Turbulence

CEFRC Combustion Summer School

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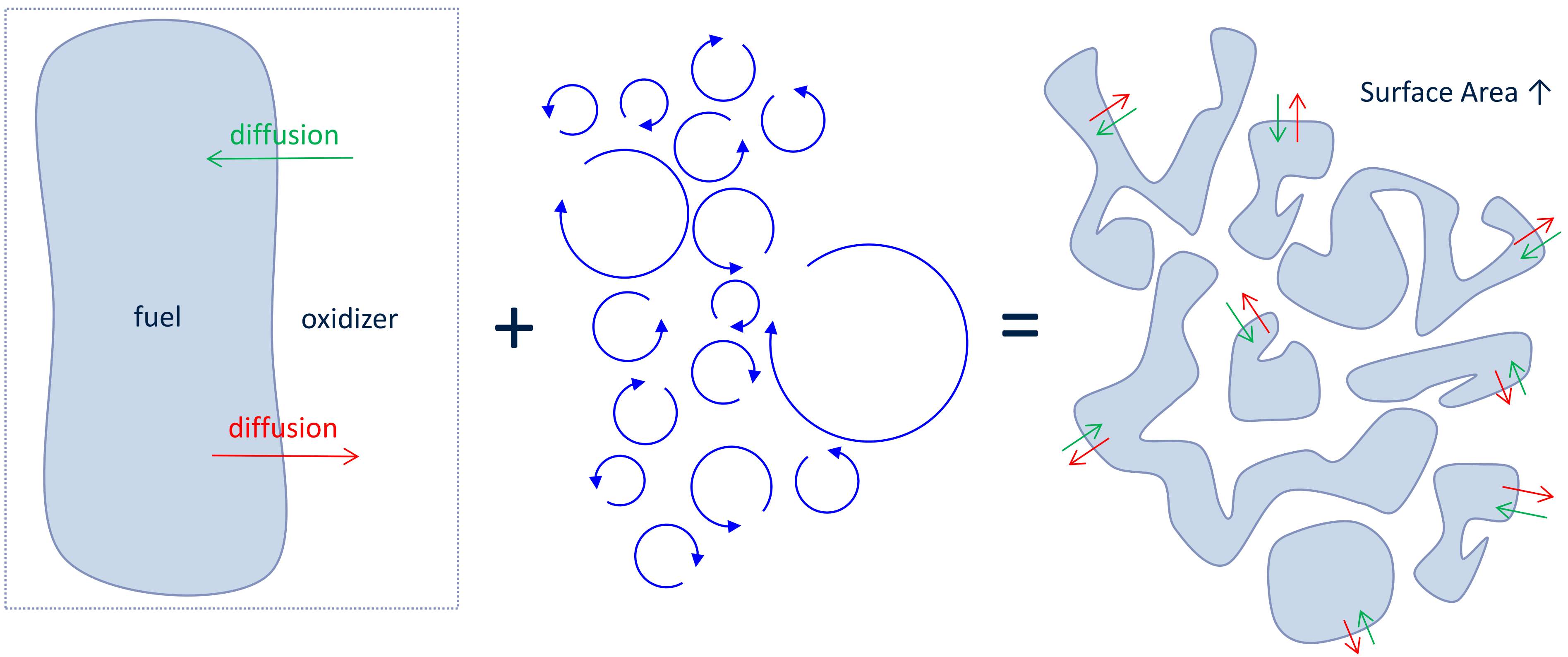
Turbulent Mixing

- Combustion requires mixing at the molecular level
- Turbulence: convective transport ↑ → molecular mixing ↑



Course Overview

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Modelling Turbulent Combustion
- Applications

- Characteristics of Turbulent Flows
- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
- Types of turbulence
- Mean-flow Equations
- Reynolds Stress Equations
- *k*-Equation
- Turbulence Models
- Scales of Turbulent Flows/Energy Cascade
- Kolmogorov Hypotheses
- Scalar Transport Equations
- Large Eddy Simulation

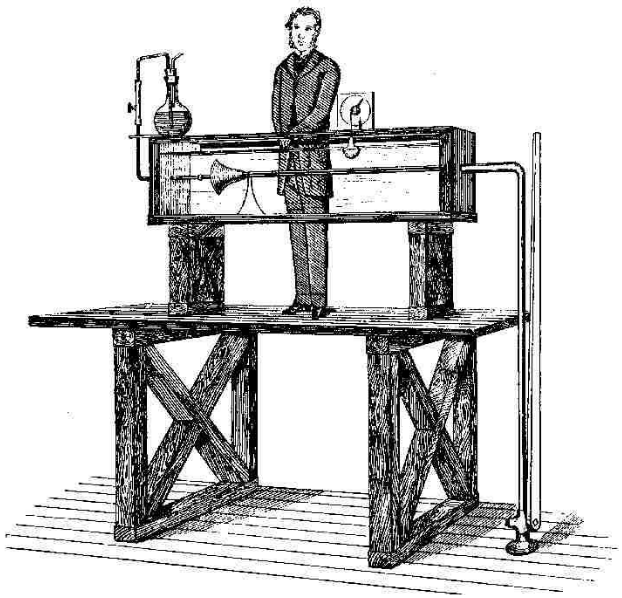
Characteristics of Turbulent Flows

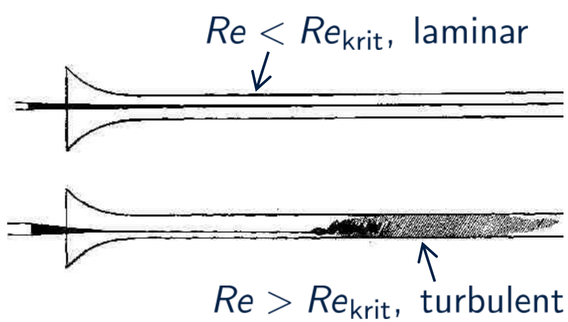
Transition to turbulence

- From observations: laminar flow becomes turbulent
  - Characteristic length $d\uparrow$
  - Flow velocity $u\uparrow$
  - Viscosity $\nu\downarrow$

→ Dimensionless number: Reynolds number *Re*

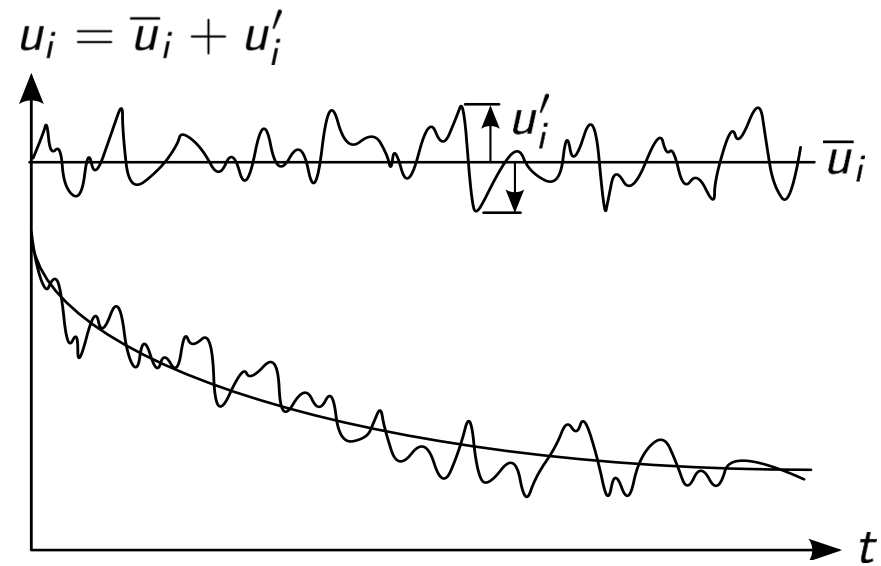
$$Re = \frac{ud}{\nu}$$





Characteristics of turbulent flows:

- Random
- 3D
- Has Vorticity
- Large *Re*



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Statistical Description of Turbulent Flows

Conventional Averaging/Reynolds Decomposition

- Averaging
  - Ensemble average

$$\overline{u}_i(x,y,z,t) = \frac{1}{N}\sum_{k=1}^{N} u_i^k(x,y,z,t), \quad i = 1,2,3$$

  - Time average

$$\overbrace{\overline{u}_i(x,y,z)}^{\neq f(t)} = \frac{1}{\Delta t}\int_t^{t+\Delta t} u_i(x,y,z,t)\,\mathrm{d}t, \quad i = 1,2,3$$

(N and Δt sufficiently large)

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

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

Reynolds-Zerlegung

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

$$\overline{u_i'} = 0, \quad i = 1, 2, 3, \quad \overline{p'} = 0, \ldots$$

- Mean of squared fluctuation differs from zero:

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

- These averages are named RMS-values (root mean square)

Favre averaging (density weighted averaging)

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

- Reynolds decomposition (for $\rho \neq$ const.)

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

- Favre averaging

$$u_i = \widetilde{u}_i + u_i'', \quad i = 1, 2, 3$$

→ By definition: mean of density weighted fluctuation → 0

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

→ Density weighted mean velocity

$$\overline{\rho u_i} = \overline{\rho(\widetilde{u}_i + u_i'')} = \overline{\rho}\widetilde{u}_i + \cancel{\overline{\rho u_i''}} \quad \Leftrightarrow \quad \boxed{\widetilde{u}_i = \frac{\overline{\rho u_i}}{\overline{\rho}}}$$

Favre average ↔ conventional average

- Favre average as a function of conventional mean and fluctuation

$$\widetilde{u}_i = \frac{\overline{\rho u_i}}{\overline{\rho}} = \frac{\overline{(\overline{\rho} + \rho')(\overline{u}_i + u_i')}}{\overline{\rho}} = \overline{u}_i + \frac{\overline{\rho' u_i'}}{\overline{\rho}}, \quad i = 1, 2, 3$$

and for the fluctuating quantity

$$u_i'' = u_i' - \frac{\overline{\rho' u_i'}}{\overline{\rho}} \quad \text{and} \quad \overline{u_i''} = -\frac{\overline{\rho' u_i'}}{\overline{\rho}}$$

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

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Types of Turbulence

Statistically Homogeneous Turbulence

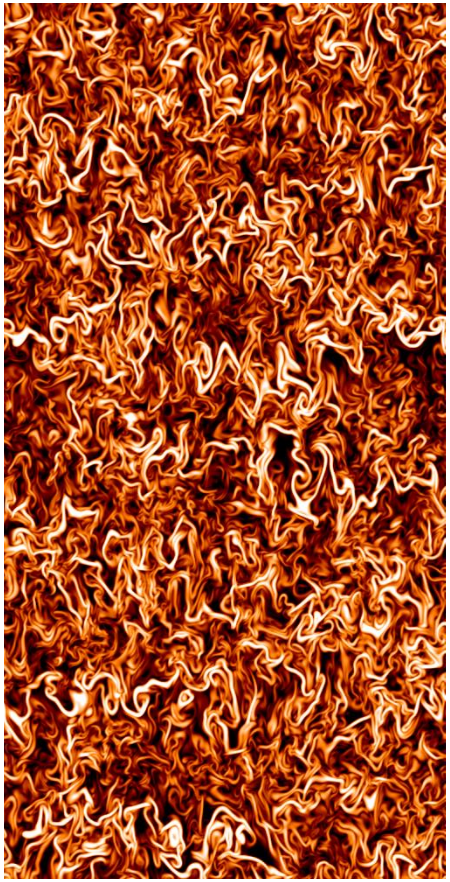
- All statistics of fluctuating quantities are invariant under translation of the coordinate system

  → for averaged fluctuating quantities $\overline{u_i' u_j'}$ (more generally $\overline{u_i' u_j' u_k' \ldots}$) applies

$$\overline{u_i'(x_k) u_j'(x_k)} = \overline{u_i'(x_k + \Delta x_k) u_j'(x_k + \Delta x_k)}, \quad i, j, k = 1, 2, 3$$

- Constant gradients of the mean velocity are permitted:

$$\frac{\partial}{\partial x_l} \overline{u}_i(x_k) = \frac{\partial}{\partial x_l} \overline{u}_i(x_k + \Delta x_k), \quad i, k, l = 1, 2, 3$$



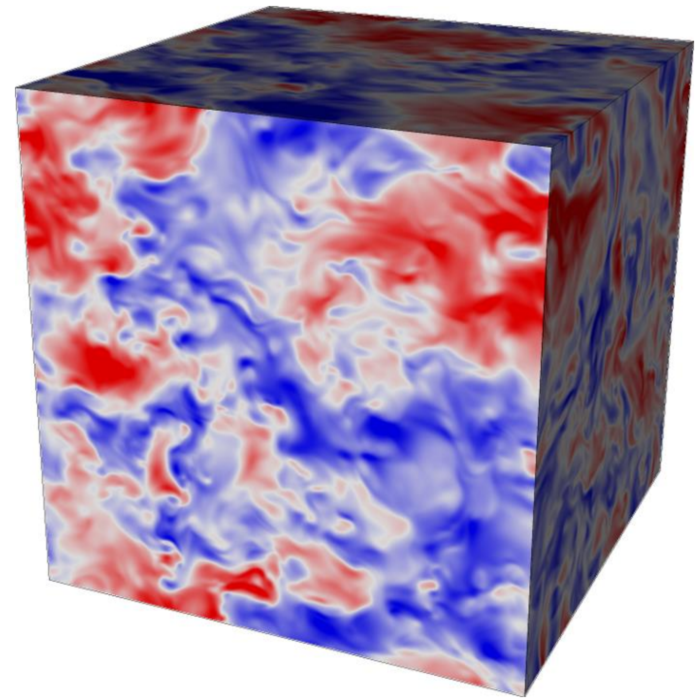
Scalar dissipation rate in statistically homogeneous turbulent flow

Statistically Isotropic Turbulence

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

$$\overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2}\,, \quad \overline{u_i' u_j'} = 0 \quad \text{für} \quad i \neq j$$

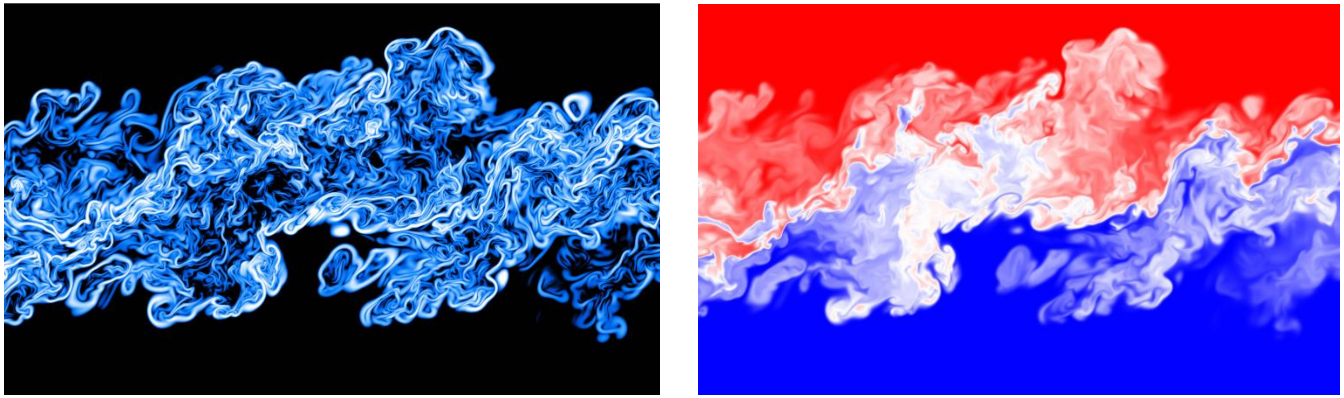
- Mean velocities = 0
- Isotropy requires homogeneity
- Relevance of this flow case:
  - Simplifications allow theoretical conclusions about turbulence
  - Turbulent motions on small scales are typically assumed to be isotropic (Kolmogorov hypotheses)



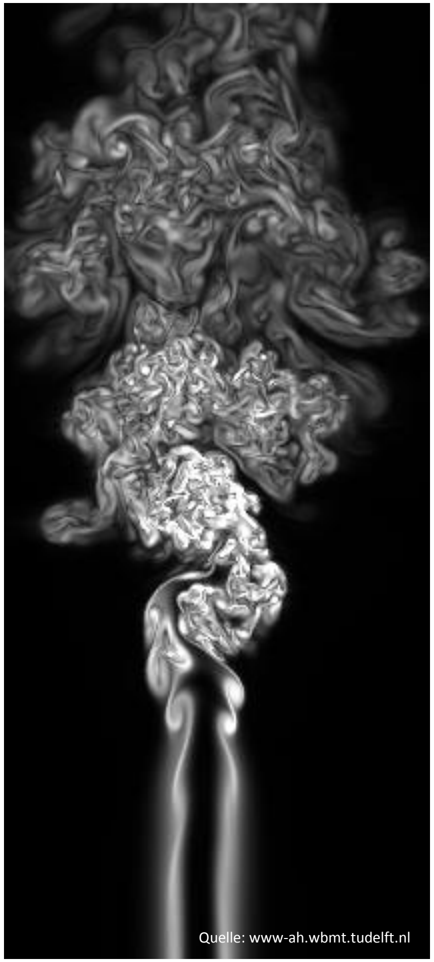
DNS of statistically homogeneous and isotropic turbulence: x_1-component of the velocity

Turbulent Shear Flow

- 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

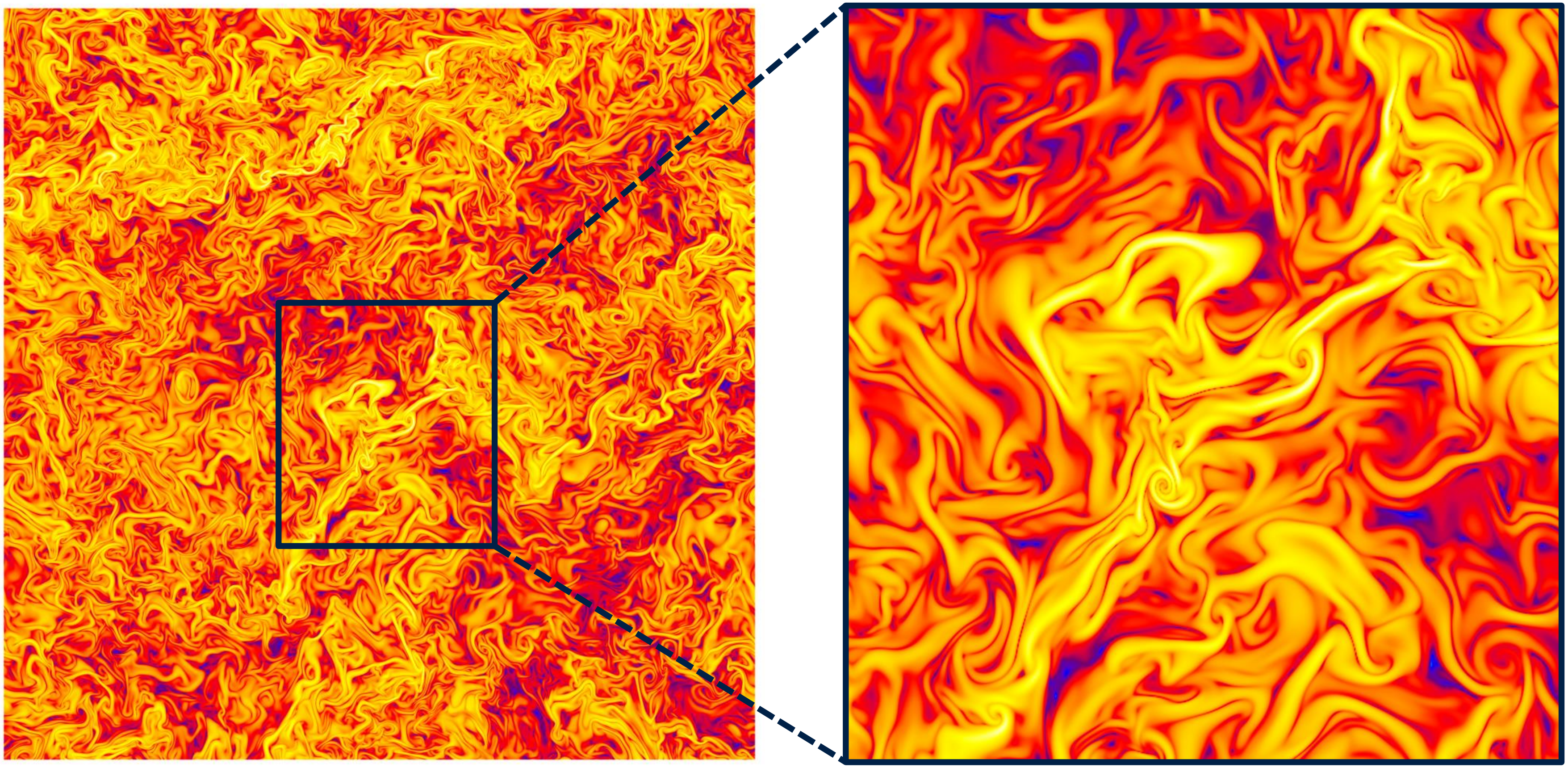


„Temporally evolving shear layer“: Scalar dissipation rate χ (left), mixture fraction Z (rechts)



Turbulent jet: magnitude of vorticity

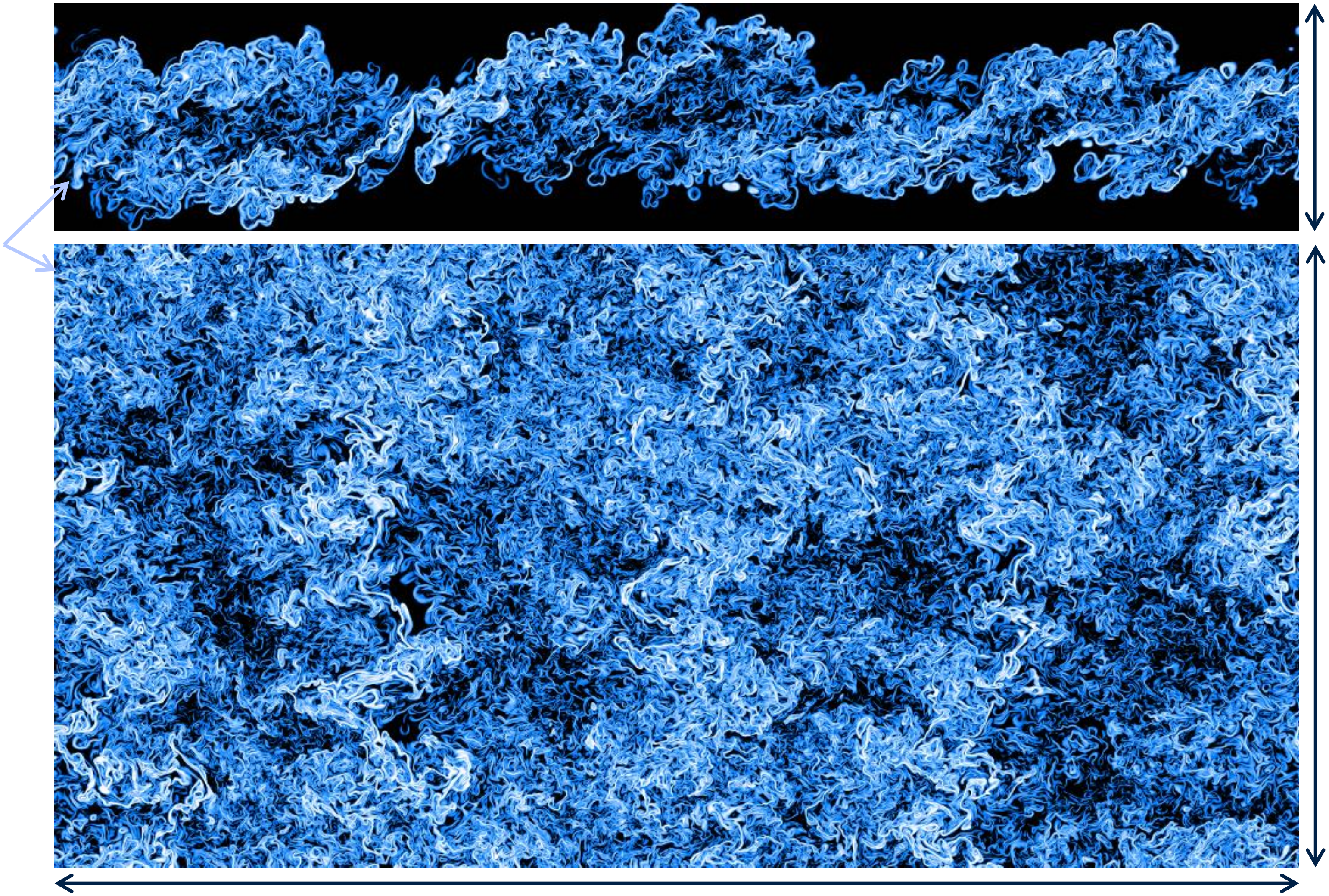
Example: DNS of Homogeneous Shear Turbulence



Scalar dissipation rate in homogeneous shear turbulence
2048x2048x2048 collocation points

Close-up/detail

Example: DNS of a Shear Flow



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Mean-flow Equations

- Starting from the Navier-Stokes-equations for incompressible fluids

$$\frac{\partial u_j}{\partial x_j} = 0 \qquad \text{(continuity)}$$

$$\frac{\partial u_j}{\partial t} + u_i \frac{\partial u_j}{\partial x_i} = -\frac{1}{\rho}\frac{\partial p}{\partial x_j} + \nu \frac{\partial^2 u_j}{\partial x_i^2} \qquad \text{(momentum)}$$

→ Four unknowns within four equations: u_1, u_2, u_3, p

- Reynolds decomposition

$$u_j = \overline{u}_j + u_j'$$

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

Averaged Continuity Equation

1. From continuity equation it follows

$$\frac{\partial \overline{u_j}}{\partial x_j} = 0$$

and

$$\frac{\partial u_j'}{\partial x_j} = 0$$

→ Linearity of the continuity equation: no correlations of fluctuating quantities

Averaged Momentum Equation

2. This does not apply for the momentum equation!
   - Convective term

$$u_i \frac{\partial u_j}{\partial x_i} \overset{\text{Contin.}}{=} \frac{\partial}{\partial x_i}(u_i u_j) = \frac{\partial}{\partial x_i}\left[(\overline{u}_i + u_i')(\overline{u}_j + u_j')\right]$$
$$= \frac{\partial}{\partial x_i}\left[\overline{u}_i \overline{u}_j + \overline{u}_i u_j' + u_i' \overline{u}_j + u_i' u_j'\right], \quad j = 1, 2, 3.$$

   - Time-averaging yields

$$\overline{u_i \frac{\partial u_j}{\partial x_i}} = \frac{\partial}{\partial x_i}(\overline{u}_i \overline{u}_j) + \frac{\partial}{\partial x_i}\overline{(u_i' u_j')} \overset{\text{Contin.}}{=} \overline{u}_i \frac{\partial \overline{u}_j}{\partial x_i} + \frac{\partial}{\partial x_i}\overline{(u_i' u_j')}$$

→ This term includes product of components of fluctuating velocities: this is due to the non-linearity of the convective term

Reynolds Stress Tensor

- Averaging of the other terms → averaged momentum equation:

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

- The additional term, resulting from convective transport, is added to the viscous term on the right hand side (divergence of a second order tensor)

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

is called Reynolds stress tensor

Closure Problem in Statistical Turbulence Theory

- This leads to the closure problem in turbulence theory!
- The Reynolds Stress Tensor

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

needs to be expressed as a function of mean flow quantities

- A first idea: derivation of a transport equation for $\tau_{ij,\mathrm{turb}}$ ...

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*Transport Equation for Reynolds Stress Tensor

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

$-$

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

$=$

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

*Transport Equation for Reynolds Stress Tensor

Multiplication of the equation

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

with the fluctuating velocity $u_k',\ k = 1,2,3$ and a corresponding equation for $u_k',\ k = 1,2,3$ with $u_j',\ j = 1,2,3$ leads after summation to

$$\frac{\partial u_j' u_k'}{\partial t} + \overline{u}_i \frac{\partial u_j' u_k'}{\partial x_i} + u_i' u_k' \frac{\partial \overline{u}_j}{\partial x_i} + u_i' u_j' \frac{\partial \overline{u}_k}{\partial x_i} + \frac{\partial}{\partial x_i}(u_i' u_j' u_k') =$$
$$-\frac{1}{\rho}\left(u_k' \frac{\partial p'}{\partial x_j} + u_j' \frac{\partial p'}{\partial x_k}\right) + \nu\left(u_k' \frac{\partial^2 u_j'}{\partial x_i^2} + u_j' \frac{\partial^2 u_k'}{\partial x_i^2}\right)$$
$$+ u_k' \frac{\partial \overline{u_i' u_j'}}{\partial x_i} + u_j' \frac{\partial \overline{u_i' u_k'}}{\partial x_i}, \quad i,j,k = 1,2,3$$

*Transport Equation for Reynolds Stress Tensor

The viscous terms on the right hand side of

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

$$- \frac{1}{\rho}\left(u_k' \frac{\partial p'}{\partial x_j} + u_j' \frac{\partial p'}{\partial x_k} \right) + \nu \left(u_k' \frac{\partial^2 u_j'}{\partial x_i^2} + u_j' \frac{\partial^2 u_k'}{\partial x_i^2} \right)$$

$$+ u_k' \frac{\partial \overline{u_i' u_j'}}{\partial x_i} + u_j' \frac{\partial \overline{u_i' u_k'}}{\partial x_i}, \quad i, j, k = 1, 2, 3$$

can be transformed into

$$u_k' \frac{\partial^2 u_j'}{\partial x_i^2} + u_j' \frac{\partial^2 u_k'}{\partial x_i^2} = \frac{\partial^2}{\partial x_i^2}(u_k' u_j') - 2 \frac{\partial u_k'}{\partial x_i} \frac{\partial u_j'}{\partial x_i}$$

*Transport Equation for Reynolds Stress Tensor

Splitting of the pressure-terms in

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

$$- \frac{1}{\rho} \left(u_k' \frac{\partial p'}{\partial x_j} + u_j' \frac{\partial p'}{\partial x_k} \right) + \nu \left(u_k' \frac{\partial^2 u_j'}{\partial x_i^2} + u_j' \frac{\partial^2 u_k'}{\partial x_i^2} \right)$$

$$+ u_k' \frac{\partial \overline{u_i' u_j'}}{\partial x_i} + u_j' \frac{\partial \overline{u_i' u_k'}}{\partial x_i}, \quad i, j, k = 1, 2, 3$$

with Kronecker delta $\delta_{\alpha\beta}$

$$u_k' \frac{\partial p'}{\partial x_j} + u_j' \frac{\partial p'}{\partial x_k} = \frac{\partial}{\partial x_j}(p' u_k') - p' \frac{\partial u_k'}{\partial x_j} + \frac{\partial}{\partial x_k}(p' u_j') - p' \frac{\partial u_j'}{\partial x_k}$$

$$= -p' \left(\frac{\partial u_k'}{\partial x_j} + \frac{\partial u_j'}{\partial x_k} \right) + \frac{\partial}{\partial x_i} \left(p' (\delta_{ij} u_k' + \delta_{ik} u_j') \right)$$

*Transport Equation for Reynolds Stress Tensor

Averaging and rearranging leads to →

$$\underbrace{\frac{\partial}{\partial t}\overline{(u_j' u_k')}}_{\text{L}} + \underbrace{\overline{u_i}\frac{\partial \overline{u_j' u_k'}}{\partial x_i}}_{\text{C}} = \underbrace{-\overline{u_i' u_k'}\frac{\partial \overline{u_j}}{\partial x_i} - \overline{u_i' u_j'}\frac{\partial \overline{u_k}}{\partial x_i}}_{\text{P}}$$

$$\underbrace{-2\nu\overline{\frac{\partial u_k'}{\partial x_i}\frac{\partial u_j'}{\partial x_i}}}_{\text{DS}} + \underbrace{\overline{\frac{p'}{\rho}\left(\frac{\partial u_j'}{\partial x_k} + \frac{\partial u_k'}{\partial x_j}\right)}}_{\text{PSC}}$$

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

→ Six new equations, but far more new unknowns

*Transport Equation for Reynolds Stress Tensor

The meaning and name of the single terms are listed below:

- „L“: Local change

$$\frac{\partial}{\partial t}\overline{(u_j' u_k')}$$

- „C“: Convective transport

$$\overline{u_i}\frac{\partial \overline{u_j' u_k'}}{\partial x_i}$$

- „P“: Production of Reynolds stresses (negative product of Reynolds-stress tensor and the gradient of time-averaged velocity)

$$-\overline{u_i' u_k'}\frac{\partial \overline{u_j}}{\partial x_i} - \overline{u_i' u_j'}\frac{\partial \overline{u_k}}{\partial x_i}$$

*Transport Equation for Reynolds Stress Tensor

- „DS“: (Pseudo-)dissipation of Reynolds stresses

$$-2\nu \overline{\frac{\partial u'_k}{\partial x_i} \frac{\partial u'_j}{\partial x_i}}$$

- „PSC“: pressure-rate-of-strain correlation. It contributes to the redistribution of Reynolds stresses in a similar way the diffusion term does

$$\overline{\frac{p'}{\rho} \left(\frac{\partial u'_j}{\partial x_k} + \frac{\partial u'_k}{\partial x_j} \right)}$$

*Transport Equation for Reynolds Stress Tensor

- „DF“: diffusion of the Reynolds stresses. It includes all terms under the divergence operator

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

- In this balance production and dissipation are the most important terms
- The mean velocity gradients are responsible for the production of turbulence („P“)

Transport equation for Reynolds stress tensor

$$
\underbrace{\frac{\partial}{\partial t}\overline{(u'_j u'_k)}}_{\text{L}} + \underbrace{\overline{u_i}\frac{\partial \overline{u'_j u'_k}}{\partial x_i}}_{\text{C}} = \underbrace{-\overline{u'_i u'_k}\frac{\partial \overline{u_j}}{\partial x_i} - \overline{u'_i u'_j}\frac{\partial \overline{u_k}}{\partial x_i}}_{\text{P}}
$$

$$
\underbrace{-2\nu\overline{\frac{\partial u'_k}{\partial x_i}\frac{\partial u'_j}{\partial x_i}}}_{\text{DS}} + \underbrace{\overline{\frac{p'}{\rho}\left(\frac{\partial u'_j}{\partial x_k} + \frac{\partial u'_k}{\partial x_j}\right)}}_{\text{PSC}}
$$

$$
+ \underbrace{\frac{\partial}{\partial x_i}\left[-\overline{u'_i u'_j u'_k} + \nu\frac{\partial}{\partial x_i}\overline{(u'_j u'_k)} - \overline{\frac{p'}{\rho}(\delta_{ij}u'_k + \delta_{ik}u'_j)}\right]}_{\text{DF}}
$$

→ Six new equations, but far more new unknowns

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Transport Equation for Turbulent Kinetic Energy

Derivation of an equation for the turbulent kinetic energy (TKE)

- TKE is defined as

$$\overline{k} = \frac{1}{2}\overline{u_j'^2} = \frac{1}{2}(\overline{u_1'^2} + \overline{u_2'^2} + \overline{u_3'^2}).$$

- Contraction $j = k$ (← k: index, not TKE) in Reynolds equation yields

$$\underbrace{\frac{\partial \overline{k}}{\partial t}}_{\mathrm{L}} + \underbrace{\overline{u_i}\frac{\partial \overline{k}}{\partial x_i}}_{\mathrm{C}} = \underbrace{-\overline{u_i' u_j'}\frac{\partial \overline{u_j}}{\partial x_i}}_{\mathrm{P}} \underbrace{- \quad \overline{\varepsilon}}_{\mathrm{DS}} + \underbrace{\frac{\partial}{\partial x_i}\left[\overline{-u_i'\left(k + \frac{p'}{\rho}\right)} + \nu\frac{\partial \overline{k}}{\partial x_i} + \nu\frac{\partial}{\partial x_j}\overline{\left(u_i' u_j'\right)}\right]}_{\mathrm{DF}}$$

Transport Equation for Turbulent Kinetic Energy

- Continuity equation→ pressure-rate-of-strain correlation PSC = 0
- Dissipation

$$\overline{\frac{\partial u_j'}{\partial x_i}\frac{\partial u_j'}{\partial x_i}} = \overline{\frac{\partial u_j'}{\partial x_i}\left(\frac{\partial u_j'}{\partial x_i} + \frac{\partial u_i'}{\partial x_j}\right)} - \frac{\partial^2}{\partial x_j x_i}\overline{\left(u_j' u_i'\right)}$$

- Mean dissipation of turbulent kinetic energy

$$\overline{\varepsilon} = \nu\overline{\left(\frac{\partial u_j'}{\partial x_i} + \frac{\partial u_i'}{\partial x_j}\right)\frac{\partial u_j'}{\partial x_i}}$$

Transport Equation for Turbulent Kinetic Energy

- The transport equation for turbulent kinetic energy

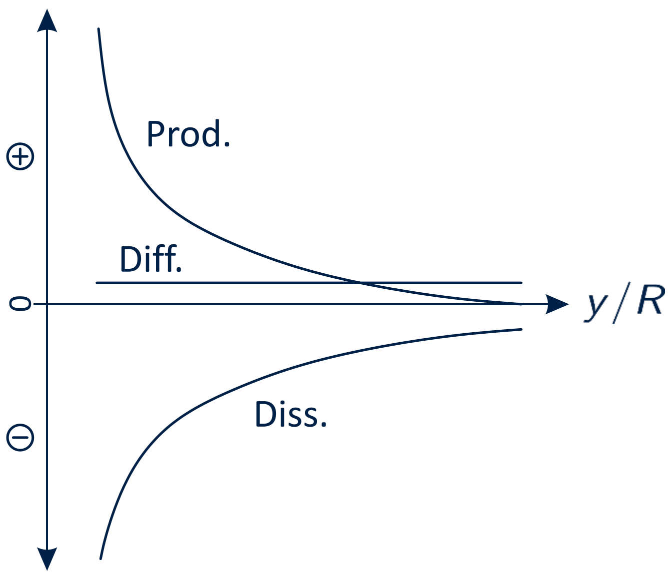
$$\underbrace{\frac{\partial \overline{k}}{\partial t}}_{\text{L}} + \underbrace{\overline{u_i}\frac{\partial \overline{k}}{\partial x_i}}_{\text{C}} = \underbrace{-\overline{u_i' u_j'}\frac{\partial \overline{u_j}}{\partial x_i}}_{\text{P}} - \underbrace{\overline{\varepsilon}}_{\text{DS}} + \underbrace{\frac{\partial}{\partial x_i}\left[-\overline{u_i'\left(u_j' u_j' + \frac{p'}{\rho}\right)} + \nu\frac{\partial \overline{k}}{\partial x_i} + \nu\frac{\partial}{\partial x_j}\overline{\left(u_i' u_j'\right)}\right]}_{\text{DF}}$$

can be interpreted just as the transport equation for the Reynolds stress tensor

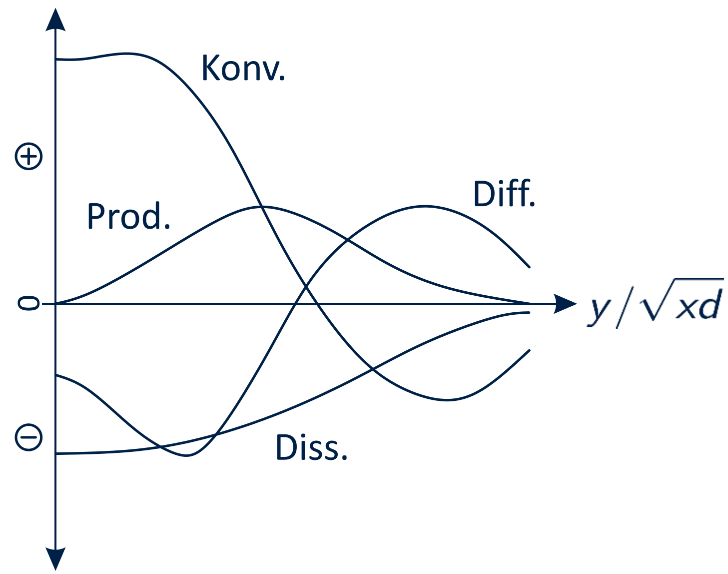
  - Local change and convection of turbulent kinetic energy (lhs)
  - Production, dissipation and diffusion (rhs)
  - PSC → 0

Transport Equation for Turbulent Kinetic Energy

example: pipe-flow



example: free jet



Transport Equation for Turbulent Kinetic Energy

- Transport equation

$$\underbrace{\frac{\partial \overline{k}}{\partial t}}_{\text{L}} + \underbrace{\overline{u_i}\frac{\partial \overline{k}}{\partial x_i}}_{\text{C}} = \underbrace{-\overline{u_i' u_j'}\frac{\partial \overline{u_j}}{\partial x_i}}_{\text{P}} - \underbrace{\overline{\varepsilon}}_{\text{DS}} + \underbrace{\frac{\partial}{\partial x_i}\left[-\overline{u_i'\left(u_j' u_j' + \frac{p'}{\rho}\right)} + \nu\frac{\partial \overline{k}}{\partial x_i} + \nu\frac{\partial}{\partial x_j}\overline{\left(u_i' u_j'\right)}\right]}_{\text{DF}}$$

- BUT: Closure problem is not solved
  - Triple correlations
  - Derivation of equations for such correlations → even higher correlations…

Course Overview

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- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
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- Mean-flow Equations
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Turbulence Models

Turbulent Viscosity

- The derived averaged equations are not closed → turbulent stress tensor has to be modeled

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

- Analogy to Newton approach for molecular shear stress → gradient transport model:

$$-\overline{u_i'u_j'} = \nu_\mathrm{t}\left(\frac{\partial\overline{u}_i}{\partial x_j} + \frac{\partial\overline{u}_j}{\partial x_i}\right) - \frac{2}{3}\overline{k}\delta_{ij}$$

- ν_t is eddy viscosity/turbulent viscosity (important: ≠ molecular viscosity!)

Turbulent-viscosity models

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

$$\nu_t = l_m^2 \left|\overline{S_{ij}}\right| \qquad S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- TKE models: e.g. Prandtl-Kolmogorov

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

- *k*-*ε*-Modell (Jones, Launder)

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

Algebraic Model: Prandtl´s Mixing-length Concept

- Eddy viscosity

$$\nu_\mathrm{t} = l_\mathrm{m}^2 \left|\overline{S_{ij}}\right|, \quad \overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u}_j}{\partial x_i} + \frac{\partial \overline{u}_i}{\partial x_j}\right)$$

- Based on dimensional analysis
- All unknown proportionalities → mixing-length
- Empirical methods for determining l_m
- Assumption: l_m = const.

TKE model: Prandtl-Kolmogorov

- Eddy viscosity

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

  - Model constant C_μ (often: $C_\mu = 0{,}09$)
  - l_{pk}: characteristic length scale → determined empirically

- Equation for TKE

Two-equation-model: *k*-*ε*-model

- Eddy viscosity

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

- Solving one equation each for
  - TKE

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

  - dissipation

$$\frac{\partial \overline{\varepsilon}}{\partial t} + \overline{u_i} \frac{\partial \overline{\varepsilon}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{Pr_\varepsilon}\frac{\partial \overline{\varepsilon}}{\partial x_i}\right) + \frac{\overline{\varepsilon}}{\overline{k}}\left(c_{\varepsilon 1} P_k - c_{\varepsilon 2}\overline{\varepsilon}\right)$$

  - the model parameters need to be determined empirically

$$c_{\varepsilon 1} = 1{,}44, \quad c_{\varepsilon 2} = 1{,}9, \quad Pr_\varepsilon = 1{,}3, \quad Pr_k = 1{,}0$$

Two-equation-model: *k*-*ε*-model

Assumptions:

- Turbulent transport term

$$\frac{\partial}{\partial x_i}\left[-\overline{u_i'\left(u_j'u_j' + \frac{p'}{\rho}\right)} \cancel{+ \nu \frac{\partial \overline{k}}{\partial x_i} + \nu \frac{\partial}{\partial x_j}\overline{\left(u_i'u_j'\right)}}\right] = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{Pr_k}\frac{\partial \overline{k}}{\partial x_i}\right)$$

→ Influence of correlation between velocity- and pressure fluctuations is not considered

→ Molecular transport is assumed to be much smaller than turbulent transport and is therefore neglected

- Production

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

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- Applications

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- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
- Types of turbulence
- Mean-flow Equations
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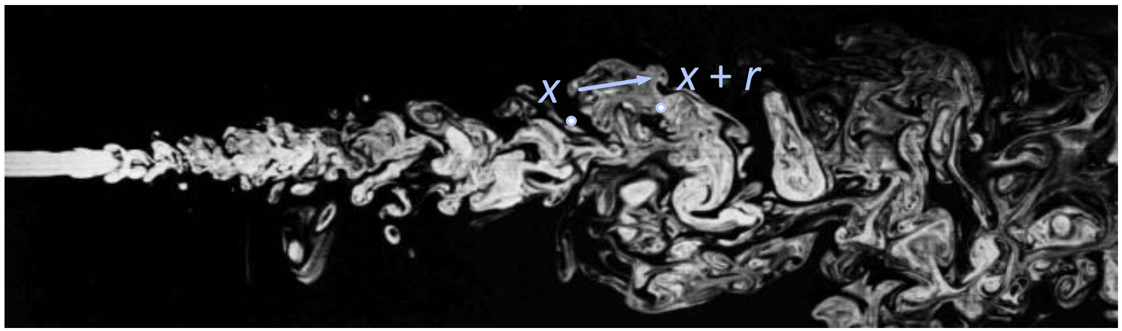
Scales of Turbulent Flows/Energy Cascade

Two-Point Correlation

- Characteristic feature of turbulent flows: eddies exist at different length scales



Turbulent round jet: Reynolds number $Re \approx 2300$

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

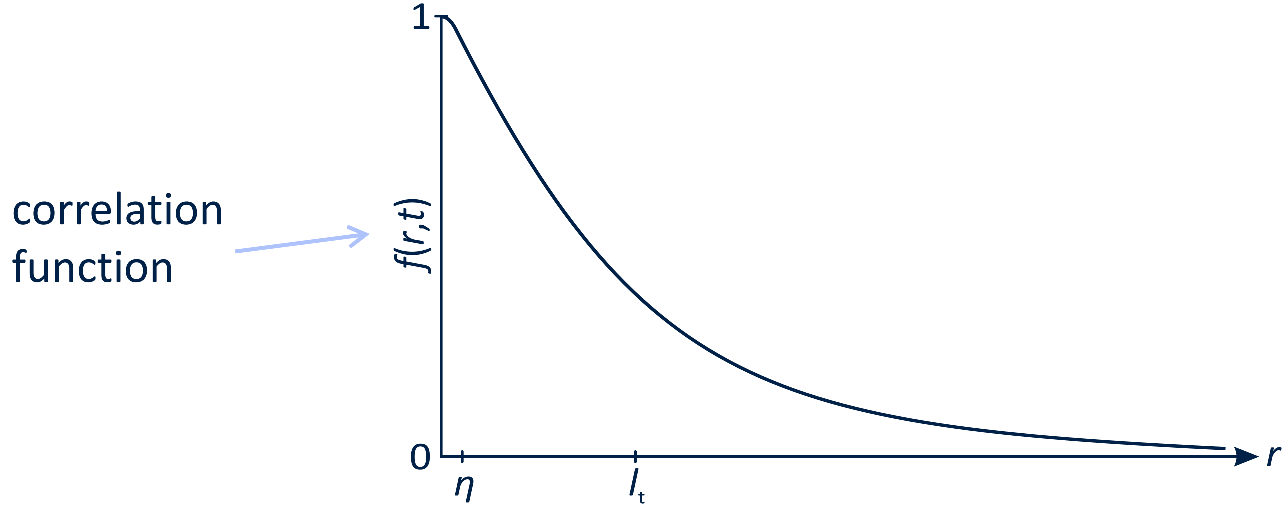
$$R_{ij}(\vec{x}, \vec{r}, t) = \overline{u_i'(\vec{x}, t)\, u_j'(\vec{x}+\vec{r}, t)}$$

Correlation Function

- Homogeneous isotropic turbulence: $\vec{r} \longrightarrow r \;, \;\; \overline{u_1'^2} = \overline{u_2'^2} = \overline{u_3'^2}$
- Two-point correlation normalized by its variance

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

- Degree of correlation of stochastic signals



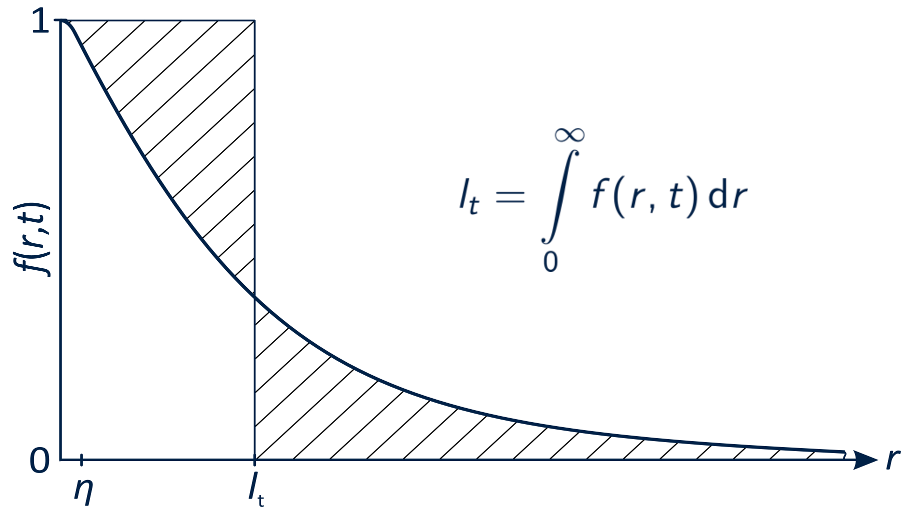
Integral Turbulent Scales

- Largest scales: physical scale of the problem
  $\underbrace{\text{Largest scales}}_{\sim l_t}$
  - Integral length scale l_t (largest eddies)
  - Integral velocity scale

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

  - Integral time scale

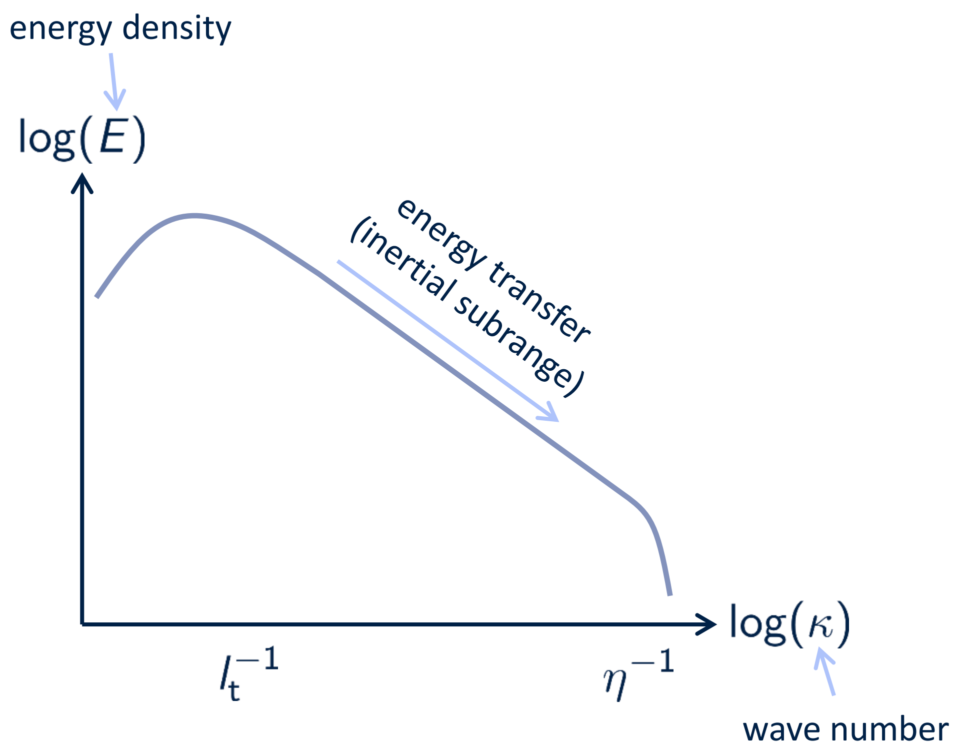
$$\tau = \frac{l_t}{u'}$$



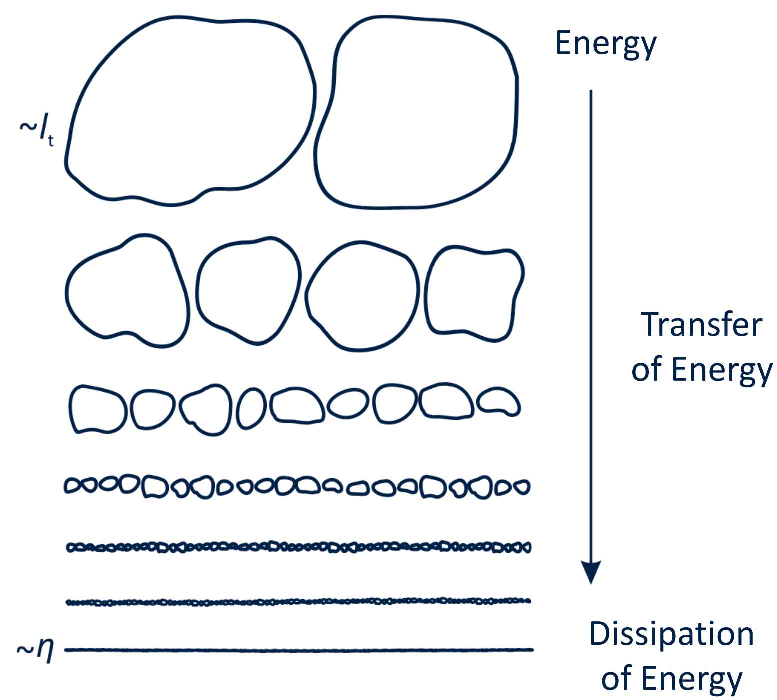
$$l_t = \int_0^\infty f(r,t)\,\mathrm{d}r$$

Energy Spectrum

Energy Spectrum (logarithmic)



Energy Cascade



Course Overview

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Modelling Turbulent Combustion
- Applications

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- Mean-flow Equations
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Kolmogorov Hypotheses

First Kolmogorov Hypothesis

- At sufficiently high Reynolds numbers, small-scale eddies have a universal form. They are determined by two parameters
  - Dissipation $\bar{\varepsilon}$
  - Kinematic viscosity ν
- Dimensional analysis $f(\bar{\varepsilon}, \nu)$ →
  - Length η
  - Time τ_η
  - Velocity u_η

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

$$\tau_\eta = \left(\frac{\nu}{\bar{\varepsilon}}\right)^{1/2}$$

$$u_\eta = \frac{\eta}{\tau_\eta} = (\nu\bar{\varepsilon})^{1/4}$$

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

Second Kolmogorov Hypothesis

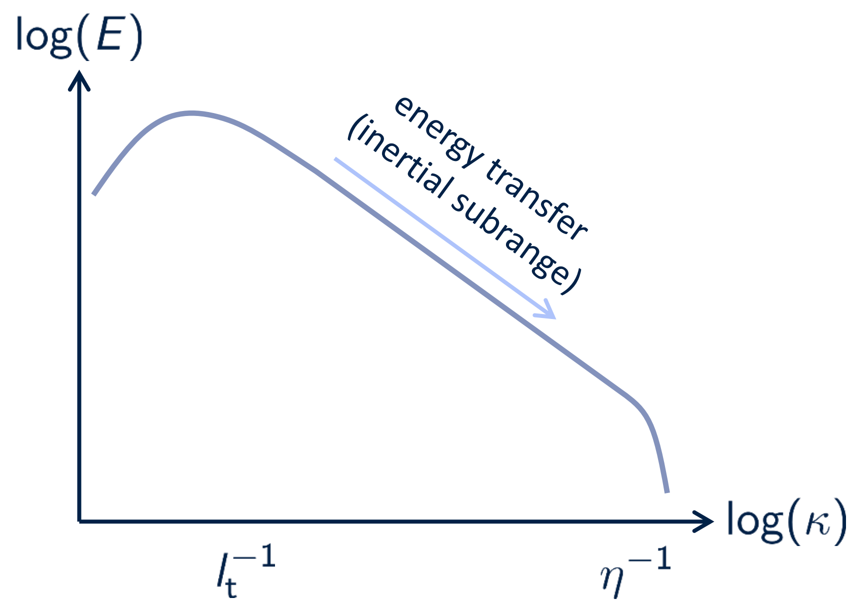
- At sufficiently high Reynolds numbers, the statistics of the motions of scale r in the range $\eta << r << l_t$ have a universal form that is uniquely determined by
  - Dissipation $\overline{\varepsilon}$
  - But independent of kinematic viscosity ν

→ Inertial subrange
  - Integral length scale

$$l_t = \frac{\overline{k}^{3/2}}{\overline{\varepsilon}} \quad \Rightarrow \quad Re_t = \frac{u' l_t}{\nu}$$

  - Ratio η / l_t

$$\frac{\eta}{l_t} \sim Re_t^{-3/4}$$



Course Overview

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Modelling Turbulent Combustion
- Applications

- Characteristics of Turbulent Flows
- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
- Types of turbulence
- Mean-flow Equations
- Reynolds Stress Equations
- *k*-Equation
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- Kolmogorov Hypotheses
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Scalar Transport Equations

- Transport equation for mixture fraction Z

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

- Favre averaging →

not closed

$$\overline{\rho}\frac{\partial \widetilde{Z}}{\partial t} + \overline{\rho}\widetilde{u}_i \frac{\partial \widetilde{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\overline{\left(\rho D \frac{\partial Z}{\partial x_i}\right)} - \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{u_i'' Z''}\right)$$

molecular transport

turbulent transport

Transport Equation for Mixture Fraction

- Neglecting molecular transport (assumption: *Re*↑)
- Gradient transport model for turbulent transport

$$-\widetilde{u_i''Z''} = D_\mathrm{t}\frac{\partial \widetilde{Z}}{\partial x_i}$$

  – D_t: Turbulent diffusivity

$$D_\mathrm{t} = \frac{\nu_\mathrm{t}}{Sc_\mathrm{t}}$$

  – Sc_t: Turbulent Schmidt number

→ Transport equation for mean mixture fraction

$$\rho\frac{\partial \widetilde{Z}}{\partial t} + \rho\widetilde{u}_i\frac{\partial \widetilde{Z}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}D_\mathrm{t}\frac{\partial \widetilde{Z}}{\partial x_i}\right)$$

Transport Equation for Mixture Fraction

- Variance equation
- First step: equation for $Z'' = Z - \widetilde{Z}$

$$\rho \frac{\partial Z}{\partial t} + \rho u_i \frac{\partial Z}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Z}{\partial x_i}\right) \qquad -$$

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

$$\frac{\partial Z''}{\partial t} + (\widetilde{u}_i + u_i'') \frac{\partial Z''}{\partial x_i} + u_i'' \frac{\partial \widetilde{Z}}{\partial x_i} = \frac{1}{\rho} \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Z}{\partial x_i}\right) - \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_i} \overline{\left(\rho D \frac{\partial Z}{\partial x_i}\right)} + \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_i}\left(\bar{\rho} \widetilde{u_i'' Z''}\right)$$

Transport Equation for Mixture Fraction

- By neglecting the derivatives of ρ and D and their mean values, then multiplying this equation by $2\rho Z''$, applying continuity equation, averaging and neglecting the molecular transport results in

$$-D_t \frac{\partial \widetilde{Z''^2}}{\partial x_i} \qquad D_t \frac{\partial \widetilde{Z}}{\partial x_i} \qquad \text{not closed}$$

$$\underbrace{\overline{\rho}\frac{\partial \widetilde{Z''^2}}{\partial t}}_{\text{L}} + \underbrace{\overline{\rho}\widetilde{u}_i \frac{\partial \widetilde{Z''^2}}{\partial x_i}}_{\text{C}} = \underbrace{-\frac{\partial}{\partial x_i}\left(\overline{\rho}\, \widetilde{u_i'' Z''^2}\right)}_{\text{turb. DF}} + \underbrace{2\overline{\rho}\left(-\widetilde{u_i'' Z''}\right)\frac{\partial \widetilde{Z}}{\partial x_i}}_{\text{P}} - \underbrace{\overline{\rho}\,\widetilde{\chi}}_{\text{DS}} \qquad \widetilde{\chi} = 2D\widetilde{\left(\frac{\partial Z''}{\partial x_i}\right)^2}$$

- Favre averaged scalar dissipation $\widetilde{\chi}$

Modeling of Scalar Dissipation

Scalar dissipation rate has to be modeled

- Integral time τ_Z (dimensional analysis)

$$\tau_Z \sim \frac{\widetilde{Z''^2}}{\widetilde{\chi}}, \quad \text{with} \quad [\widetilde{\chi}] = \frac{1}{\mathrm{s}}$$

- Typically proportional to τ

$$\tau = \frac{\widetilde{k}}{\widetilde{\varepsilon}} = c_\chi \tau_Z \quad \text{and} \quad 1{,}5 \leq c_\chi \leq 3$$

- This leads to →

$$\widetilde{\chi} = c_\chi \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z''^2}$$

Transport Equation for Reactive Scalars

- Assumptions:
  - Specific heat $c_{p,\alpha} = c_p =$ const.
  - Pressure $p =$ const., heat transfer by radiation is neglected
  - Lewis number $Le_\alpha = Le = Sc/Pr = 1$
- Temperature equation

$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) + \omega_T$$

- Source term ω_T due to chemical reactions (heat release)

$$\omega_T = -\frac{1}{c_p} \sum_{\alpha=1}^{N} h_\alpha \dot{m}_\alpha'''$$

Transport Equation for Reactive Scalars

- Temperature equation

$$\rho \frac{\partial T}{\partial t} + \rho u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial T}{\partial x_i}\right) + \omega_T$$

is similar to the equation for the mass fraction of component α

$$\rho \frac{\partial Y_\alpha}{\partial t} + \rho u_i \frac{\partial Y_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Y_\alpha}{\partial x_i}\right) + \dot{m}_\alpha'''$$

Transport Equation for Reactive Scalars

- The term „reactive scalar“ includes
  - Mass fractions Y_α of all components $\alpha = 1, \dots N$
  - Temperature T

$$\psi_i = (Y_1, Y_2, \dots Y_N, T)^\mathrm{T}$$

- Balance equations for $\psi_i, \; i = 1, \dots N+1$

$$\rho \frac{\partial \psi_i}{\partial t} + \rho u_j \frac{\partial \psi_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_i \frac{\partial \psi_i}{\partial x_j}\right) + \rho S_i$$

  - D_i: mass diffusivity, thermal diffusivity
  - S_i: mass/temperature source term

Transport Equation for Reactive Scalars

- Derivation of a transport equation for $\widetilde{\psi}_i$
- Favre decomposition

$$\psi_i = \widetilde{\psi}_i + \psi_i''$$

and averaging of

$$\rho \frac{\partial \psi_i}{\partial t} + \rho u_j \frac{\partial \psi_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_i \frac{\partial \psi_i}{\partial x_j}\right) + \rho S_i, \quad i = 1, 2, \ldots, N+1$$

leads to

not closed

$$\overline{\rho} \frac{\partial \widetilde{\psi}_i}{\partial t} + \overline{\rho}\widetilde{u}_j \frac{\partial \widetilde{\psi}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \overline{\left(\rho D_i \frac{\partial \psi_i}{\partial x_j}\right)} - \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u_j''\psi_i''}\right) + \overline{\rho}\widetilde{S}_i$$

molecular transport

turbulent transport

averaged source term

Transport Equation for Reactive Scalars

- Neglecting the molecular transport (assumption: *Re*↑)
- Gradient transport model for the turbulent transport term

$$-\widetilde{u_j''\psi_i''} = D_\mathrm{t}\frac{\partial\widetilde{\psi}_i}{\partial x_j} \quad \text{where} \quad D_\mathrm{t} = \frac{\nu_\mathrm{t}}{Sc_\mathrm{t}}$$

→ Averaged transport equation

Not closed → chapter „Modelling of Turbulent Combustion“

$$\overline{\rho}\frac{\partial\widetilde{\psi}_i}{\partial t} + \overline{\rho}\widetilde{u}_j\frac{\partial\widetilde{\psi}_i}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\overline{\rho}D_\mathrm{t}\frac{\partial\widetilde{\psi}_i}{\partial x_j}\right) + \boxed{\overline{\rho}\widetilde{S}_i}$$

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Part II: Turbulent Combustion

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- Applications

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- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
- Types of turbulence
- Mean-flow Equations
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Large-Eddy Simulation

Direct Numerical Simulation (DNS)

- Solve NS-equations
- No models

- For turbulent flows
  - Computational domain has to be at least of order of integral length scale l
  - Mesh spacing has to resolve smallest scales η
    - Minimum number of cells per direction $n_x = l/\eta = Re_t^{3/4}$
    - Minimum number of cells total $n_t = n_x^3 = Re_t^{9/4}$

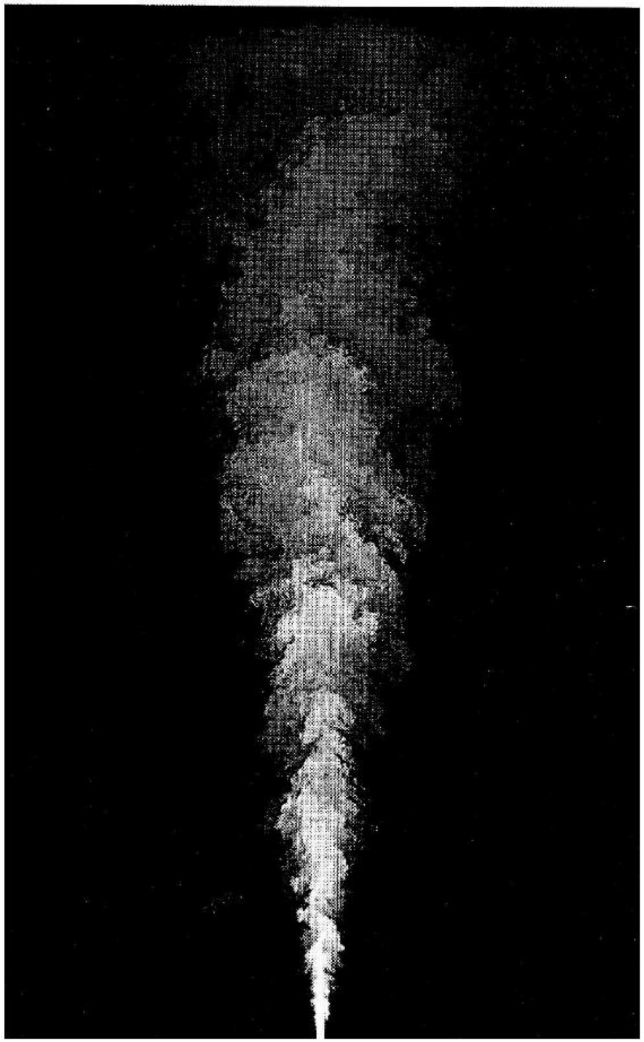
Large-Eddy Simulation

- Example: Turbulent Jet with Re = 15000

$$\mathrm{Re}_t = \mathrm{Re}/50$$

$$n_t = \frac{\mathrm{Re}}{50}^{9/4} \approx 375000$$

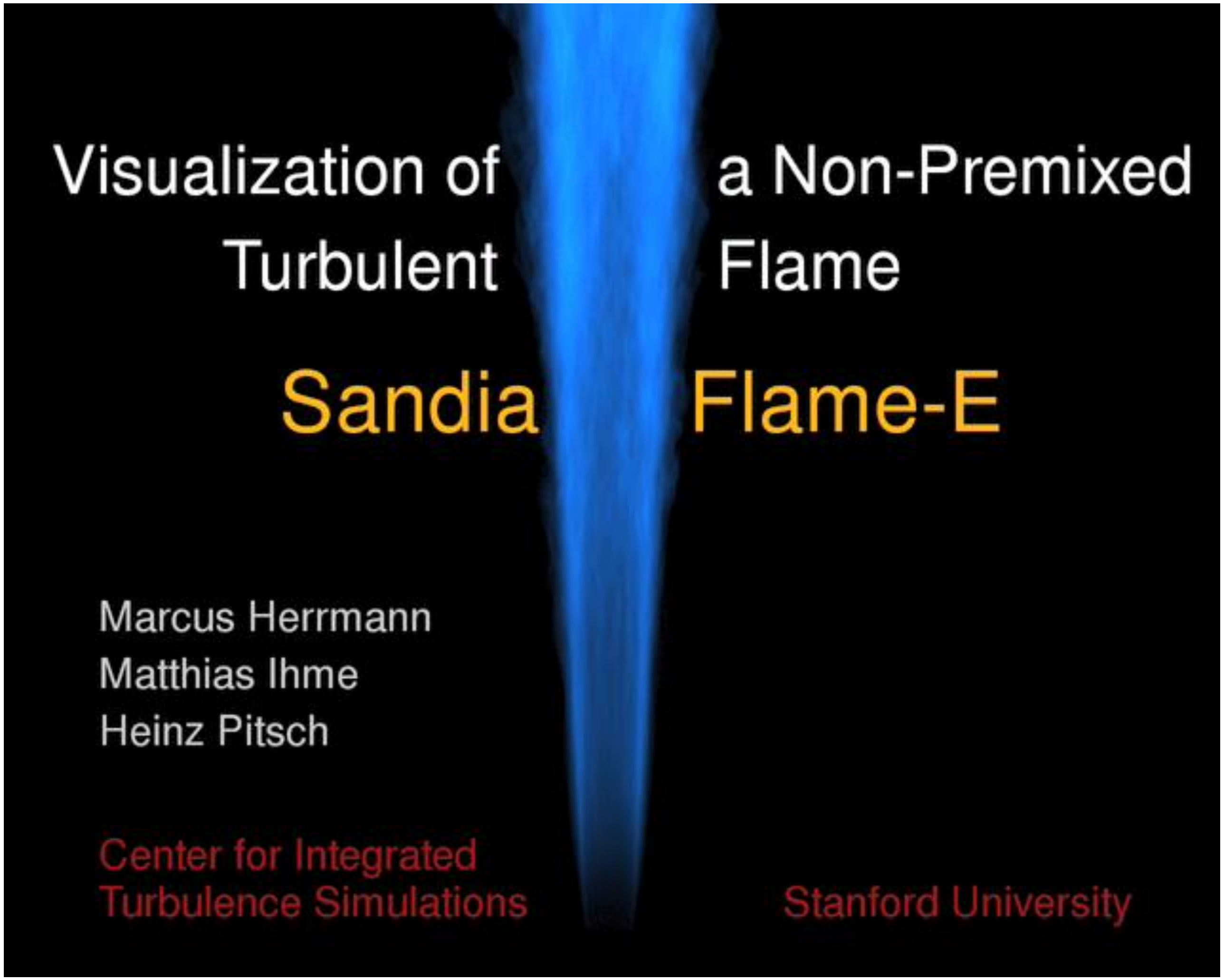
- This is for one integral length scale only!



Pope, „Turbulent Flows“

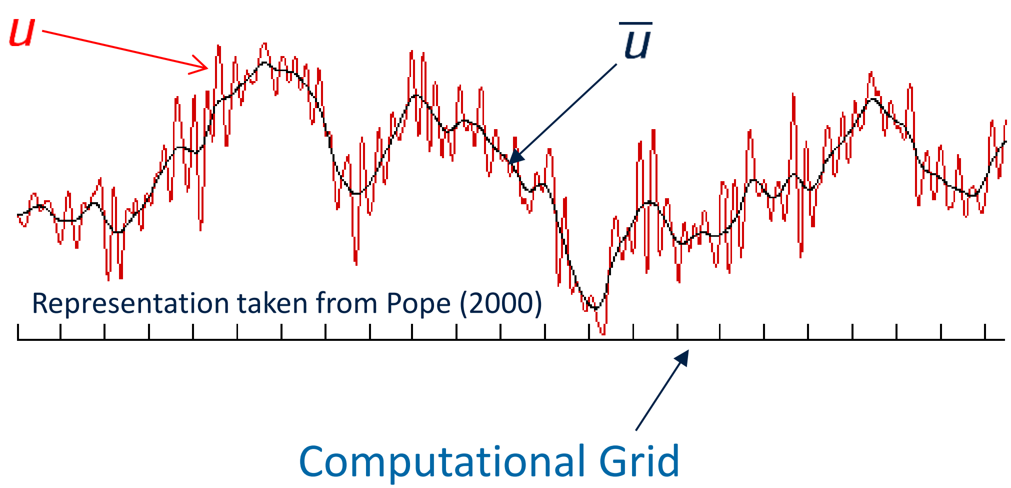
Large-Eddy Simulation (LES)

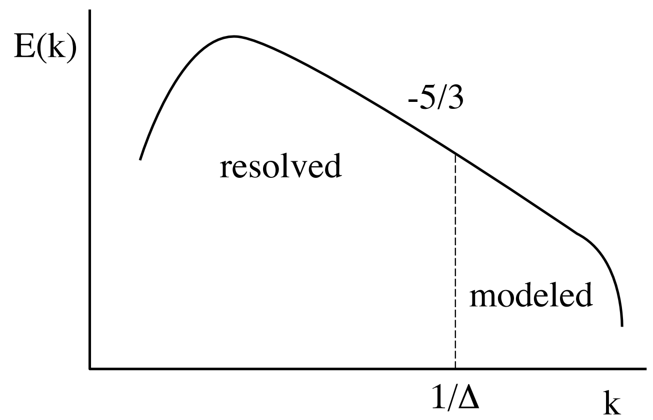
- Spatial filtering as opposed to RANS-ensemble averaging
- Sub-filter modeling as opposed to DNS


Visualization of
Turbulent
a Non-Premixed
Flame
Sandia
Flame-E
Marcus Herrmann
Matthias Ihme
Heinz Pitsch
Center for Integrated
Turbulence Simulations
Stanford University

- Spatial filtering rather than ensemble average

$$\overline{u} = \int G(x, x')u(x')\mathrm{d}x'$$





- Scales smaller than filter scale absent from the filtered quantities
- Filtered signal can be discretized using a mesh substantially smaller than the DNS mesh

- For example:
- Box filter in 1D:

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

- Sharp spectral filter:

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

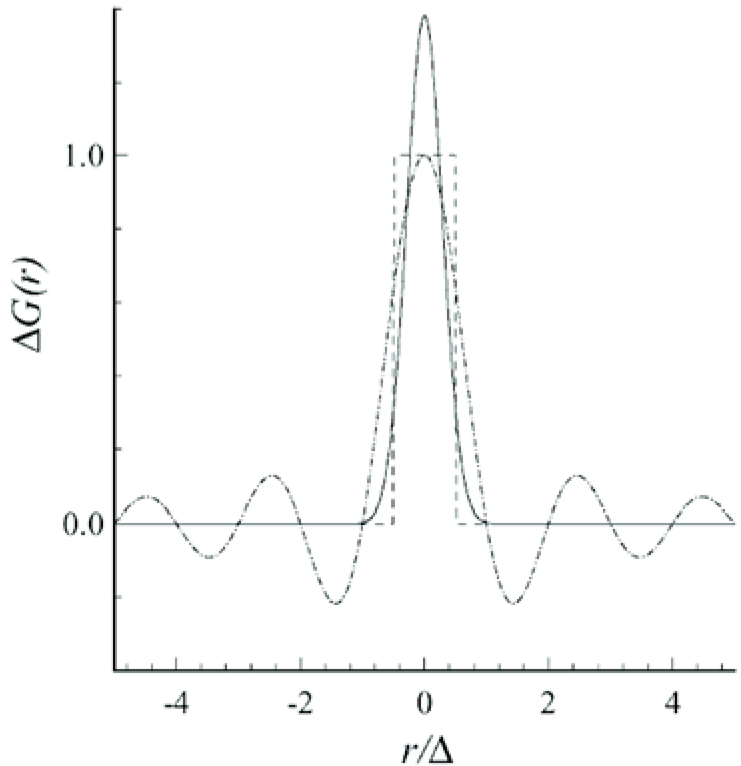


Figure 13.1: Filters $G(r)$: box filter, dashed line; Gaussian filter, solid line; sharp spectral, dot-dashed line.

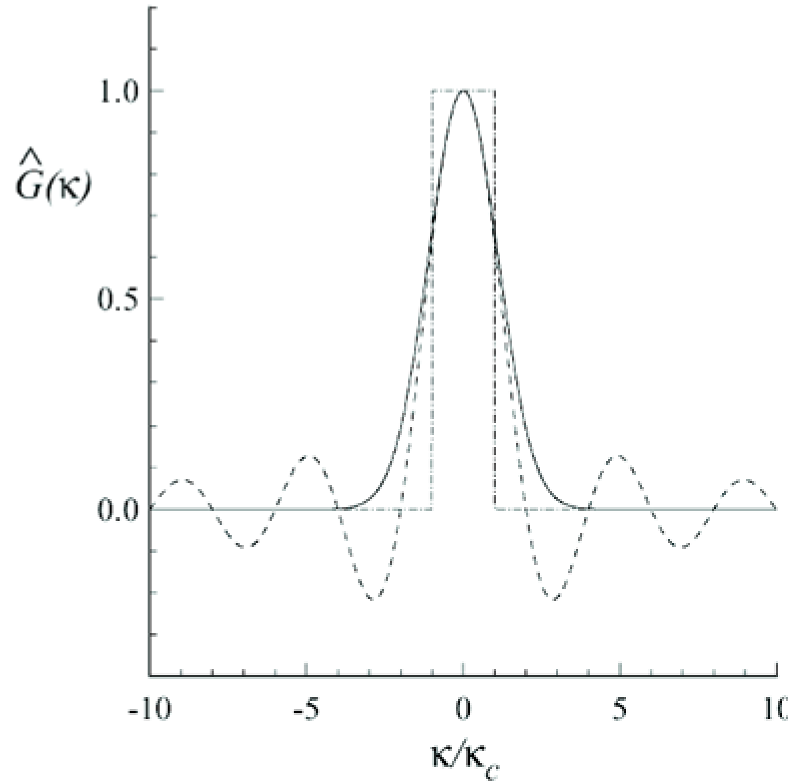


Figure 13.2: Filter transfer functions $\hat{G}(\kappa)$: box filter, dashed line; Gaussian filter, solid line; sharp spectral, dot-dashed line.

Pope, „Turbulent Flows“

Large-Eddy Simulation

- Filtered momentum equation: $$\frac{\partial \overline{U}_j}{\partial t} + \frac{\partial \overline{U_i U_j}}{\partial x_i} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_j} + \nu \frac{\partial^2 \overline{U}_j}{\partial x_i^2}$$

- Define residual stress tensor: $$\tau_{ij}^R \equiv \overline{U_i U_j} - \overline{U_i}\ \overline{U_j}$$

$$\Rightarrow \frac{\partial \overline{U}_j}{\partial t} + \frac{\partial \overline{U}_i \overline{U}_j}{\partial x_i} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_j} + \nu \frac{\partial^2 \overline{U}_j}{\partial x_i^2} - \frac{\partial \tau_{ij}^R}{\partial x_i}$$

Sub-filter Modeling

- *Eddy viscosity model* for τ_{ij}^{r}

- Filtered strain rate tensor

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

$$\tau_{ij}^{r} = -\nu_r \left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) = -2\nu_r \overline{S}_{ij}$$

- *Smagorinsky model* for ν_r
  (in analogy to mixing length model)

- Sub-filter eddy viscosity $\nu_r = u'_\Delta l_\Delta = u'_\Delta l_S$

- Sub-filter velocity fluctuation $u'_\Delta = l_S \overline{S}$

  with filtered rate of strain $\overline{S} = \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2}$

$$\Rightarrow \nu_r = l_S^2 \overline{S}$$

Large-Eddy Simulation

- Smagorinsky length scale

$$l_S = C_S \Delta$$

$$\Rightarrow \nu_r = \left(C_S \Delta\right)^2 \overline{S}$$

$$\Rightarrow \tau_{ij}^r = \left(C_S \Delta\right)^2 \overline{S}\ \overline{S}_{ij}$$

- Similar equations can be derived for scalar transport

→ System of equations closed!

Summary

Part II: Turbulent Combustion

- Turbulence
- Turbulent Premixed Combustion
- Turbulent Non-Premixed Combustion
- Modelling Turbulent Combustion
- Applications

- Characteristics of Turbulent Flows
- Statistical Description of Turbulent Flows
  - Reynolds decomposition
  - Favre decomposition
- Types of turbulence
- Mean-flow Equations
- Reynolds Stress Equations
- *k*-Equation
- Turbulence Models
- Scales of Turbulent Flows/Energy Cascade
- Kolmogorov Hypotheses
- Scalar Transport Equations
- Large Eddy Simulation