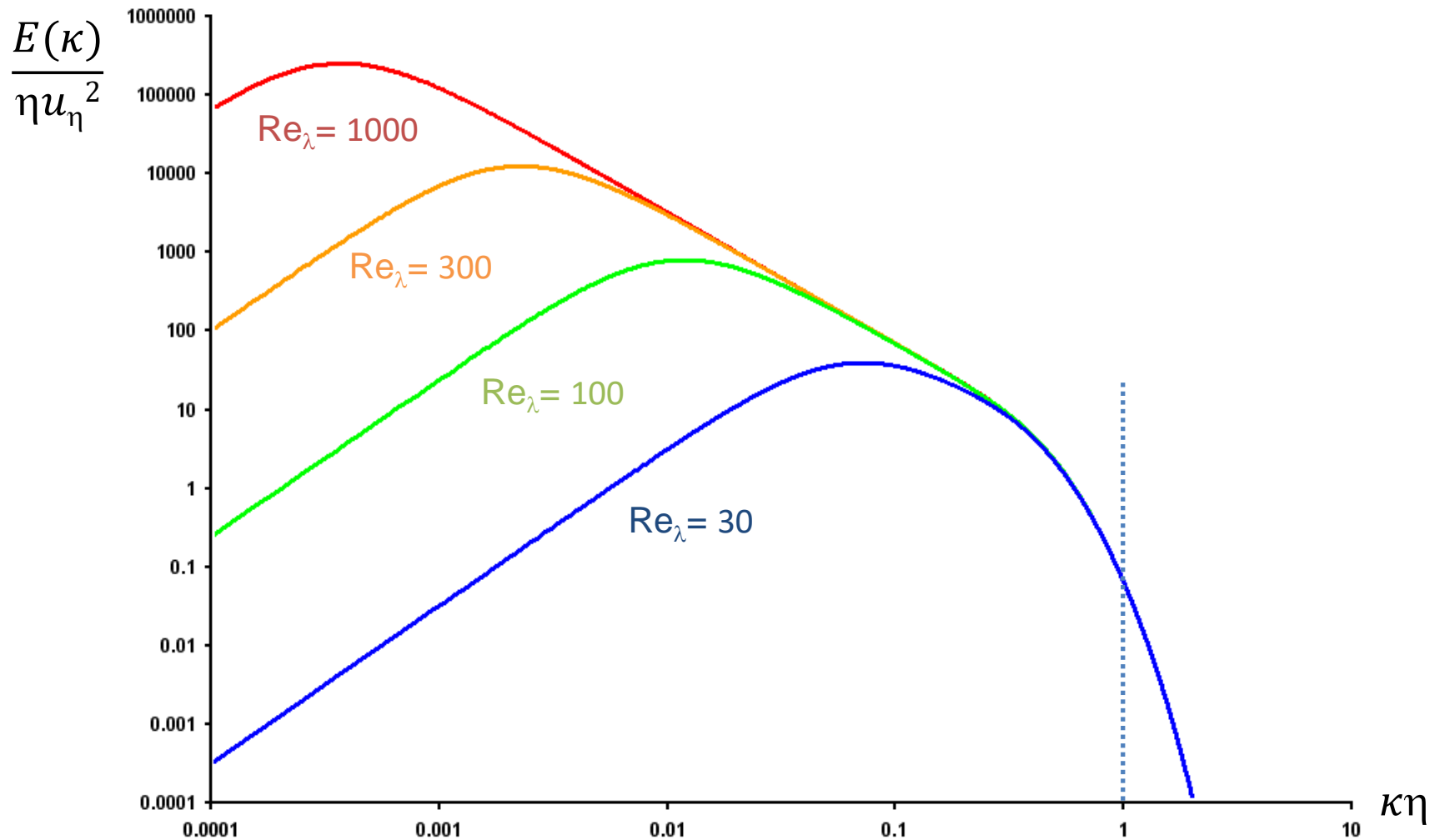
The Kolmogorov's scale can be correlated to the integral scale:

$$\frac{l_0}{\eta} = \frac{l_0}{11\left(\dfrac{\nu^3}{\varepsilon}\right)^{1/4}} = \frac{l_0}{11\left(\nu^3 \dfrac{l_0}{3.1 v_{rms}'^3}\right)^{1/4}} = 0.07\left(\frac{l_0 v_{rms}'}{\nu}\right)^{3/4} = 0.07\,Re_{l_0}^{0.75}$$

If we change the mean velocity, i.e. the mean Reynolds' number, we are changing the ratio between the scales of turbulence. Usually macroscales are unchanged (because they mainly depend on the geometry), but microscales becomes smaller and smaller by increasing the Reynolds' number.
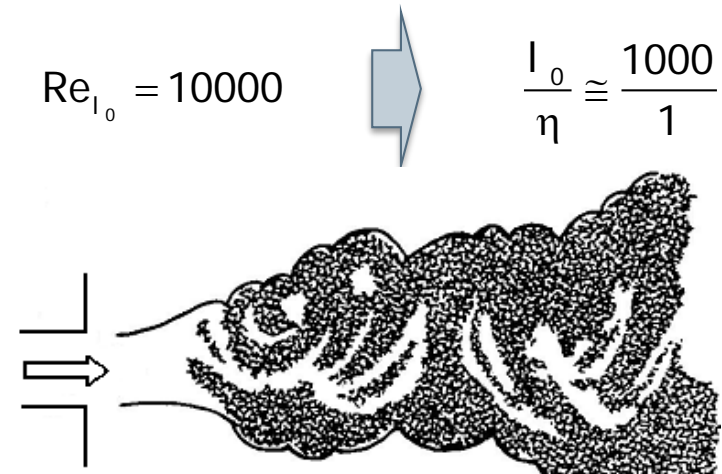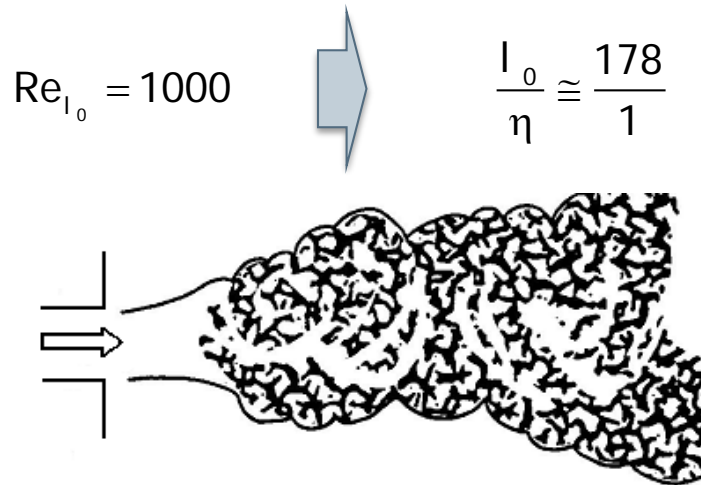
$Re_{l_0} = 1000$ ➡ $\dfrac{l_0}{\eta} \cong \dfrac{178}{1}$ $Re_{l_0} = 10000$ ➡ $\dfrac{l_0}{\eta} \cong \dfrac{1000}{1}$

Outline

1. **Introduction to turbulent flows**

2. **Statistical description of turbulent flows**
   a) Reynolds and Favre average
   b) 2-point correlations
   c) Turbulent eddies and energy cascade

3. **Kolmogorov's Theory**
   a) Kolmogorov's similarity hypotheses
   b) Kolmogorov's scales
   c) Energy spectrum

4. **Transport equations for mean variables**
   a) Need of mean/filtered equations
   b) Favre's averaged transport equations for continuity and momentum
   c) Closure models for turbulent flows: $\kappa - \varepsilon$ model
   d) Favre's averaged transport equations for passive scalars and species
   e) Large Eddy Simulation (LES)

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The evolution of turbulent systems is still described through the usual conservation equations we already derived:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla p + \nabla \cdot \mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T - \frac{2}{3} (\nabla \cdot \boldsymbol{u}) I \right) + \rho \boldsymbol{g}$$

$$\rho \frac{\partial Y_i}{\partial t} + \rho \boldsymbol{u} \cdot \nabla Y_i = \nabla \cdot (\rho \mathcal{D}_i \nabla Y_i) + \dot{\Omega}_i$$

$$\rho C_P \frac{DT}{Dt} = \frac{Dp}{Dt} + \nabla \cdot \lambda \nabla T - \sum \rho \boldsymbol{u}_i^d Y_i C_{Pi} \cdot \nabla T + \dot{Q}$$

Such conservation equations still requires proper sub-models to close them (thermodynamic equation of state, radiative heat transfer equation, kinetic mechanism, etc.)

Solution of transport equations

The turbulent flows are described by the usual conservation equations of mass, species, momentum and energy

In principle, after assigning the proper boundary and initial conditions, we can solve the transport equations using the numerical techniques we discussed, in order to estimate the relevant variables in every point of the computational domain.

Problem! The number of grid points to describe the details of turbulent flows is huge, because of the wide range of scales (from the Kolmogorov's scale to the macroscale)

10^{-7} m   1

Kolmogorov's   Macroscale
scale
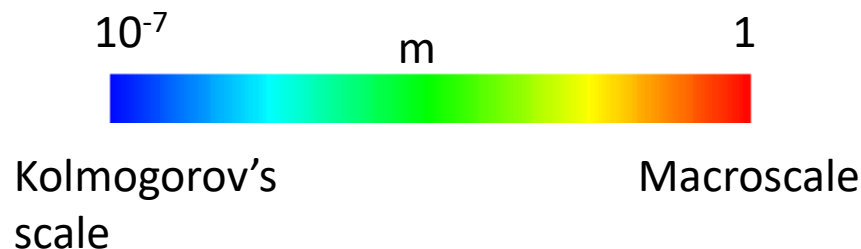
This direct approach (DNS or Direct Numerical Solution) is possible only for simple flows and for small Reynolds numbers:

DNS: Direct Numerical Simulation

Ratio between the Kolmogorov's and the integral scales:

$$\frac{\eta}{l_0} = Re_t^{-3/4}$$

Example
Turbulent jet
$$Re_{l_0} = 5,000$$

Number of points per direction
$$\frac{l_0}{\eta} = n \sim 600$$

Total number of mesh points:
$$n^3 \sim 0.21 \cdot 10^9$$

Craske, John. (2016). The properties of integral models for planar and axisymmetric unsteady jets. IMA Journal of Applied Mathematics. 82. hxw043. 10.1093/imamat/hxw043.

Numerical modeling of turbulent flows

Semi-empirical correlations: this methodology is very simple and useful for some applications of interest for Chemical Engineering. However, this approach is not very general (it is valid only for the conditions for which the correlation was developed) and not always it is very useful for the understanding of the phenomenon under investigation
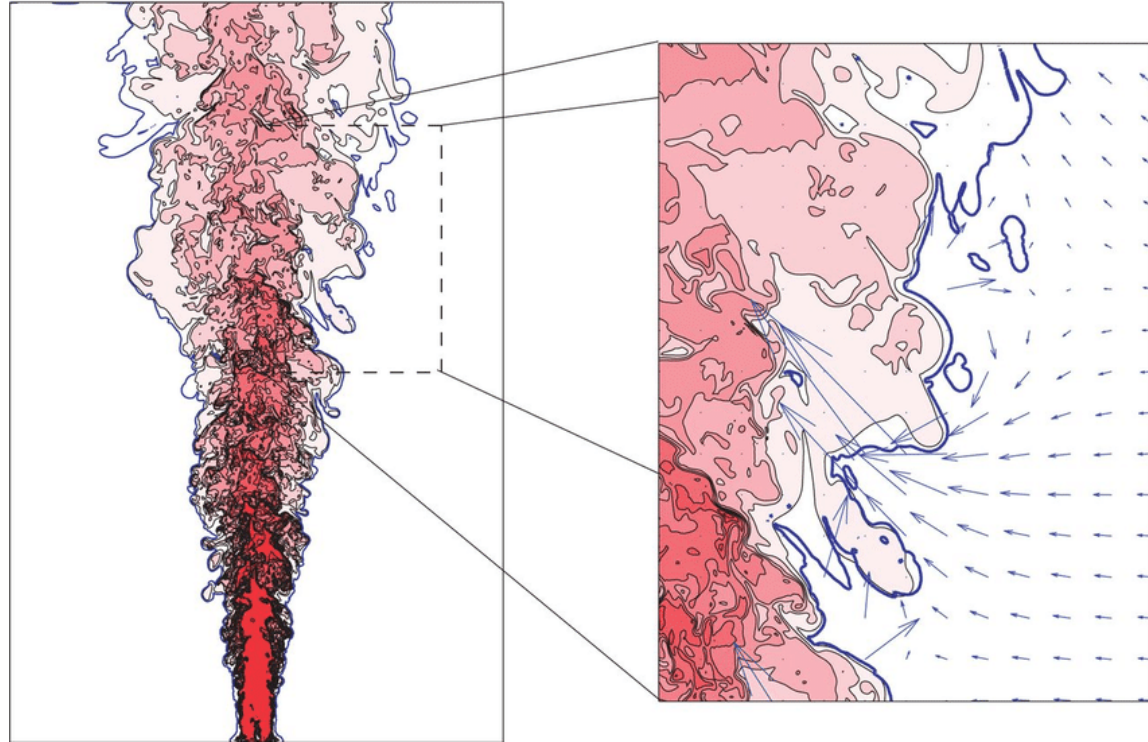
Integral equations: they can be derived from the integration of conservation equations along one or more than one coordinates; the resulting problem to be solved is describe by one or more differential equations

Reynolds Averaged Navier-Stokes (RANS): this methodology consists of a system of PDE (partial differential equations) which is derived from a proper averaging in time of conservation equations of relevant variables (momentum, pressure, energy and species). The RANS equations however need a proper closure, i.e. sub-models describing non-linear effects

Large Eddy Simulation (LES): in this approach a new set of partial differential equations is solved, in which the new variables are filtered in space (i.e. only the scales larger than a so called filter width are solved). Only LES approach requires a proper closure, i.e. submodels describing the effescts of small scales (which are not resolved

Direct Numerical Simulation (DNS): the transport equations of relevant species are solved directly

Computational cost

Numerical modeling of turbulence (I)

DNS
Direct Numerical Simulation

The transport equations are resolved as they are, with any filtering or averaging

LES
Large Eddy Simulation

Only largest vortices are transported. Computational cells are too large to describe small vortices, which are modeled using proper sub-grid scale models

RANS
Reynolds-Averaged Navier-Stokes

Only the mean quantities are transported. The transport equations require closure models.

Q(t)

DNS

RANS

LES

time
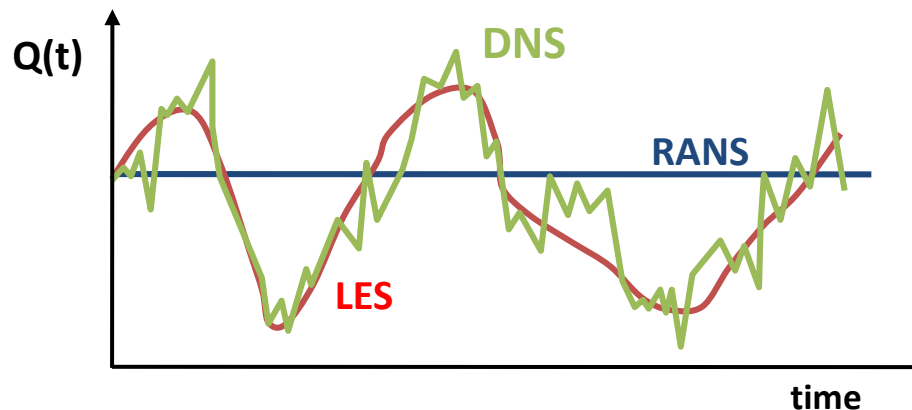
RANS

Advantages: computational cost very low

Disadvantages: inaccuracy of closure models

DNS (a) LES (b) RANS (c)
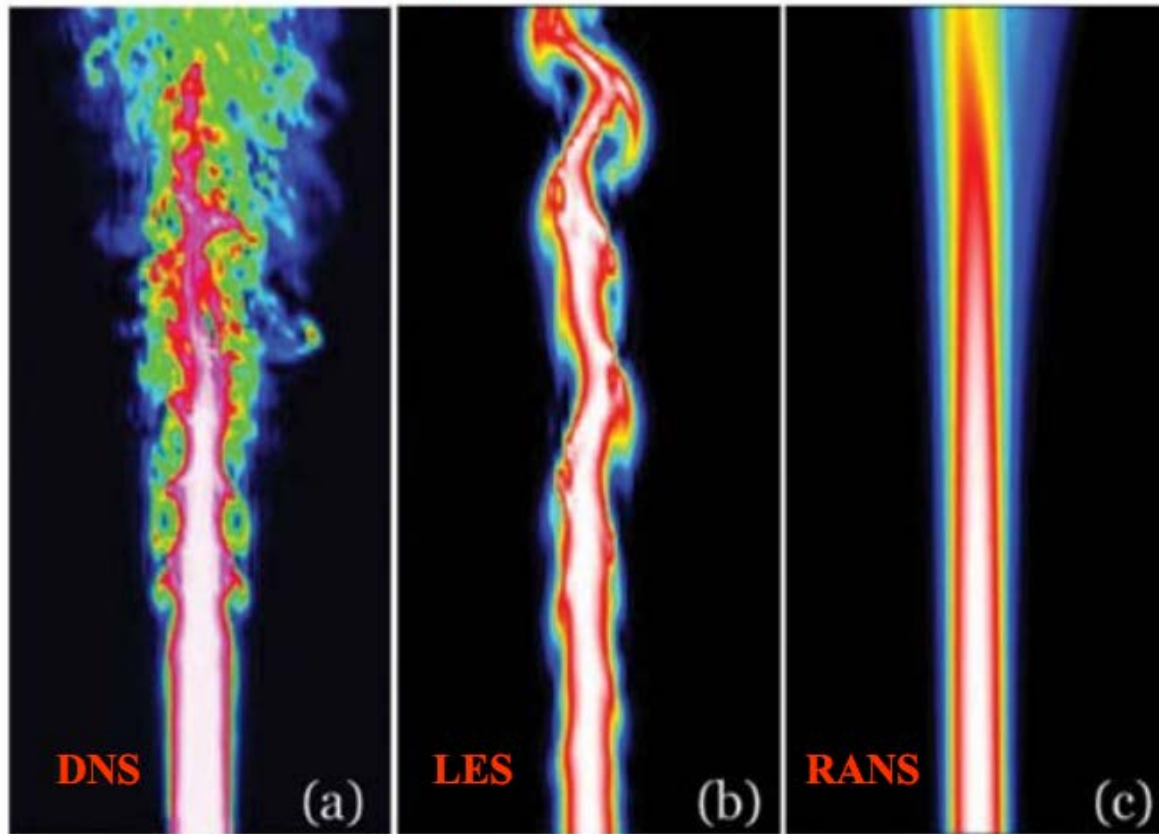
Small vortices are not transported, but modelled

Only mean quantities are available in RANS

Mean flow equations

Let us start from the Navier-Stokes equations for incompressible fluids, i.e. for fluids with constant density:

$$\begin{cases} \dfrac{\partial u_j}{\partial x_j} = 0 \\[4mm] \dfrac{\partial u_j}{\partial t} + u_i \dfrac{\partial u_j}{\partial x_i} = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial x_j} + v\dfrac{\partial^2 u_j}{\partial x_i^2} \qquad j = 1,2,3 \end{cases}$$

The equations above are written using the Einstein's notation, which implies summation over a set of repeated indices terms in a formula, thus achieving notational brevity

Remember the definition of Reynolds' decomposition

$$\begin{cases} u_i = \bar{u}_i + u_i' \qquad i = 1,2,3 \\[3mm] \qquad\quad p = \bar{p} + p' \end{cases}$$

Averaged continuity equation

Let us apply the Reynolds' average to the continuity equation:

$$\overline{\frac{\partial u_j}{\partial x_j}} = \frac{\partial \bar{u}_j}{\partial x_j} + \frac{\partial \overline{u'_j}}{\partial x_j} = \frac{\partial \bar{u}_j}{\partial x_j} = 0$$

The result above comes directly from the definition of Reynolds' averaging, according to which the average of fluctuation is identically equal to zero:

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

Thus, because of the linearity of the continuity equation, there are no correlations of fluctuating quantities. The Reynolds' averaged continuity equation becomes:

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0$$ Reynolds' averaged continuity equation

Unfortunately this is not true for the momentum equations, because of the non linearity of the convective term $u_i \dfrac{\partial u_j}{\partial x_i}$:

$$u_i \frac{\partial u_j}{\partial x_i} = \frac{\partial u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_i}\left[(\bar{u}_i + u_i')(\bar{u}_j + u_j')\right] = \frac{\partial}{\partial x_i}\left[\bar{u}_i\bar{u}_j + \bar{u}_j u_i' + \bar{u}_i u_j' + u_i' u_j'\right]$$

When we apply the Reynolds' averaging operator, an additional term is created:

$$\overline{u_i \frac{\partial u_j}{\partial x_i}} = \overline{\frac{\partial u_i u_j}{\partial x_i}} = \frac{\partial}{\partial x_i}\left[\overline{\bar{u}_i\bar{u}_j} + \overline{\bar{u}_j u_i'} + \overline{\bar{u}_i u_j'} + \overline{u_i' u_j'}\right] = \frac{\partial}{\partial x_i}\left[\overline{\bar{u}_i\bar{u}_j} + \overline{u_i' u_j'}\right]$$

$$\frac{\partial}{\partial x_i}\overline{u_i' u_j'} \neq 0$$

Thus, the averaged convective term is the sum of two terms:

$$\overline{u_i \frac{\partial u_j}{\partial x_i}} = \frac{\partial}{\partial x_i}\bar{u}_i\bar{u}_j + \frac{\partial}{\partial x_i}\overline{u_i' u_j'} = \bar{u}_i \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial}{\partial x_i}\overline{u_i' u_j'}$$

The remaining terms in the momentum equations do not represent an issue, since they are linear. So, the averaged momentum equations become:

$$\frac{\partial \bar{u}_j}{\partial t} + \bar{u}_i \frac{\partial \bar{u}_j}{\partial x_i} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_j}{\partial x_i^2} - \frac{\partial}{\partial x_i} \overline{u_i' u_j'} \qquad j = 1,2,3$$

$$\frac{\partial \bar{u}_j}{\partial t} + \bar{u}_i \frac{\partial \bar{u}_j}{\partial x_i} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_i} \left(\nu \frac{\partial \bar{u}_j}{\partial x_i} - \overline{u_i' u_j'} \right) \qquad j = 1,2,3$$

The additional term, resulting from convective transport, is added to the viscous term on the right hand side (divergence of a second order tensor) and is called **Reynolds Stress Tensor**:

$$\tau_{ij}^{turb} = -\overline{u_i' u_j'} \qquad j = 1,2,3$$

- This leads to the closure problem in turbulence theory!

- The Reynolds Stress Tensor

$$\tau_{ij}^{turb} = -\overline{u_i' u_j'} \quad j = 1,2,3$$

    needs to be expressed as a function of mean flow quantities

- A first idea: derivation of a transport equation for τ_{ij}^{turb}. This can be done analytically, starting from the momentum equations, and properly applying multiplications with the velocity components and averaging operations. The derivation is not here reported, but it can be easily found in many textbooks on turbulent flows or in [Pitsch2018].

Reynolds stress tensor equations

We have 6 new equations for the Reynolds' Stress Tensor components:

$$\frac{\partial}{\partial t}\left(\overline{u_j' u_k'}\right) + \bar{u}_i \frac{\partial}{\partial x_i}\left(\overline{u_j' u_k'}\right) = -\overline{u_i' u_k'}\frac{\partial \bar{u}_j}{\partial x_i} - \overline{u_i' u_j'}\frac{\partial \bar{u}_k}{\partial x_i} + \cdots$$

$$-2\upsilon \overline{\frac{\partial u_k'}{\partial x_i}\frac{\partial u_j'}{\partial x_i}} + \overline{\frac{p'}{\rho}\left(\frac{\partial u_j'}{\partial x_k} + \frac{\partial u_k'}{\partial x_j}\right)} + \cdots$$

$$+ \frac{\partial}{\partial x_i}\left[-\overline{u_i' u_j' u_k'} + \upsilon \frac{\partial}{\partial x_i}\left(\overline{u_j' u_k'}\right) - \overline{\frac{p'}{\rho}\left(\delta_{ij} u_k' + \delta_{ik} u_j'\right)}\right]$$

However, they are not closed, but they contains additional unknowns and correlation terms of third-order!

Transport Equation for Turbulent Kinetic Energy

Derivation of an equation for the Turbulent Kinetic Energy (TKE)

TKE is defined as:

$$\bar{k} = \frac{1}{2}\overline{u_i'^2} = \frac{1}{2}\left(\overline{u_1'^2} + \overline{u_2'^2} + \overline{u_3'^2}\right)$$

From the equations for the Reynolds' Stress Tensor components it is relatively easy to get the equation governing the evolution of the TKE:

convection   production

$$\frac{\partial \bar{k}}{\partial t} + \bar{u}_i\frac{\partial \bar{k}}{\partial x_i} = -\overline{u_i'u_j'}\frac{\partial \bar{u}_j}{\partial x_i} - \varepsilon + \frac{\partial}{\partial x_i}\left[-\overline{u_i'\left(k+\frac{p'}{\rho}\right)} + v\frac{\partial \bar{k}}{\partial x_i} + v - \frac{\partial}{\partial x_i}\left(\overline{u_i'u_j'}\right)\right]$$

Local change
(unsteady)

diffusion

Dissipation

$$\varepsilon = v\,\overline{\frac{\partial u_j'}{\partial x_i}\frac{\partial u_j'}{\partial x_i}}$$

ε is the rate at which turbulence kinetic energy is converted into thermal internal energy.

Turbulence models: turbulent viscosity

The derived averaged equations are not closed

turbulent stress tensor τ_{ij}^{turb} has to be modeled

$$\tau_{ij}^{turb} = -\overline{u_i' u_j'} \quad j = 1,2,3$$

Analogy to Newton approach for molecular shear stress

Gradient Transport Model:

$$-\overline{u_i' u_j'} = v_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \bar{k} \delta_{ij}$$

v_t is **eddy viscosity/turbulent viscosity** (important: ≠ molecular viscosity!)

Turbulent viscosity models

- Algebraic models: e.g. Prandtl's mixing-length concept

$$v_t = l_m^2 \left| \overline{S_{ij}} \right| = l_m^2 \left| \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \right|$$

- TKE models: e.g. Prandtl-Kolmogorov

$$v_t = C_\mu l_{pk} \sqrt{k}$$

- Two equation models: e.g. $k - \varepsilon$ model (Jones, Launder)

$$v_t = C_\mu \frac{k^2}{\varepsilon}$$

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$$v_t = l_m^2 |\overline{S_{ij}}| = l_m^2 \left|\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right|$$

- Based on a dimensional analysis
- The mixing-length l_m becomes the unique parameter
- Empirical methods for determining the mixing length l_m
- Assumption: $l_m = const$

- Important for LES (Large Eddy Simulation)

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$$v_t = C_\mu l_{pk} \sqrt{k}$$

- Model constant C_μ (typically $C_\mu = 0.09$)
- l_{pk} is a characteristic length scale determined empirically
- An equation for TKE is needed

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$$v_t = C_\mu \frac{k^2}{\varepsilon}$$

- Equation for TKE

$$\frac{\partial \bar{k}}{\partial t} + \bar{u}_i \frac{\partial \bar{k}}{\partial x_i} = P_k - \bar{\varepsilon} + \frac{\partial}{\partial x_i} \left(\frac{v_t}{Pr_k} \frac{\partial \bar{k}}{\partial x_i} \right)$$

- Equation for dissipation

$$\frac{\partial \bar{\varepsilon}}{\partial t} + \bar{u}_i \frac{\partial \bar{\varepsilon}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{v_t}{Pr_\varepsilon} \frac{\partial \bar{\varepsilon}}{\partial x_i} \right) + \frac{\bar{\varepsilon}}{\bar{k}} (C_{\varepsilon 1} P_k - C_{\varepsilon 2} \bar{\varepsilon})$$

- Empirically determined parameters

$$C_{\varepsilon 1} = 1.44 \qquad C_{\varepsilon 2} = 1.90 \qquad Pr_\varepsilon = 1.30 \qquad Pr_k = 1.0$$

In the model, the turbulent transport term in the turbulent kinetic energy equation is simplified:

$$\frac{\partial \bar{k}}{\partial t} + \bar{u}_i \frac{\partial \bar{k}}{\partial x_i} = -\overline{u'_i u'_j} \frac{\partial \bar{u}_j}{\partial x_i} - \varepsilon + \frac{\partial}{\partial x_i}\left[\overline{-u'_i \left(k + \frac{p'}{\rho} \right)} + v \frac{\partial \bar{k}}{\partial x_i} + v - \frac{\partial}{\partial x_i}\left(\overline{u'_i u'_j} \right) \right]$$

$$\frac{\partial}{\partial x_i}\left[\overline{-u'_i \left(k + \frac{p'}{\rho} \right)} + v \frac{\partial \bar{k}}{\partial x_i} + v - \frac{\partial}{\partial x_i}\left(\overline{u'_i u'_j} \right) \right] \approx \frac{\partial}{\partial x_i}\left[\overline{-u'_i \left(k + \frac{p'}{\rho} \right)} \right] \approx \frac{\partial}{\partial x_i}\left(\frac{v_t}{Pr_k} \frac{\partial \bar{k}}{\partial x_i} \right)$$

The production term is expanded according to the gradient assumption and the turbulent viscosity concept:

$$P_k = -\overline{u'_i u'_j} \frac{\partial \bar{u}_j}{\partial x_i} = v_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_j}{\partial x_i}$$

Let us consider the transport equation for a passive scalar ϕ, i.e. a scalar without any source term and without impact on the main fluid dynamic variables (velocity, pressure, and density). Let us also consider the general case of a compressible fluid:

$$\rho \frac{\partial \phi}{\partial t} + \rho u_i \frac{\partial \phi}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D}_\phi \frac{\partial \phi}{\partial x_i}\right)$$

If we apply the Reynolds average to every term and we consider the definition of Favre average (i.e. density-weighted average), we get the following averaged equation:

$$\bar{\rho}\frac{\partial \tilde{\phi}}{\partial t} + \bar{\rho}\tilde{u}_i\frac{\partial \tilde{\phi}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho \mathcal{D}_\phi \frac{\partial \phi}{\partial x_i}}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i''\phi''}\right)$$

Unclosed terms

molecular transport   **turbulent transport**

A typical simplification is to assume that the molecular transport is negligible with respect to the turbulent transport (this simplification implies the assumption of high Reynolds' number)

The turbulent transport term is usually modelled using the gradient transport model:

$$\widetilde{u_i'' \phi''} = -\mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i}$$

$\mathcal{D}_t$ is the turbulent diffusivity, proportional to the turbulent viscosity:

$$\mathcal{D}_t = \frac{\upsilon_t}{Sc_t}$$

Thus, the transport equation for the mean passive scalar is:

$$\bar{\rho} \frac{\partial \tilde{\phi}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{\phi}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho} \mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i} \right)$$

It is possible to derive a transport equation for the variance of a passive scalar ϕ. The demonstration is reported in many textbooks and in [Pitsch2018]:

$$\bar{\rho}\frac{\partial \widetilde{\phi''^2}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \widetilde{\phi''^2}}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i''\phi''^2}\right) + 2\bar{\rho}\left(-\widetilde{u_i''\phi''}\right)\frac{\partial \tilde{\phi}}{\partial x_i} - 2\bar{\rho}\mathcal{D}_\phi \left(\widetilde{\frac{\partial \phi''}{\partial x_i}}\right)^2$$

dissipation

$$\widetilde{u_i''\phi''^2} = -\mathcal{D}_t \frac{\partial \widetilde{\phi''^2}}{\partial x_i}$$

Turbulent transport

$$\widetilde{u_i''\phi''} = -\mathcal{D}_t \frac{\partial \tilde{\phi}}{\partial x_i}$$

production

$$\bar{\rho}\frac{\partial \widetilde{\phi''^2}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \widetilde{\phi''^2}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_t \frac{\partial \widetilde{\phi''^2}}{\partial x_i}\right) + 2\bar{\rho}\mathcal{D}_t \left(\frac{\partial \tilde{\phi}}{\partial x_i}\right)^2 - \bar{\rho}\chi$$

Scalar dissipation $\quad \chi \overset{\text{def}}{=} 2\mathcal{D}_\phi \left(\widetilde{\frac{\partial \phi''}{\partial x_i}}\right)^2$

Integral time τ_ϕ (dimensional analysis, $[\chi] = s^{-1}$)

$$\tau_\phi \sim \frac{\widetilde{\phi''^2}}{\chi}$$

Typically proportional to τ

$$\tau = \frac{\tilde{k}}{\tilde{\varepsilon}} = C_\chi \tau_\phi \qquad 1.5 \leq C_\chi \leq 3$$

This leads to

$$\chi = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{\phi''^2}$$

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Transport equation for mean passive scalar ϕ:

$$\bar{\rho}\frac{\partial\tilde{\phi}}{\partial t} + \bar{\rho}\tilde{u}_i\frac{\partial\tilde{\phi}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_t\frac{\partial\tilde{\phi}}{\partial x_i}\right)$$

Transport equation for mean variance of passive scalar ϕ:

$$\bar{\rho}\frac{\partial\widetilde{\phi''^2}}{\partial t} + \bar{\rho}\tilde{u}_i\frac{\partial\widetilde{\phi''^2}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_t\frac{\partial\widetilde{\phi''^2}}{\partial x_i}\right) + 2\bar{\rho}\mathcal{D}_t\left(\frac{\partial\tilde{\phi}}{\partial x_i}\right)^2 - \bar{\rho}C_\chi\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{\phi''^2}$$

Let us consider the transport equation for a reactive species whose mass fraction is Y_k:

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D}_k \frac{\partial Y_k}{\partial x_i}\right) + \rho S_k$$

The "only" difference with the passive scalar case is the presence of the source term S_k due to the chemical reactions (actually we will see this is a huge difference). If we apply the averaging, we have:

$$\bar{\rho}\frac{\partial \widetilde{Y_k}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \widetilde{Y_k}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho \mathcal{D}_k \frac{\partial Y_k}{\partial x_i}}\right) - \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i'' Y_k''}\right) + \rho \tilde{S}_k$$

Unclosed terms

molecular transport   **turbulent transport**   **source term**

Reactive species transport equations (II)

We can proceed similarly to what we already did for the passive scalar case. In particular, we can neglect the molecular transport contribution and we can use the gradient transport model for the turbulent transport term:

$$\bar{\rho}\frac{\partial \widetilde{Y_k}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \widetilde{Y_k}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}\mathcal{D}_t \frac{\partial \widetilde{Y_k}}{\partial x_i}\right) + \boxed{\rho\tilde{S}_k}$$

Unclosed terms

source term

The source term is unclosed. Its modeling is quite complex, because it is a strongly non linear function of temperature and composition. Moreover, its expression is not general, but it depends on the kinetic mechanism describing the reactions in which the species is involved.

Modeling of turbulent combustion!

The averaged temperature transport equation presents the same features of the averaged transport equations for reactive species. In particular, it is easy to demonstrate that if we neglect the heat fluxes due to the molecular diffusion of species (which is reasonable for high Reynolds' number), the temperature equation become:

$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \mathcal{D}_T \frac{\partial T}{\partial x_i}\right) + \frac{\dot{Q}}{C_P}$$

$\mathcal{D}_T$ is the thermal diffusion coefficient $\mathcal{D}_T = \frac{\lambda}{\rho C_P}$ and $\dot{Q}$ is the heat release due to the chemical reactions: $\dot{Q} = -\sum h_k \dot{\Omega}_k$. After applying the proper averaging operations and the usual simplifications:

$$\bar{\rho} \frac{\partial \tilde{T}}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \tilde{T}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho} \mathcal{D}_t \frac{\partial \tilde{T}}{\partial x_i}\right) + \boxed{\frac{\overline{\dot{Q}}}{C_P}} \quad \textbf{Unclosed terms}$$

Outline

1. **Introduction to turbulent flows**

2. **Statistical description of turbulent flows**
   a) Reynolds and Favre average
   b) 2-point correlations
   c) Turbulent eddies and energy cascade

3. **Kolmogorov's Theory**
   a) Kolmogorov's similarity hypotheses
   b) Kolmogorov's scales
   c) Energy spectrum

4. **Transport equations for mean variables**
   a) Need of mean/filtered equations
   b) Favre's averaged transport equations for continuity and momentum
   c) Closure models for turbulent flows: $\kappa - \varepsilon$ model
   d) Favre's averaged transport equations for passive scalars and species
   e) **Large Eddy Simulation (LES)**

- In Large-Eddy Simulation (LES) of turbulence, the time and space dependence of the fluid motions are resolved down to some prescribed **length-scale Δ**.
- The motion is separated into small and large scales, often by spatially filtering the velocity field with a filter kernel function (or simply a kernel) $G(x, \Delta)$ (Leonard 1974).
- The convolution kernel eliminates scales smaller than Δ . The eliminated scales are called subfilter or subgrid-scale (SGS) motions.
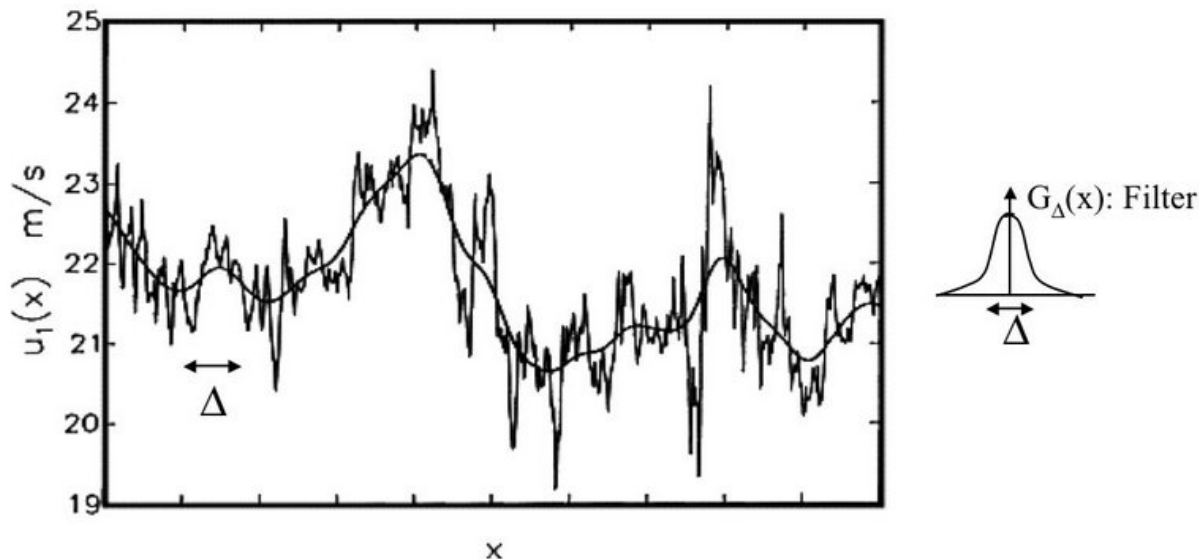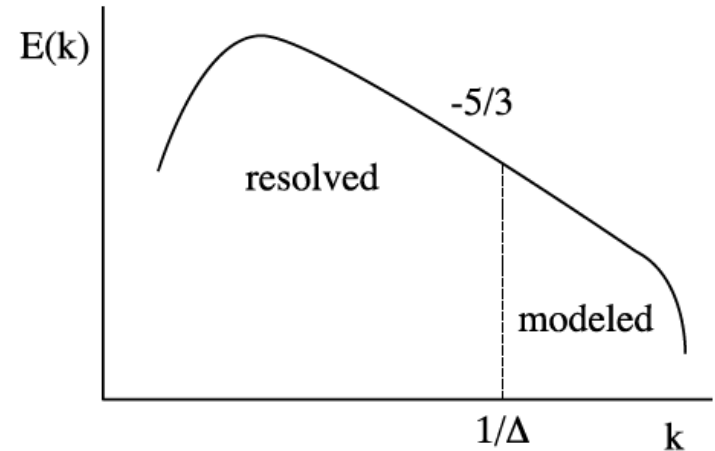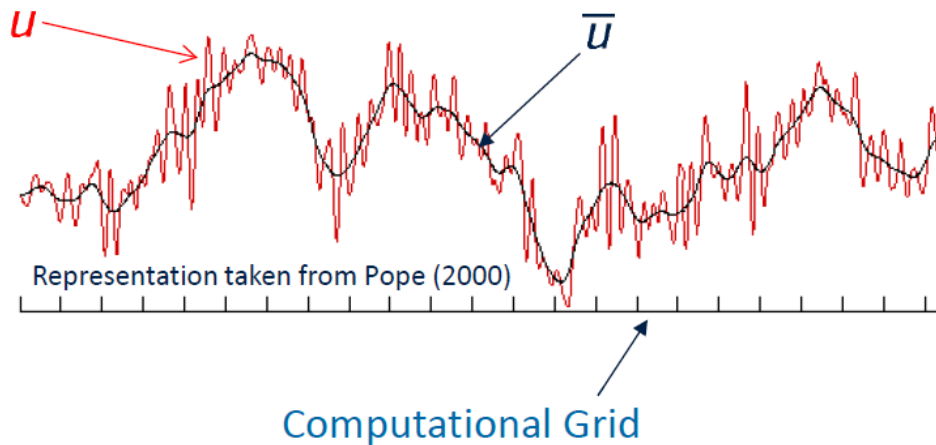

Unfiltered and filtered turbulent field showing decomposition used in LES. In subgrid-scale modeling, the effects of the difference between the two signals upon the dynamics of the large scale signal must be modeled.

Spatial filtering opposed to Reynolds' (or Favre's) averaging

$$\bar{\psi} = \mathcal{L}(\psi) \stackrel{\text{def}}{=} \int G(\boldsymbol{x}, \boldsymbol{x}')\psi(\boldsymbol{x}')\boldsymbol{dx}'$$

Representation taken from Pope (2000)

Computational Grid

- $G(\boldsymbol{x}, \boldsymbol{x}')$ is the **filter kernel function**
- Scales smaller than **filter scale** Δ absent from the filtered quantities
- Filtered signal can be discretized using a mesh substantially smaller than the DNS mesh
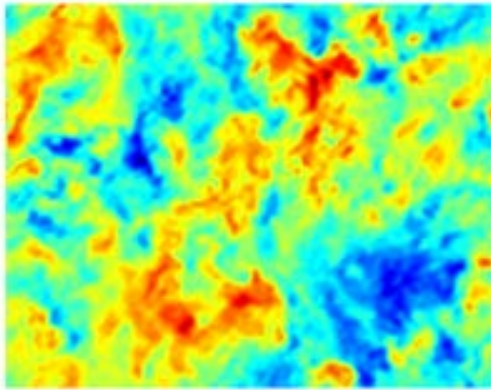
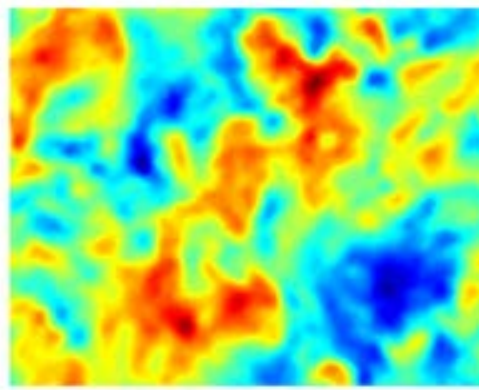A velocity field produced by a direct numerical simulation (DNS) of homogeneous decaying turbulence. The domain size is L^3.

The same DNS velocity field filtered using a box filter and $\Delta = L/32$
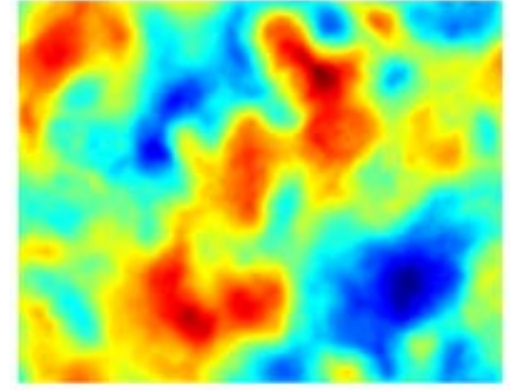
The same DNS velocity field filtered using a box filter and $\Delta = L/16$

The filter kernel function G uses a cutoff length scale Δ. Scales smaller than this Δ are eliminated from $\overline{\psi}$. Using this definition, any field ψ may be split up into a filtered and sub-filtered (denoted with a prime) portion, as:

$$\psi = \overline{\psi} + \psi'$$

Box filter in 1D

$$G(r) = \frac{1}{\Delta} H\left(\frac{1}{2}\Delta - |r|\right) = \begin{cases} \dfrac{1}{\Delta} & if \ |r| \leq \dfrac{1}{2} \\ \\ 0 & otherwise \end{cases}$$

Sharp spectral filter

$$G(\kappa) = H\left(\frac{\pi}{\Delta} - |\kappa|\right)$$

The LES equations (or filtered NS) can be discretized numerically by employing a spatial resolution that is on the order of Δ. When Δ is chosen to be much larger than the Kolmogorov scale η_K LES is typically far less expensive than Direct Numerical Simulation (DNS) which requires resolutions near η_K.

Filtered Momentum Equations

Momentum equations or instantaneous variables (incompressible fluid)

$$\frac{\partial u_j}{\partial t} + \frac{\partial}{\partial x_i}\left(u_i u_j\right) = -\frac{1}{\rho}\frac{\partial p}{\partial x_j} + v\frac{\partial^2 u_j}{\partial x_j^2}$$

Filtered momentum equations

$$\frac{\partial \bar{u}_j}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{u_i u_j}\right) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_j} + v\frac{\partial^2 \bar{u}_j}{\partial x_j^2}$$

Residual stress tensor

$$\tau_{ij}^R \overset{\text{def}}{=} \overline{u_i u_j} - \bar{u}_i \bar{u}_j$$

$$\frac{\partial \bar{u}_j}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{u}_i \bar{u}_j\right) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_j} + v\frac{\partial^2 \bar{u}_j}{\partial x_j^2} - \frac{\partial \tau_{ij}^R}{\partial x_i}$$

A sub-filter model is needed to close the equations

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Eddy-viscosity (or functional models) focus only on dissipating energy at a rate that is physically correct. These are based on an artificial eddy viscosity approach, where the effects of turbulence are lumped into a turbulent viscosity.

The approach treats dissipation of kinetic energy at sub-grid scales as analogous to molecular diffusion:

$$\tau_{ij}^{R} = -v_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) = -2v_t \bar{S}_{ij}$$

v_t is the so-called turbulent eddy viscosity and $\bar{S}_{ij}$ is the filtered strain rate tensor:

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

Based on dimensional analysis, the eddy viscosity v_t must have units of m^2/s. Most eddy viscosity SGS models model the eddy viscosity as the product of a characteristic length scale and a characteristic velocity scale.

Smagorinsky-Lilly Model

The units of the eddy viscosity are velocity times a characteristic length-scale (or kinetic energy density) multiplied by a time-scale:

$$v_t \sim \ell v$$

The best known eddy-viscosity model bears the name of J. Smagorinsky. In the Smagorinsky model (1963) the eddy viscosity is expressed as the characteristic scale $\ell = C_s \Delta$ times a velocity scale $v = \ell |\bar{S}|$, where $|\bar{S}| \stackrel{\text{def}}{=} \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{\frac{1}{2}}$ represents an estimation of velocity differences over length-scales of order Δ:

$$v_t = (C_s \Delta)^2 |\bar{S}|$$

The model contains a dimensionless empirical parameter (the so-called Smagorinsky coefficient C_s). Lilly (1967) derived from theoretical arguments $C_s \approx 0.16$. This result is valid for locally isotropic turbulence, when Δ falls in the inertial range of turbulence. Numerical simulations of isotropic turbulence with this value yield very realistic decay rates of kinetic energy and energy spectra with realistic features, except close to the cutoff-wavenumber of the LES.

Dynamic Smagorinsky-Lilly Model

Germano et al. (1991) and subsequently Lilly (1992) conceived a procedure in which the Smagorinsky model constant C_s is dynamically computed based on the information provided by the resolved scales of motion. The dynamic procedure thus obviates the need for users to specify the model constant C_s in advance.

The concept of the dynamic procedure is to apply a second filter (called the test filter) to the equations of motion. The new filter width $\widehat{\Delta}$ is equal to twice the grid filter width Δ. Both filters produce a resolved flow field. The difference between the two resolved fields is the contribution of the small scales whose size is in between the grid filter and the test filter.

Germano, M., Piomelli, U., Moin, P., Cabot, W., A dynamic subgrid-scale eddy viscosity model, Physics of Fluids A, 3(7): 1760–1765 (1991)

D. K. Lilly, A Proposed Modification of the Germano Subgrid-Scale Closure Model. *Physics of Fluids*, 4: 633-635 (1992)

Other models

The original and dynamic Smagorinsky-Lilly models are essentially algebraic models in which subgrid-scale stresses are parameterized using the resolved velocity scales. The underlying assumption is the local equilibrium between the transferred energy through the grid-filter scale and the dissipation of kinetic energy at small subgrid scales.
Many other models have been proposed and applied in order to overcome the limitations of original and dynamic Smagorinsky-Lilly models.

Wall-Adapting Local Eddy-Viscosity (WALE) Model
WALE model is designed to return the correct wall asymptotic behavior for wall bounded flows.
F. Nicoud and F. Ducros, *Subgrid-Scale Stress Modelling Based on the Square of the Velocity Gradient Tensor*, Flow, Turbulence, and Combustion, 62(3):183-200 (1999)

Dynamic Kinetic Energy Subgrid-Scale Model
W.W. Kim and S. Menon, *Application of the localized dynamic subgrid-scale model to turbulent wall-bounded flows*, Technical Report AIAA-97-0210, American Institute of Aeronautics and Astronautics, 35th Aerospace Sciences Meeting, Reno (1997)