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Università degli Studi di Napoli "Federico II"

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Turbulent Reactive Flows - I

Gennaro Coppola

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Navier–Stokes equations — I

- Mass and momentum balance:

$$\begin{cases} \nabla \cdot \mathbf{V} &= 0 \\ \\ \rho \dfrac{D\mathbf{V}}{Dt} &= \nabla \cdot \boldsymbol{\tau} + \mathbf{f} \end{cases}$$

where $\mathbf{V} = \mathbf{V}(\mathbf{x}, t)$, $\rho = \text{const.}$, $\dfrac{D}{Dt} = \dfrac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$

- For Newtonian and incompressible flows:

$$\boldsymbol{\tau} = -p\mathbf{I} + 2\mu \left(\frac{\nabla \mathbf{V} + (\nabla \mathbf{V})^T}{2} \right)$$

Navier–Stokes equations — II

- Navier–Stokes equations (Navier 1822, Stokes 1845):

$$\begin{cases} \nabla \cdot \mathbf{V} = 0 \\ \dfrac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} = -\dfrac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{V} + \mathbf{f} \end{cases} \qquad (\mathbf{NS})$$

- "Indicial notation":

$$\begin{cases} \dfrac{\partial U_j}{\partial x_j} = 0 \\ \dfrac{\partial U_j}{\partial t} + U_i \dfrac{\partial U_j}{\partial x_i} = -\dfrac{1}{\rho}\dfrac{\partial p}{\partial x_j} + \nu \dfrac{\partial^2 U_j}{\partial x_i^2} + f_j \end{cases} \qquad (\mathrm{NS})_j$$

Navier–Stokes equations — III

- When body forces admit a potential ($\mathbf{f} = \nabla\varphi$), defining the *modified pressure* $P = p/\rho + \varphi$ and exploiting incompressibility:

$$\frac{\partial \mathbf{V}}{\partial t} + \nabla \cdot (\mathbf{V}\mathbf{V}) = -\nabla P + \nu \nabla^2 \mathbf{V}$$

- Non dimensional formulation is:

$$\frac{\partial \mathbf{V}^*}{\partial t^*} + \nabla^* \cdot (\mathbf{V}^*\mathbf{V}^*) = -\nabla^* P^* + \frac{1}{\mathrm{Re}} \nabla^{*2} \mathbf{V}^*$$

where $\mathrm{Re} = \dfrac{V_{ref} L_{ref}}{\nu}$

Definitions – I

- Decomposition of the tensor $\nabla \mathbf{V} = \mathbf{S} + \mathbf{\Omega}$:

$$\mathbf{S} = \underbrace{\frac{\nabla \mathbf{V} + (\nabla \mathbf{V})^T}{2}}_{\textit{rate of strain}} \qquad \mathbf{\Omega} = \underbrace{\frac{\nabla \mathbf{V} - (\nabla \mathbf{V})^T}{2}}_{\textit{rate of rotation}}$$

- In indicial notation...: $\dfrac{\partial U_i}{\partial x_j} = S_{ij} + \Omega_{ij}$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \qquad \Omega_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i}\right)$$

Definitions – II

- $\mathbf{S}$ e $\boldsymbol{\Omega}$ arise for example in the relations:

$$\boldsymbol{\tau} = -p\mathbf{I} + 2\mu\mathbf{S} \qquad \tau_{ij} = -p\delta_{ij} + 2\mu S_{ij}$$

$$\boldsymbol{\Omega}\cdot\mathbf{A} = \frac{1}{2}\boldsymbol{\omega}\wedge\mathbf{A} \qquad \Omega_{ij} = -\frac{1}{2}\epsilon_{ijk}\,\omega_k$$

$$2\nabla\cdot\mathbf{S} = \nabla\left(\nabla\cdot\mathbf{V}\right) + \nabla^2\mathbf{V} \qquad 2\frac{\partial S_{ij}}{\partial x_i} = \frac{\partial}{\partial x_j}\frac{\partial U_i}{\partial x_i} + \frac{\partial^2 U_j}{\partial x_i^2}$$

$$\nabla\cdot\mathbf{S} = -\frac{1}{2}\mathrm{curl}\boldsymbol{\omega} + \nabla\left(\nabla\cdot\mathbf{V}\right) \qquad \frac{\partial S_{ij}}{\partial x_i} = -\frac{1}{2}\epsilon_{jki}\frac{\partial \omega_i}{\partial x_k} + \frac{\partial}{\partial x_j}\frac{\partial U_i}{\partial x_i}$$

with $\boldsymbol{\omega} = \mathrm{curl}\mathbf{V}$ (i. e. $\omega_i = \epsilon_{ijk}\dfrac{\partial U_k}{\partial x_j}$)

Conserved passive scalars

- Convection-diffusion equation for a passive scalar:

$$\frac{\partial \phi}{\partial t} + \mathbf{V} \cdot \nabla \phi = \Gamma \nabla^2 \phi$$

- Conservative form of the conservation equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{F}(\phi) = 0$$

with $\mathbf{F}(\phi) = \mathbf{V}\phi - \Gamma \nabla \phi$

Induced equations — I

- Poisson equation for pressure (divergence of (**NS**)):

$$\nabla^2 p = -\rho \nabla \cdot (\mathbf{V} \cdot \nabla \mathbf{V})$$

- Vorticity equation (curl of (**NS**)):

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \mathbf{V} \cdot \nabla \boldsymbol{\omega} = \boldsymbol{\omega} \cdot \nabla \mathbf{V} + \nu \nabla^2 \boldsymbol{\omega}$$

$\boldsymbol{\omega} \cdot \nabla \mathbf{V}$ is the "stretching" term

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Induced equations — II

- Evolution equation for (unit mass) kinetic energy: $E = \dfrac{|\mathbf{V}|^2}{2}$

$$\frac{\partial E}{\partial t} + \mathbf{V} \cdot \nabla E + \nabla \cdot \left[\left(\mathbf{V} \frac{p}{\rho} \right) - 2\nu \mathbf{V} \cdot \mathbf{S} \right] = -\Phi$$

  with $\Phi = 2\nu S_{ij} S_{ij}$ dissipation function.

- By considering a domain $\mathcal{D}$ with periodic or impermeable wall BCs, by integrating over $\mathcal{D}$ one has:

$$\frac{d\mathcal{E}}{dt} = -\int_{\mathcal{D}} \Phi \, d\mathcal{D} = -\nu \int_{\mathcal{D}} \omega_i^2 \, d\mathcal{D}$$

  with $\mathcal{E} = \int_{\mathcal{D}} E \, d\mathcal{D}$
  $\omega_i^2 = |\boldsymbol{\omega}|^2$ is the *enstrophy*

Turbulence: definitions(?!) — I

- *It is a well-known fact that under suitable conditions, which normally amount to a requirement that the kinematic viscosity ν be sufficiently small, some of this motions are such that the velocity at any given time and position in the fluid is not found to be the same when it is measured several times under seemingly identical conditions. In these motions the velocity takes random values which are not determined by the ostensible, or controllable, or 'macroscopic', data of the flow, although we believe that the average properties of the motion are determined uniquely by the data. Fluctuating motions of this kind are said to be turbulent.*

G. K. Batchelor, 1953

- *Turbulence is a three-dimensional time-dependent motion in which vortex stretching causes velocity fluctuations to spread to all wavelengths between a minimum determined by viscous forces and a maximum determined by the boundary conditions of the flow. It is the usual state of fluid motion except at low Reynolds numbers.*

☺ *The only short but satisfactory answer to the question "what is turbulence?" is that it is the general solution of the Navier Stokes equation.*

P. Bradshaw, 1972

- *Creation of small scale activity and dissipation, is the principle of turbulence. Classical fluid dynamical instabilities play a role of the fuel, vortex stretching is the engine, and viscous dissipation is the breaks.*

P. Constantin, 1994

Turbulence: definitions(?!) — II

- *The following definition of turbulence can thus be tentatively proposed and may contribute to avoiding the somewhat semantic discussion on this matter: a) Firstly, a turbulent flow must be unpredictable, in the sense that a small uncertainty as to its knowledge at a given initial time will amplify so as to render impossible a precise deterministic prediction of it evolution; b) Secondly, it has to satisfy the increased mixing property defined above; c) Thirdly, it must involve a wide range of spatial wave lengths.*

M. Lesieur, 1997

- *Turbulence can be defined by a statement of impotence reminiscent of the second law of thermodynamics: flow at a sufficiently high Reynolds number cannot be decelerated to rest in a steady fashion. The deceleration always produces vorticity, and the resulting vortex interactions are apparently so sensitive to the initial conditions that the resulting flow pattern changes in time and usually in stochastic fashion.*

H. W. Liepmann, 1979

- *A body of fluid is a mechanical system with an infinite number of degrees of freedom. It may therefore be expected to execute a rather random motion comparable to that of the molecules in a gas. If one regards such a chaotic motion as analyzed into harmonic components of various scales, one recognizes that frictional forces tend to dissipate the small scale oscillations and keep the motion more or less regular. Thus, when viscous forces are sufficiently strong, i.e. at sufficiently low Reynolds numbers, the motion will become laminar. On the other hand, at sufficiently high Reynolds numbers the motion will tend to become random fluctuating, even when external conditions are steady.*

C. C. Lin and H. W. Reid, 1963

Turbulence: phenomenology

Turbulence characteristics

- High vorticity and 3D
- Highly irregular in both space and time
- Randomness
- Diffusivity and dissipativity
- Wide range of spatial and temporal scales involved
- Non locality

Turbulence: statistical approach

- (Thermo)fluid-dynamic quantities are assumed as stochastic variables, unpredictable for a single experiment but with stable expected values

- For each variable we define the mathematical expectation as:

$$\langle U \rangle = \lim_{N \to \infty} \sum_{\nu=1}^{N} \frac{U_\nu}{N}$$

- Comparison with experiments (in which various *space* and/or *temporal* mean values are measured) is made under the assumption of validity of the *ergodic hypotesis*

Stochastic tools: basic concepts — I

Given Ω the *probability space*:

- At every time instant $\bar{t}$ and in every point in space $\bar{\mathbf{x}}$ the generic fluid-dynamic variable is a *random variable*.

$$U_{\bar{t},\bar{\mathbf{x}}}(\omega) : \Omega \longrightarrow \mathbb{R}$$

- Fixed the point $\bar{\mathbf{x}}$ in space, $U_{\bar{\mathbf{x}}}(t)$ is a *stochastic process*.

$$U_{\bar{\mathbf{x}}}(\omega, t) : \Omega \times [t_0, \infty[\longrightarrow \mathbb{R}$$

- Fixed a time instant $\bar{t}$, $U_{\bar{t}}(\mathbf{x})$ is a *random field*.

$$U_{\bar{t}}(\omega, \mathbf{x}) : \Omega \times \mathcal{D} \longrightarrow \mathbb{R}$$

Stochastic tools: basic concepts — II

- The characterization of a random variable is made through the specification of the *Probability Density Function* f_U in such a way that:

$$P\left(U\left(\omega\right) \in \mathcal{R}\right) = \int_{\mathcal{R}} f_U\left(u\right) \, du$$

- The characterization of N random variables is made through the specification of the *Joint Probability Density Function*:

$$f_{U_1,U_2,\ldots,U_N}$$

- The characterization of stochastic processes and/or random fields is made through the specification of the *n-point, n-time Joint Probability Density Functions*

$$f_N\left(u_1, t_1, \mathbf{x}_1; \ldots u_N, t_N, \mathbf{x}_N\right)$$

$\forall N$, $\forall \left(t_1, \ldots, t_N\right)$, $\forall \left(\mathbf{x}_1, \ldots, \mathbf{x}_N\right)$

Stochastic tools: basic concepts — III

The *synthetic characterization* is made through the specification of the *moments*

- Mean value:

$$\langle U \rangle = \int_{-\infty}^{\infty} V f_U(V)\, dV$$

- Variance:

$$\langle (U - \langle U \rangle)^2 \rangle = \int_{-\infty}^{\infty} (V - \langle U \rangle)^2 f_U(V)\, dV$$

- Central moment of order n:

$$\langle (U - \langle U \rangle)^n \rangle = \int_{-\infty}^{\infty} (V - \langle U \rangle)^n f_U(V)\, dV$$

Stochastic tools: basic concepts — IV

- Let σ be the *standard deviation* ($\sigma = \sqrt{\mathrm{var}\,(U)}$). *Standard* random variables are defined as:

$$\hat{U} = \frac{(U - \langle U \rangle)}{\sigma}$$

- Of particular interest are standard moments of order $n = 3$ and $n = 4$, respectively called *skewness* and *flatness*

$$\mathrm{Sk}\,(U) = \frac{\langle (U - \langle U \rangle)^3 \rangle}{\sigma^3} \qquad \mathrm{Fl}\,(U) = \frac{\langle (U - \langle U \rangle)^4 \rangle}{\sigma^4}$$

- In the case of a random vector $\mathbf{U} = (U_1, U_2, \ldots, U_N)$ the covariance matrix is defined as:

$$\mathrm{cov}\,(\mathbf{U}) = \langle (U_i - \langle U_i \rangle) \left(U_j - \langle U_j \rangle \right) \rangle$$

Reynolds equations

- Reynolds decomposition:

$$u_i = U_i - \langle U_i \rangle$$

- By applying the mean operator to $(\mathrm{NS})_j$ (Reynolds equations):

$$\begin{aligned} \frac{\partial \langle U_j \rangle}{\partial x_j} &= 0 \\ \frac{\partial \langle U_j \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle U_j \rangle}{\partial x_i} &= -\frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_j} + \nu \frac{\partial^2 \langle U_j \rangle}{\partial x_i^2} - \frac{\partial \langle u_i u_j \rangle}{\partial x_i} \end{aligned}$$

$\langle u_i u_j \rangle$ is the **Reynolds Stress Tensor (RST)**

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$\langle u_i u_j \rangle$ is the **Reynolds Stress Tensor (RST)**

Reynolds Stress Tensor — I

Interpretation as a stress for the RST:

- Reynolds equations can be written as::

$$\rho\left(\frac{\partial\langle U_j\rangle}{\partial t}+\langle U_i\rangle\frac{\partial\langle U_j\rangle}{\partial x_i}\right)=\frac{\partial\widetilde{\tau}_{ij}}{\partial x_i}$$

- The stress tensor $\widetilde{\tau}_{ij}$ is now given by

$$\widetilde{\tau}_{ij}=-\langle p\rangle\delta_{ij}+2\mu\langle S_{ij}\rangle-\rho\langle u_iu_j\rangle$$

Reynolds Stress Tensor — II

- In the Reynolds equations the term $\langle u_i u_j \rangle$ is unknown

- It is possible to write down balance equations for $\langle u_i u_j \rangle$; they will involve further unknowns (closure problem)

- At fixed $\mathbf{x}$ e t RST represents the covariance matrix of the random vector $\mathbf{U}$

$$\langle u_i u_j \rangle = \langle (U_i - \langle U_i \rangle) \left(U_j - \langle U_j \rangle \right) \rangle = \mathrm{cov}\,(\mathbf{U})$$

Reynolds Stress Tensor — III

- The turbulent kinetic energy k is defined as half the trace of the RST $\langle u_i u_j \rangle$:

$$k = \frac{1}{2}\langle u_i u_i \rangle$$

- The anisotropy a_{ij} is defined as the deviatoric part of the RST:

$$a_{ij} = \langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij}$$

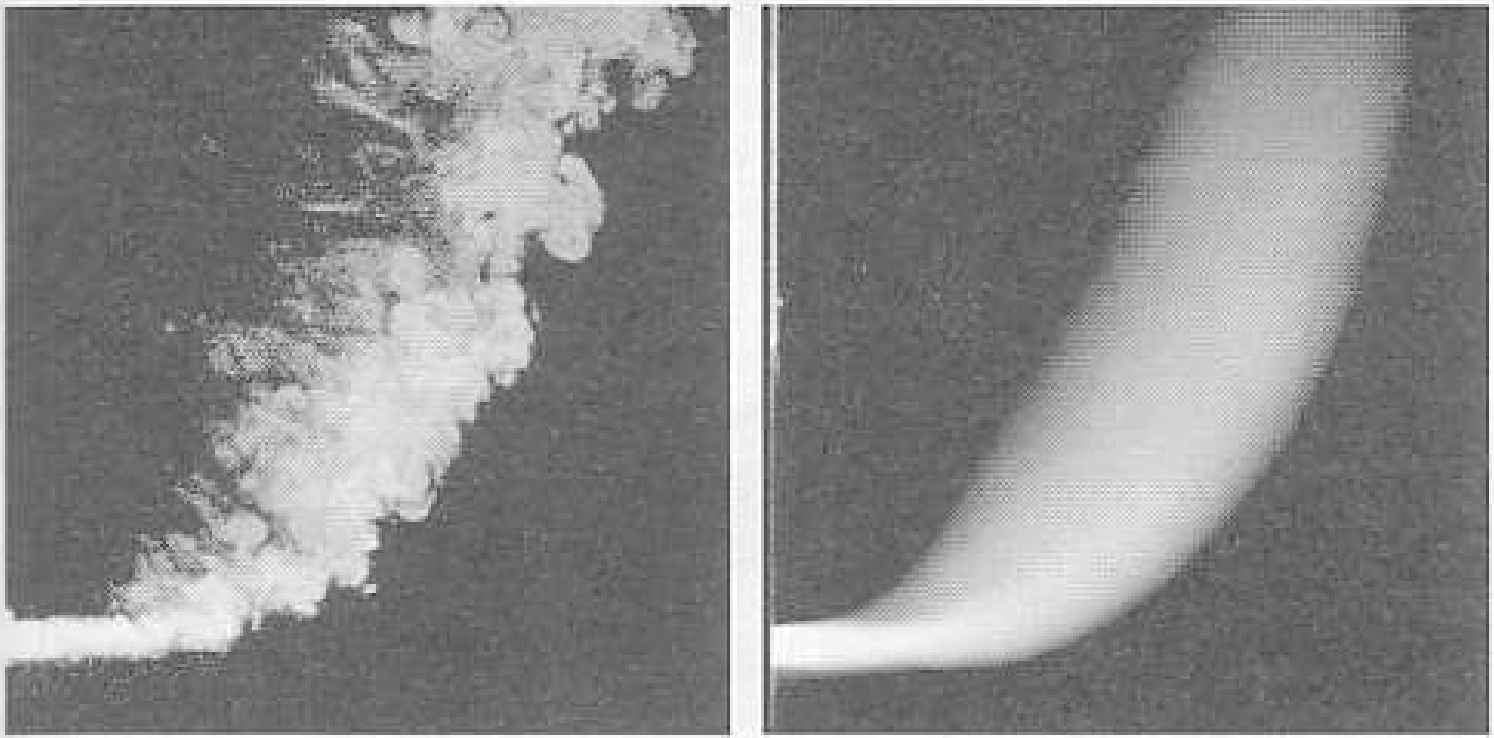

Figure 1.3 *Instantaneous and time averaged views of a jet in cross flow. The jet exits from the wall at left into a stream flowing from bottom to top (Su & Mungal, 1999).*

Instantaneous and mean scalar field

Passive scalar transport: mean equations

- The mean equation for a passive scalar reads:

$$\frac{\partial \langle \phi \rangle}{\partial t} + \langle \mathbf{V} \rangle \cdot \nabla \langle \phi \rangle + \nabla \cdot \langle \mathbf{u} \phi' \rangle = \nabla \cdot (\Gamma \nabla \langle \phi \rangle)$$

- In conservative form one has:

$$\frac{\partial \langle \phi \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{V} \rangle \langle \phi \rangle) = \nabla \cdot \left(\Gamma \nabla \langle \phi \rangle - \langle \mathbf{u} \phi' \rangle \right)$$

- Again, in addition to diffusive ($\Gamma \nabla \langle \phi \rangle$) and convective ($\langle \mathbf{V} \rangle \langle \phi \rangle$) mean fluxes, an additional unknown term due to fluctuations arises: ($-\langle \mathbf{u} \phi' \rangle$).

Energy equations

- An equation for turbulent kinetic energy k can be written from the equations of mean kinetic energy and from an equation for the transport of kinetic energy of the mean velocity field:

$$\langle E\rangle = \frac{1}{2}\langle U_i U_i\rangle \qquad \bar{E} = \frac{1}{2}\langle U_i\rangle\langle U_i\rangle \qquad k = \frac{1}{2}\langle u_i u_i\rangle$$

$$\frac{\bar{D}\langle E\rangle}{\bar{D}t} + \nabla\cdot\mathbf{T}_1 = -\bar{\varepsilon} - \varepsilon \qquad \frac{\bar{D}\bar{E}}{\bar{D}t} + \nabla\cdot\mathbf{T}_2 = -\mathcal{P} - \bar{\varepsilon}$$

$$\frac{\bar{D}k}{\bar{D}t} + \nabla\cdot\mathbf{T} = \mathcal{P} - \varepsilon$$

where:

$$\frac{\bar{D}}{\bar{D}t} = \partial_t + \langle U_i\rangle\partial_i \quad s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad \mathcal{P} = -\langle u_i u_j\rangle\frac{\partial\langle U_i\rangle}{\partial x_j} = -a_{ij}\bar{S}_{ij}$$

$\varepsilon = 2\nu\langle s_{ij}s_{ij}\rangle$ Turbulent kinetic energy dissipation (for unit mass and time)

$$\bar{\varepsilon} = 2\nu\bar{S}_{ij}\bar{S}_{ij}, \quad T_i = \frac{1}{2}\langle u_i u_j u_j\rangle + \langle u_i p'\rangle/\rho - 2\nu\langle u_j s_{ij}\rangle$$

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$$\frac{\bar{D}\langle E\rangle}{\bar{D}t} + \nabla\cdot\mathbf{T}_1 = -\bar{\varepsilon} - \varepsilon \qquad \frac{\bar{D}\bar{E}}{\bar{D}t} + \nabla\cdot\mathbf{T}_2 = -\mathcal{P} - \bar{\varepsilon}$$

$$\frac{\bar{D}k}{\bar{D}t} + \nabla\cdot\mathbf{T} = \mathcal{P} - \varepsilon$$

where:

$$\frac{\bar{D}}{\bar{D}t} = \partial_t + \langle U_i\rangle\partial_i \quad s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad \mathcal{P} = -\langle u_i u_j\rangle\frac{\partial\langle U_i\rangle}{\partial x_j} = -a_{ij}\bar{S}_{ij}$$

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Stochastic tools, again — I

- For a stochastic process one defines the *autocovariance* and the *auto-correlation function*

$$R(t,s) = \langle u(t)\, u(t+s) \rangle$$

$$\rho(t,s) = \frac{R(t,s)}{\langle u(t)^2 \rangle}$$

  For *statistically stationary* processes R and ρ depend only on s

- For a Random field one defines the *two-point correlation*

$$R_{ij}(\mathbf{x},\mathbf{r}) = \langle u_i(\mathbf{x})\, u_j(\mathbf{x}+\mathbf{r}) \rangle$$

  For a *statistically homogeneous* field R_{ij} depends only on $\mathbf{r}$.

Stochastic tools, again — II

- From the definition of autocorrelation one can define temporal scales of the flow (*integral timescale*):

$$\tau = \int_0^\infty \rho(s)\, ds$$

- From the definition of two point correlation one can define various spatial scales (*integral lengthscales*), e.g.:

$$L_{11}\left(\mathbf{x}\right) = \frac{1}{R_{11}(\mathbf{x},0)} \int_0^\infty R_{11}\left(\mathbf{x},\mathbf{r}_1\right)\, dr_1$$

Homogeneous and isotropic turbulence (Taylor, 1935)

- A turbulent field is defined *homogeneous* if all the statistical variables of the *fluctuating field* are independent on a shift in space

- A turbulent homogeneous field is defined *isotropic* if all the statistical variables are independent on reflection and rotations of the coordinate system

Homogeneous and isotropic turbulence — II

In homogeneous and isotropic fields the two-point correlation functions are independent on the direction of $\mathbf{r}$ and are hence dependent only on r.

- At $r = 0$ we have the RST, which is now a *scalar* tensor:

$$R_{ij}(0,t) = \langle u_i u_j \rangle = u'^2 \delta_{ij} \qquad u'^2 = \frac{2}{3}k$$

- It is possible to show that the most general form of the autocorrelation tensor for isotropic fields is given by

$$R_{ij}(\mathbf{r},t) = u'^2 \left(g(r,t)\,\delta_{ij} + (f(r,t) - g(r,t))\,\frac{r_i r_j}{r^2} \right)$$

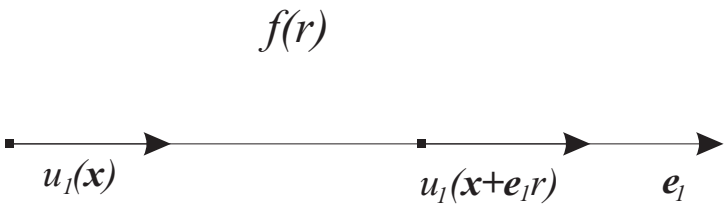
where $u'^2 = \frac{2}{3}k$ and f and g are respectively the *longitudinal* and *trasverse autocorrelation*.

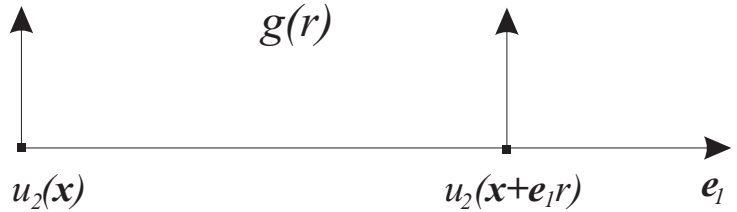
Homogeneous and isotropic turbulence — III

$$f(r,t) = \frac{R_{11}}{u'^2} = \frac{\langle u_1(\mathbf{x}+\mathbf{e}_1 r,t)u_1(\mathbf{x},t)\rangle}{\langle u_1^2\rangle}$$

$$g(r,t) = \frac{R_{22}}{u'^2} = \frac{\langle u_2(\mathbf{x}+\mathbf{e}_1 r,t)u_2(\mathbf{x},t)\rangle}{\langle u_2^2\rangle}$$

$$R_{33} = R_{22} \qquad R_{ij} = 0 \text{ per } i \neq j$$





Longitudinal and trasverse autocorrelation

Homogeneous and isotropic turbulence — IV

- Continuity imposes:

$$g(r,t) = f(r,t) + \frac{1}{2} r \frac{\partial}{\partial r} f(r,t)$$

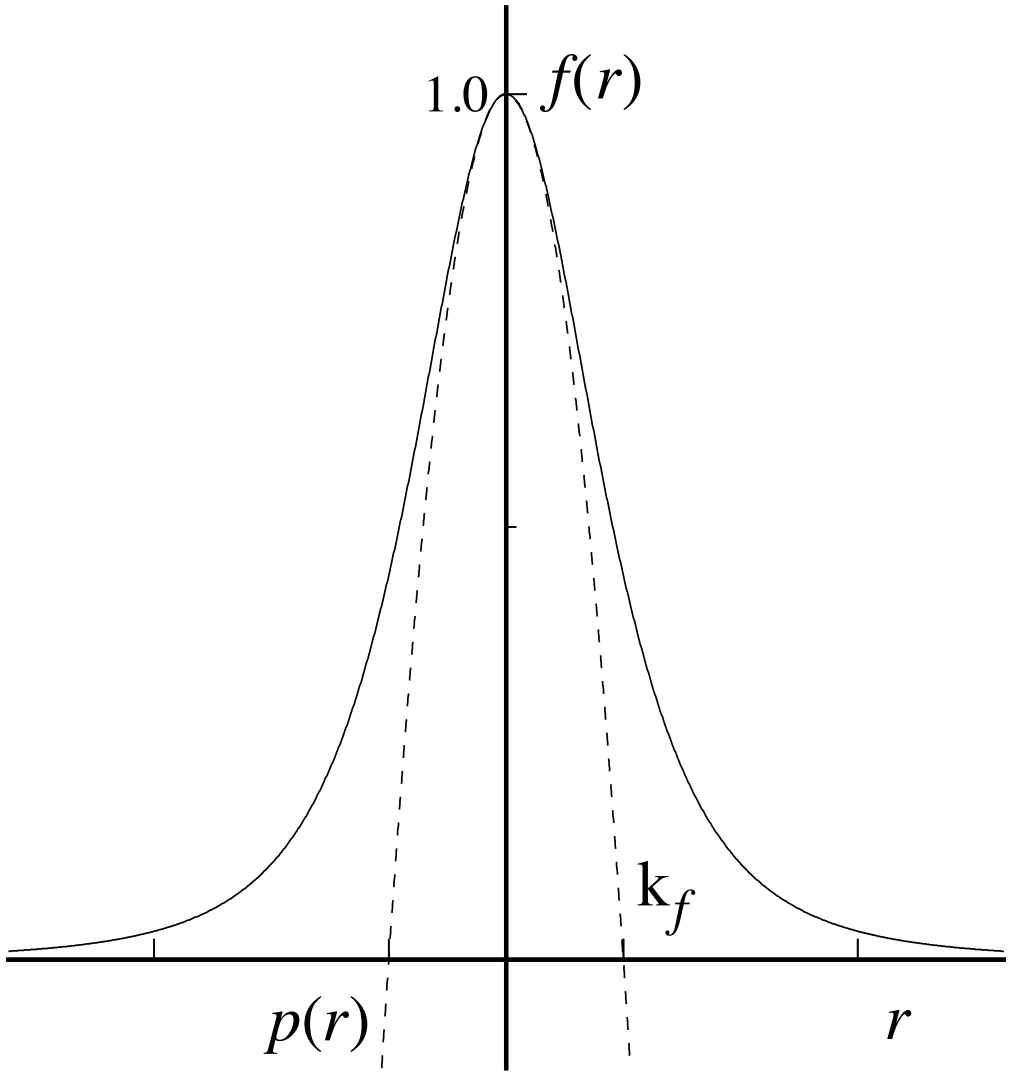
  and hence R_{ij} is univocally determined by $f(r,t)$.

- There are spatial scales based on f and g:

$$L_{11} = \int_0^\infty f(r,t)\, dr \qquad \text{(longitudinal integral scale)}$$

$$L_{22} = \int_0^\infty g(r,t)\, dr \qquad \text{(trasverse integral scale)}$$

$$\lambda_f = \left[-\frac{1}{2} f''(0,t) \right]^{\frac{1}{2}} \qquad \text{(longitudinal Taylor microscale)}$$



Longitudinal autocorrelation and Taylor microscale

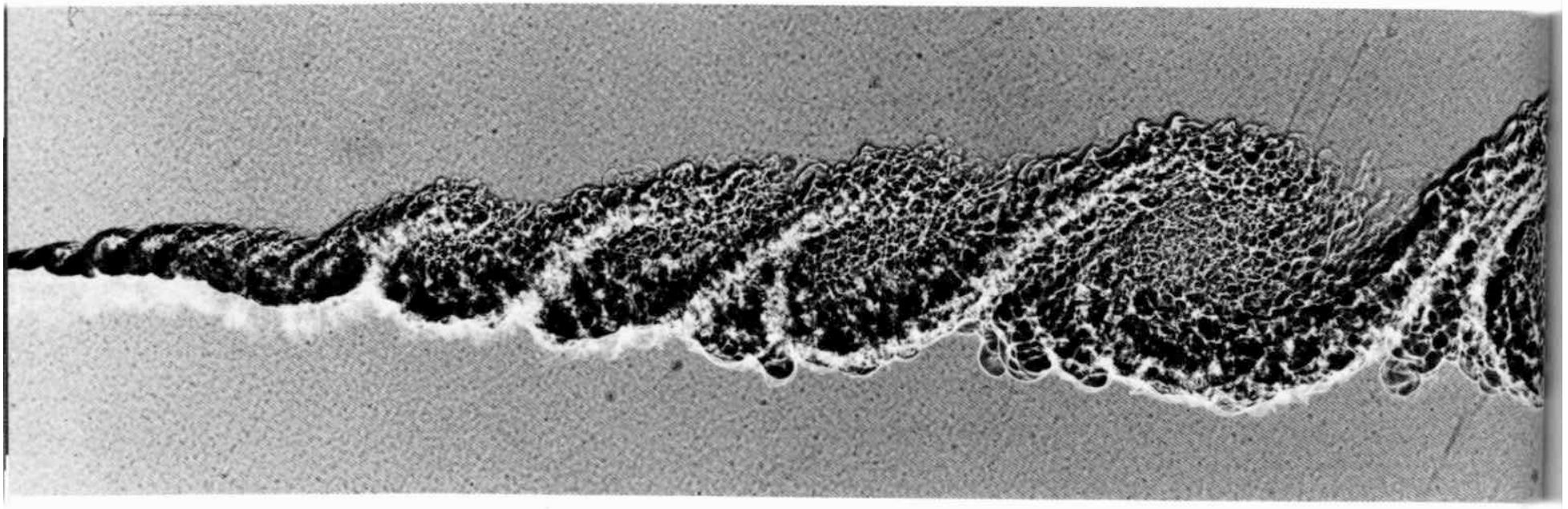
Kolmogorov (1941) theory: basic concepts

- Kolmogorov 1941 theory (K41) is based on few statistical hypotesis justified by Richardson *energy cascade* view (Richardson, 1922)

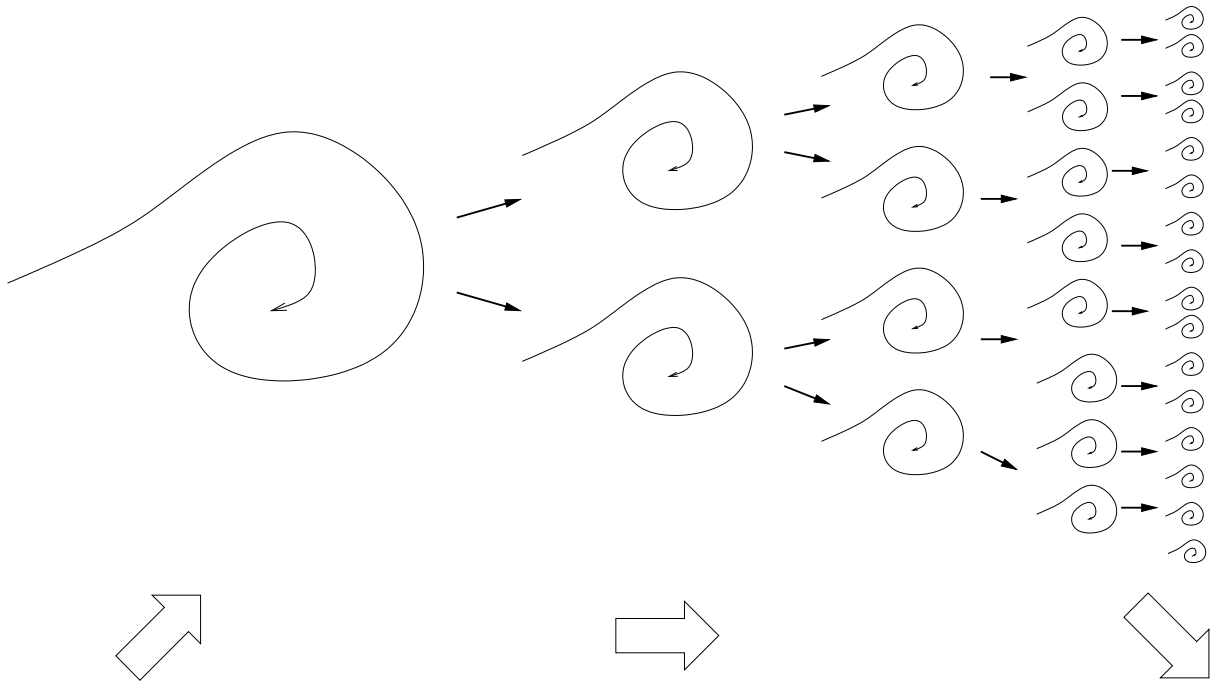
- In such a description a turbulent field can be considered to be composed of (*eddies*) of different sizes

- Large eddies are unstable and break up trasferring their energy to smaller eddies. This process is assumed to be non viscous

- The energy transfer is halted on sufficiently small scales at which viscosity is active in dissipating energy



Mixing Layer (Brown e Roshko, 1974)



Energy cascade (Richardson, 1922)

Kolmogorov (1941) theory: basic concepts

Kolmogorov theory is formulated for turbulent flows at sufficiently high Reynolds number. For such flows one assumes that:

1. Small scales are statistically isotropic (and *universal*)

2. Statistical properties of small scales (*dissipation range*) depend solely on ν and ε

3. There exist intermediate scales (*inertial subrange*) at which statistical properties are universal and depend only on ε.

Kolmogorov (1941) theory: basic concepts

- Dimensional analysis allows one to determine the following *Kolmogorov scales*

$$\begin{aligned} \eta &\equiv \left(\nu^3/\varepsilon\right)^{1/4} \\ u_\eta &\equiv (\varepsilon\nu)^{1/4} \\ \tau_\eta &\equiv (\nu/\varepsilon)^{1/2} \end{aligned}$$

- By assuming $\varepsilon \sim \mathcal{U}^3/\mathcal{L}$ one has the following scaling laws:

$$\begin{aligned} \eta/\mathcal{L} &\sim \mathrm{Re}^{-3/4} \\ u_\eta/\mathcal{U} &\sim \mathrm{Re}^{-1/4} \\ \tau_\eta/\mathcal{T} &\sim \mathrm{Re}^{-1/2} \end{aligned}$$

Kolmogorov (1941) theory: basic concepts

- Second order velocity structure function:

$$B_{ij}(\mathbf{r},\mathbf{x},t) = \langle [U_i(\mathbf{x}+\mathbf{r},t) - U_i(\mathbf{x},t)] \left[U_j(\mathbf{x}+\mathbf{r},t) - U_j(\mathbf{x},t)\right] \rangle$$

- For homogeneous and isotropic turbulence

$$B_{ij}(\mathbf{r},t) = B_{NN}(r,t)\,\delta_{ij} + [B_{LL}(r,t) - B_{NN}(r,t)]\,\frac{r_i r_j}{r^2}$$

- A consequence of continuity equation is

$$B_{NN}(r,t) = B_{LL}(r,t) + \frac{1}{2} r \frac{\partial}{\partial r} B_{LL}(r,t)\,\frac{r_i r_j}{r^2}$$

Kolmogorov (1941) theory: basic concepts

Dimensional analysis allows one to obtain the following scaling laws:

- In the dissipation range:

$$B_{LL}(r,t) = (\varepsilon r)^{2/3}\, \widehat{B}_{LL}(r/\eta)$$

- In the inertial subrange:

$$B_{LL}(r,t) = C_2\,(\varepsilon r)^{2/3} \qquad \text{“two-third law”}$$

  i.e. $\widehat{B}_{LL} \to C_2$ for $r/\eta \gg 1$

Kolmogorov (1941) theory: basic concepts

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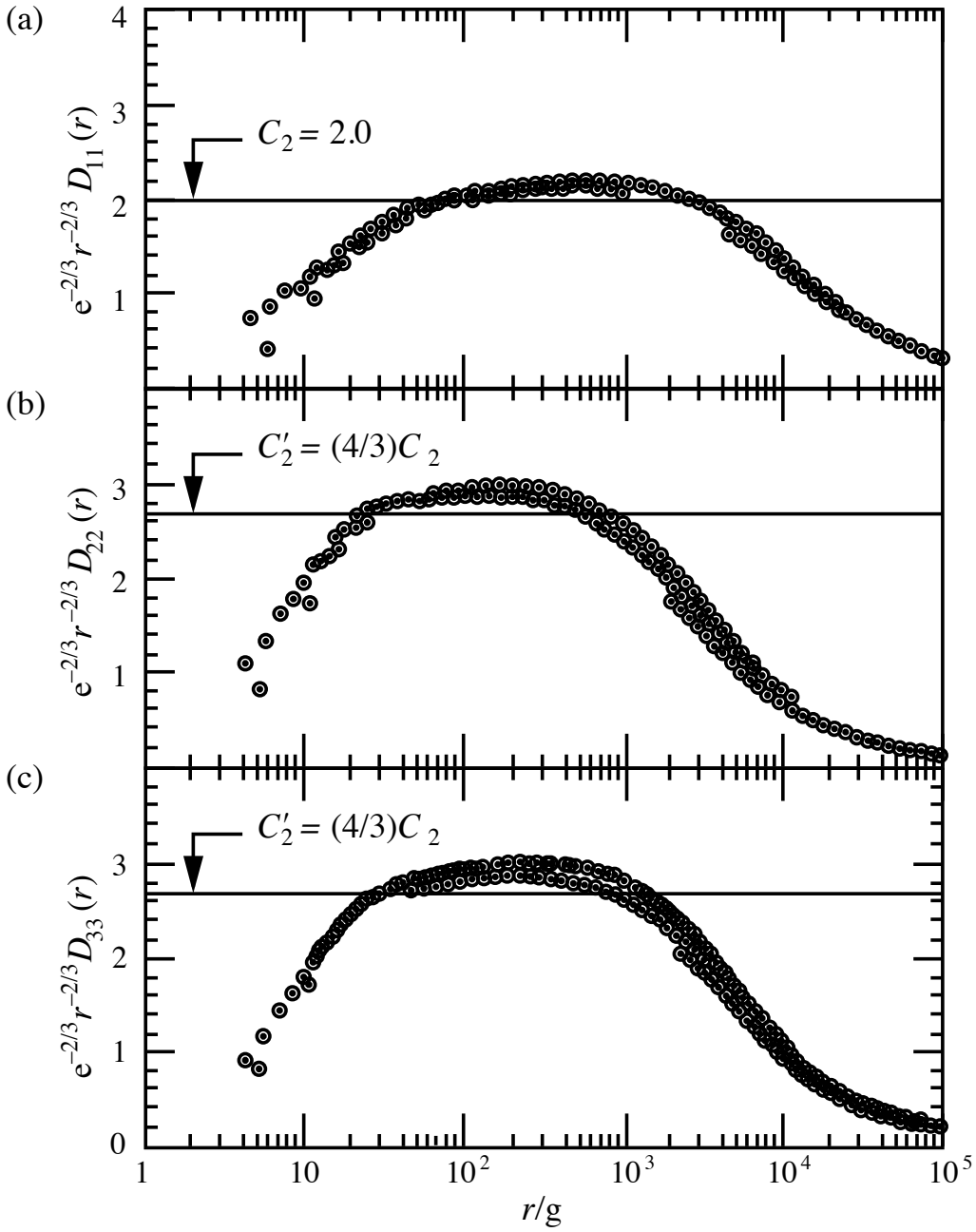

Velocity structure functions: Boundary Layer (Saddoughi e Veeravalli, 1994)

Kolmogorov (1941) theory: basic concepts

- It is possible to obtain an equation for $f(r,t)$ from **(NS)** (Karman–Howart, 1938)

$$\frac{\partial}{\partial t}\left(u'^2 f\right) - \frac{u'^3}{r^4}\frac{\partial}{\partial r}\left(r^4 \bar{k}\right) = \frac{2\nu u'^2}{r^4}\frac{\partial}{\partial r}\left(r^4 \frac{\partial f}{\partial r}\right)$$

  where $\bar{k} = \langle u_1(\mathbf{x},t)^2 u_1(\mathbf{x}+\mathbf{e}_1 r,t)\rangle / u'^3$ and $u'^2 = \frac{2}{3}k$

- Expressed in terms of the longitudinal structure function $B_{LLL}(r,t)$ on has: (Kolmogorov equation)

$$\frac{3}{r^5}\int_0^r s^4 \frac{\partial}{\partial t} B_{LL}(s,t)\, ds = 6\nu \frac{\partial B_{LL}}{\partial r} - B_{LLL} - \frac{4}{5}\varepsilon r$$

- In the inertial subrange one has:

$$B_{LLL} = -\frac{4}{5}\varepsilon r \qquad \text{“four-fifth” law}$$

Kolmogorov (1941) theory: basic concepts

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Fourier representation — I

- Fourier transform of the autocorrelation tensor is the velocity-spectrum tensor

$$\Phi_{ij}(\boldsymbol{\kappa}) = \frac{1}{(2\pi)^3} \int\int\int_{-\infty}^{\infty} R_{ij}(r) e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}}\, d\mathbf{r}$$

$$R_{ij}(r) = \int\int\int_{-\infty}^{\infty} \Phi_{ij}(\boldsymbol{\kappa}) e^{i\boldsymbol{\kappa}\cdot\mathbf{r}}\, d\boldsymbol{\kappa}$$

- The RST is given by:

$$R_{ij}(0) = \langle u_i u_j \rangle = \int\int\int_{-\infty}^{\infty} \Phi_{ij}(\boldsymbol{\kappa})\, d\boldsymbol{\kappa}$$

  which identifies Φ_{ij} as the "density" of the RST in the wavenumbers space

Fourier representation — II

- By removing all "directional" informations from $\Phi_{ij}(\boldsymbol{\kappa})$ one obtains the definition of the energy spectrum function:

$$E(\kappa) = \int_{\mathcal{S}(\kappa)} \frac{1}{2} \Phi_{ii}(\boldsymbol{\kappa}) \, d\mathcal{S}(\kappa)$$

where $\mathcal{S}(\kappa)$ is the sphere of radius κ in wavenumber space

- From the definition of $E(\kappa)$ one obtains:

$$\begin{aligned} k &= \int_0^\infty E(\kappa) \, d\kappa \\ \varepsilon &= \int_0^\infty 2\nu\kappa^2 E(\kappa) \, d\kappa \end{aligned}$$

$D(\kappa) = 2\nu\kappa^2 E(\kappa)$ is the dissipative spectrum

Fourier representation — III

By applying Kolmogorov hypotesis in the wavenumber space one obtains scaling laws analogous to the ones for the velocity structure functions.

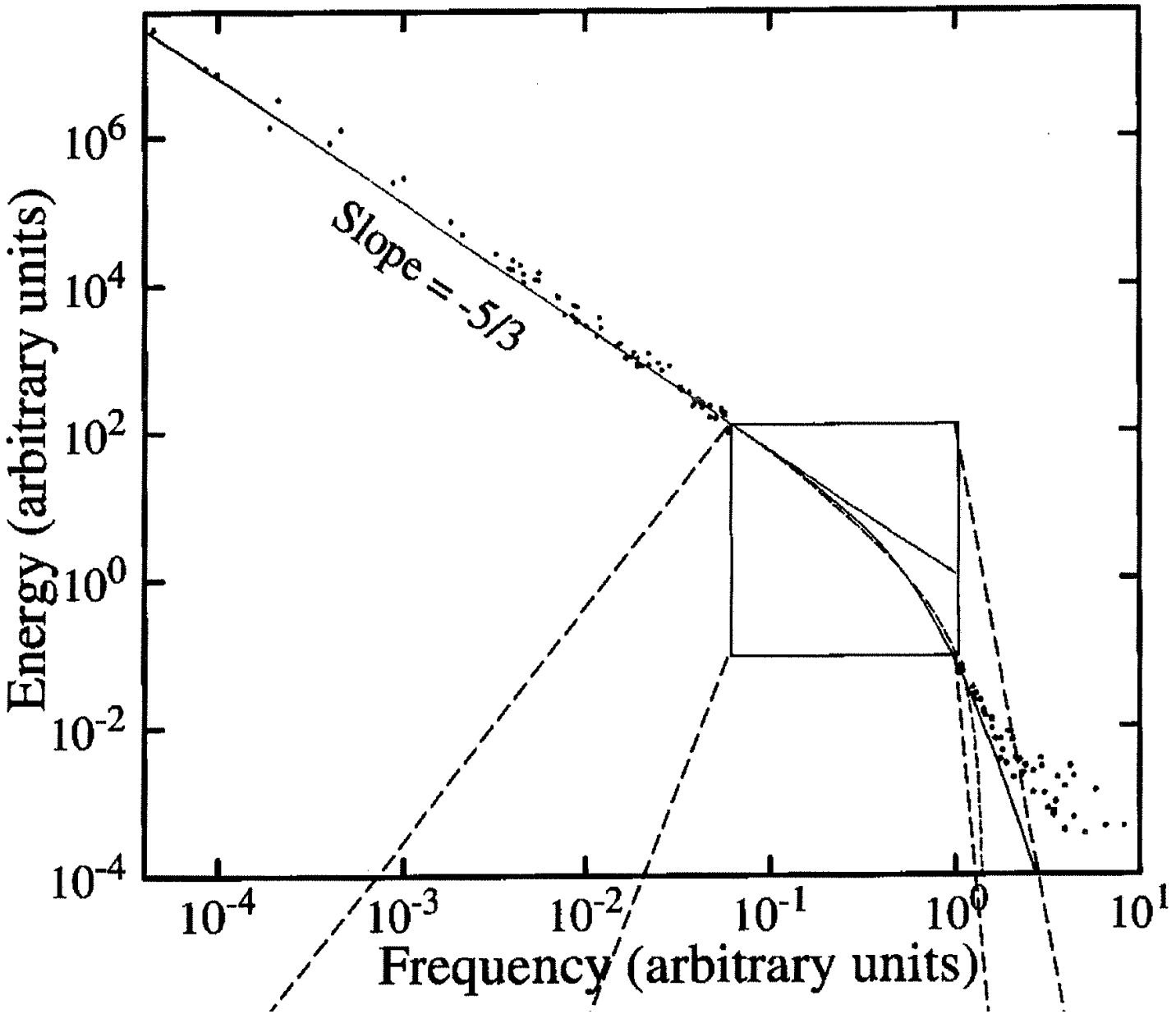
- In the dissipation range, $E(\kappa)$ is uniquely determined by ν and ε:

$$E(\kappa) = (\varepsilon\nu^5)^{1/4}\varphi(\kappa\eta)$$

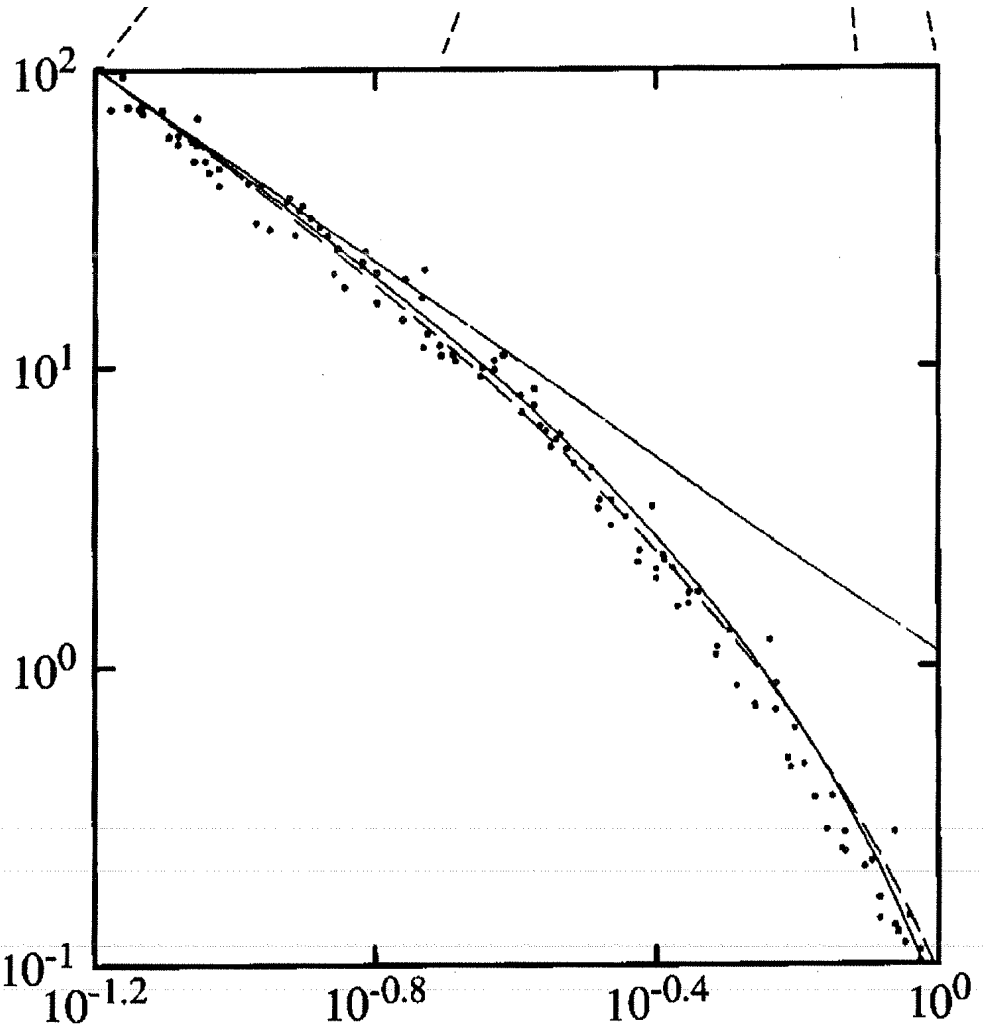
  and $\varphi(\kappa\eta)$ is an universal function.

- In the inertial subrange, $E(\kappa)$ is uniquely determined by ε:

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



Energy spectrum (Frisch, 1996)



Energy spectrum (Frisch, 1996)

Fourier representation — IV

- Experimentally, the 1D spectrum is measured

$$E_{11}(\kappa_1) = \frac{1}{\pi}\int_{\infty}^{\infty} R_{ij}\left(\mathbf{e}_1 r_1\right) e^{-i\kappa_1 r_1}\, dr_1$$

  also expressed as:

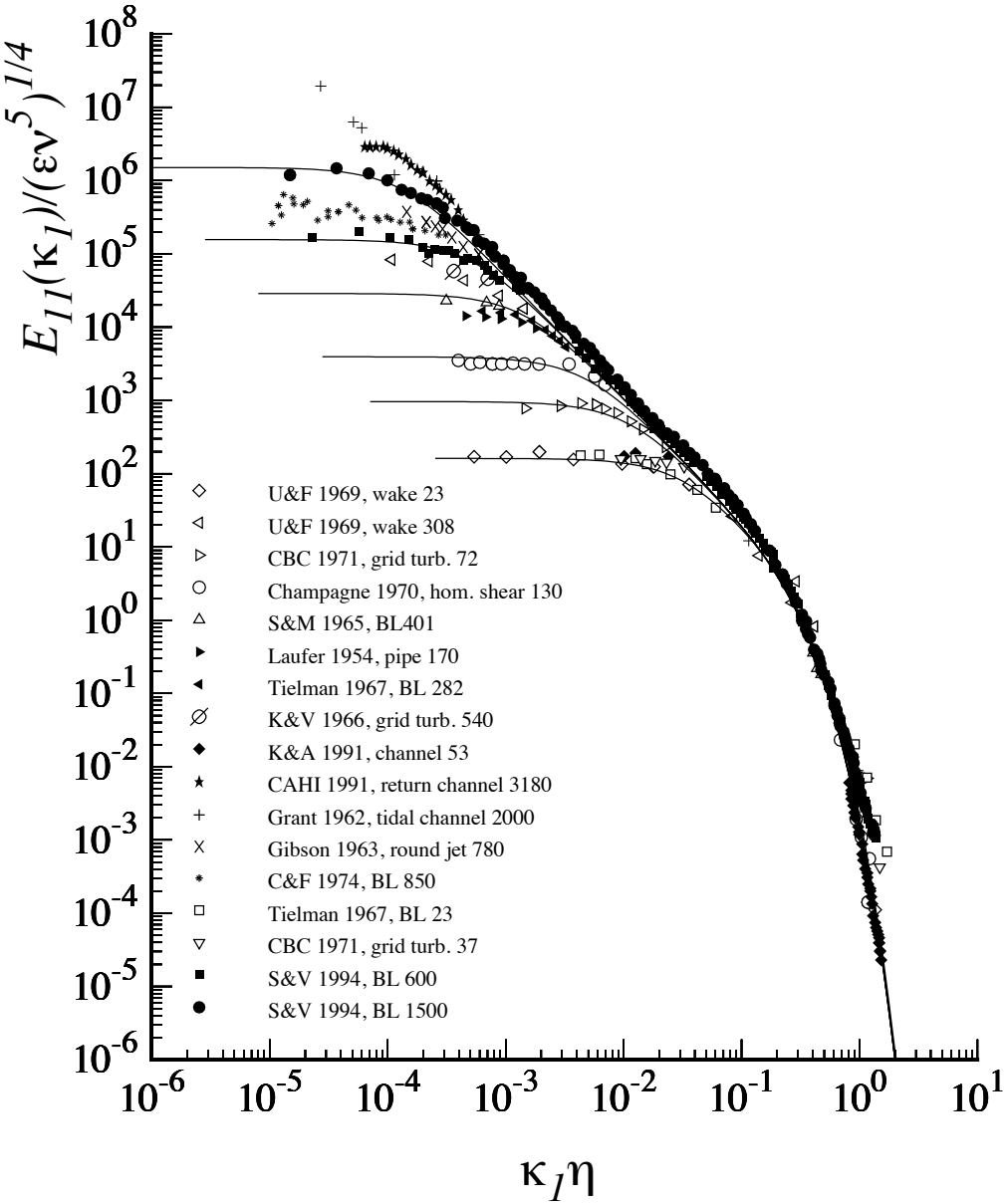
$$E_{11}(\kappa_1) = \frac{2}{\pi}\langle u_1^2\rangle \int_{0}^{\infty} f(r_1)\cos(\kappa_1 r_1)\, dr_1$$

- Scaling laws for E_{11} are given by:

$$E_{11}(\kappa_1) = \psi(\kappa_1\eta)\varepsilon^{2/3}\kappa_1^{-5/3}$$

$$E_{11}(\kappa_1) = \phi(\kappa_1\eta)\left(\varepsilon\nu^5\right)^{1/4} \qquad \text{in the dissipation range } (\kappa\eta \to 1)$$

$$E_{11}(\kappa_1) = C_1\varepsilon^{2/3}\kappa^{-5/3} \qquad \text{in the inertial range } (\kappa\eta \ll 1)$$



$E_{11}(\kappa_1)/(\varepsilon\nu^5)^{1/4}$.
Various experimental flows (Saddoughi e Veeravalli, 1994)

K41 refinements — I

Further results of K–41 for higher-order statistics:

- Scaling laws for moments of order $n \geq 3$ for the velocity structure functions:

$$\langle (\Delta U)^n \rangle = C_n \left(r \langle \varepsilon \rangle \right)^{n/3}$$

  with $\Delta U = [U_i(\mathbf{x} + \mathbf{e}_i r) - U_i(\mathbf{x})]$. In the case $n = 3$ theory has already given: $C_3 = -4/5$

- Normalized velocity derivative moments of higher order:

$$M_n = \frac{\langle \left(\frac{\partial u_i}{\partial x_i} \right)^n \rangle}{\langle \left(\frac{\partial u_i}{\partial x_i} \right)^2 \rangle^{n/2}}$$

  According to K41 M_n are universal constants.

K41 refinements — II

- Both predictions for higher order statistics are not fully verified by experiments

- Higher order moments exhibit scaling exponents different from $n/3$ and not universal. Normalized velocity derivatives have moments growing with Re

- From the point of view of the hypotesis, the critical point is the dependence of the local statistics from *averaged* dissipation (Landau 1944)

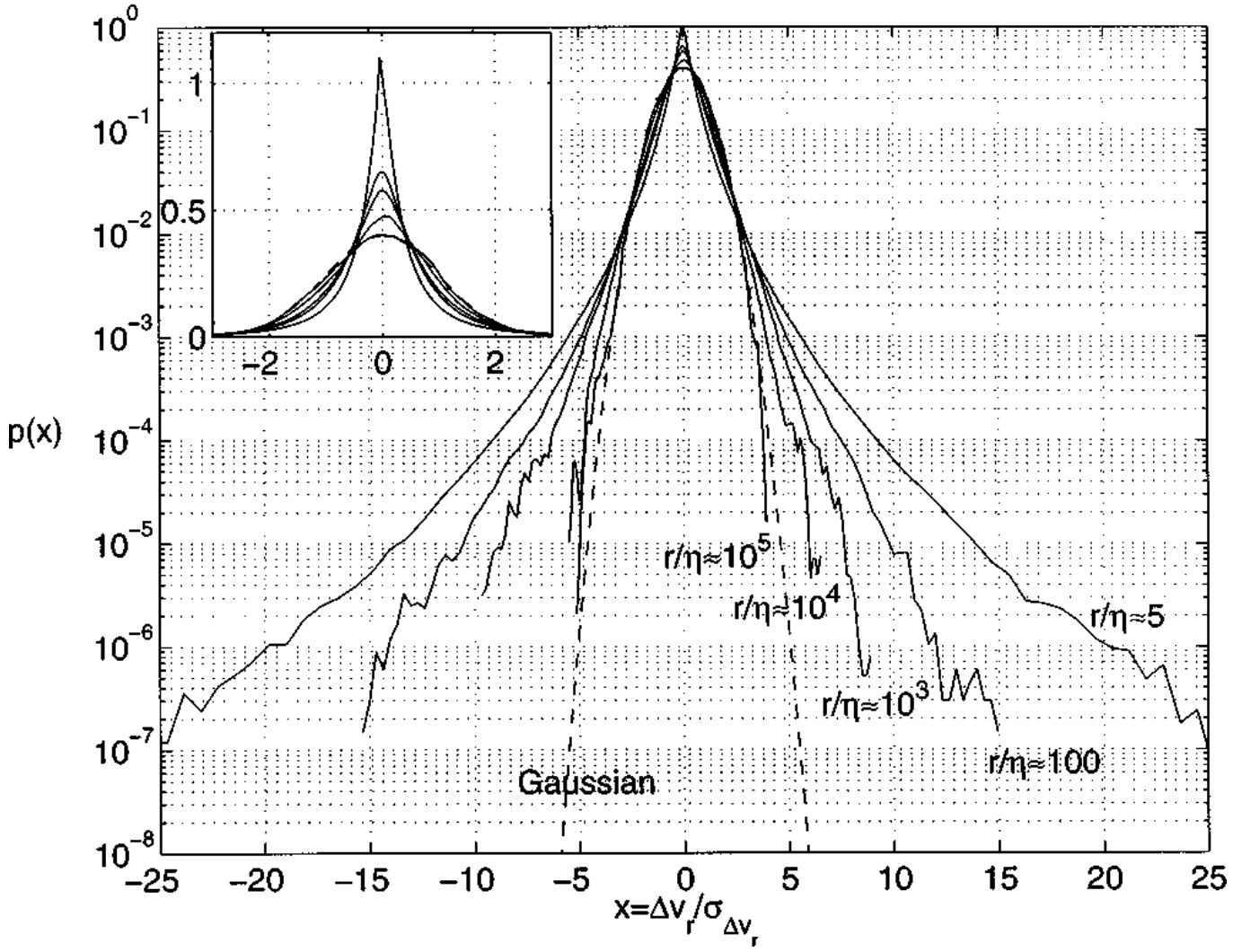
- A (partial) correction has been given by Kolmogorov himself (*refined similarity hypotesis*, 1962)

K41 refinements — III

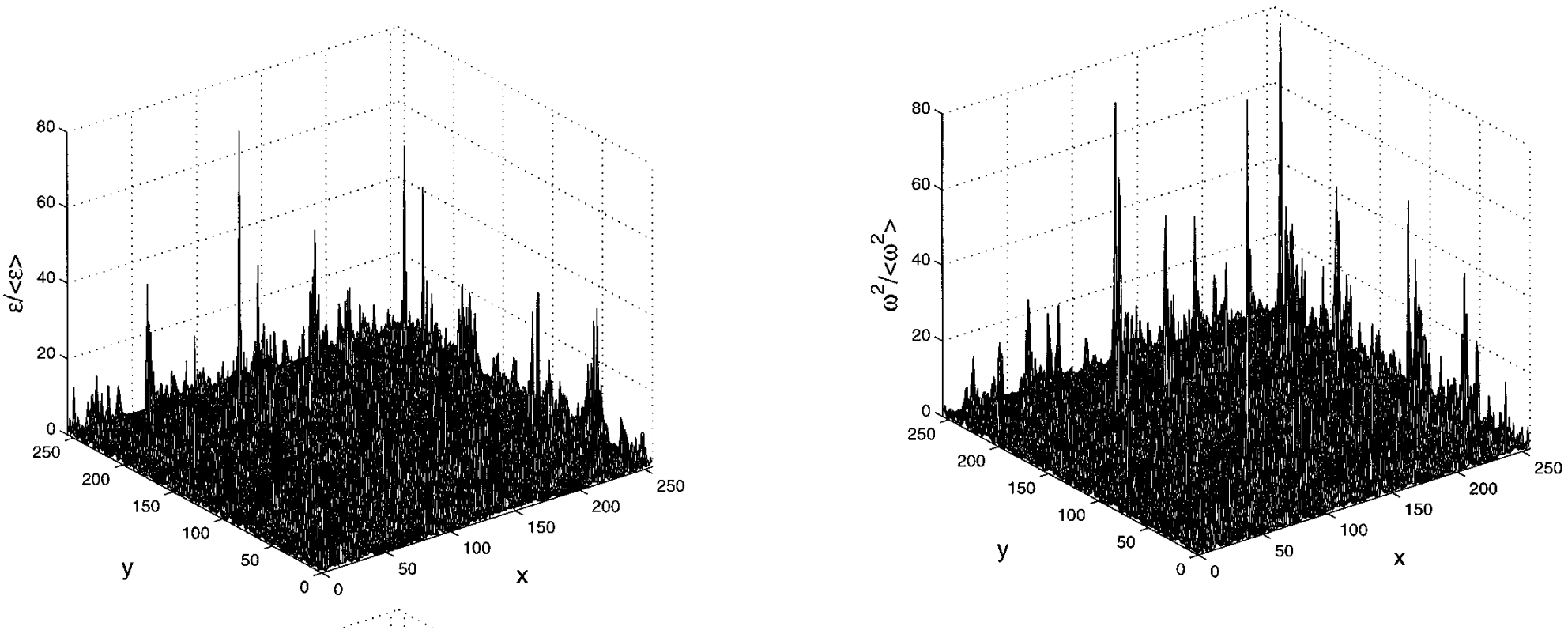
- Discrepancy between theoretical predictions and experimental results is attributed to *internal intermittency*.

- It is the tendency of turbulent flows to develop highly localized regions of intense vorticity by means of the vortex stretching mechanism, with consequent intense and localized dissipation peaks

- Statistical consequence of this phenomenon is the occurrence of rare events with high probability with exponential decay of the pdf



PDF of the difference of velocity fluctuations.
Atmosferic turbulence



Spatial distribution of vorticity dissipation in homogeneous and isotropic turbulence.
DNS, periodic box (Sreenevasan, 1999)

Turbulence: numerical simulation

These considerations justify the view that a considerable mathematical effort towards a detailed understanding of the mechanism of turbulence is called far. The entire experience with the subject indicates that the purely analytical approach is beset with difficulties, which at this moment are still prohibitive. The reason for this is probably as was indicated above: That our intuitive relationship to the subject is still too loose – not having succeeded at anything like deep mathematical penetration in any part of the subject, we are still quite disoriented as to the relevant factors, and as to the proper analytical machinery to be used.
Under these conditions there might be some hope to 'break the deadlock' by extensive, but well-planned, computational efforts. It must be admitted that the problems in question are too vast to be solved by a direct computational attack, that is, by an outright calculation of a representative family of special cases. There are, however, strong indications that we could name certain strategic points in this complex, where relevant information must be obtained by direct calculations. If this is properly done, and the operation is then repeated on the basis of broader information then becoming available, etc., there is a reasonable chance of effecting real penetrations in this complex of problems and gradually developing a useful, intuitive relationship to it. This should, in the end, make an attack with analytical methods, that is truly more mathematical, possible

J. von Neumann, 1949

Turbulence: numerical simulation — I

Numerical simulation of turbulent flows can be obtained with different approaches

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- PDF models
- RANS models, based on equations for the RST
- RANS models, based on the concept of *turbulent viscosity*

Turbulence: numerical simulation — II

For what it concerns turbulent viscosity models, here we will consider:

- Algebraic models (e.g. *mixing length* models)
- One equation models (e.g. Turbulent-kinetic-energy models)
- Two equations models (e.g. k–ε, k–ω)

Gradient diffusion hypotesis

- The mean equation for passive scalar transport can be written in conservative form as:

$$\frac{\partial \langle \phi \rangle}{\partial t} + \nabla \cdot (\langle \mathbf{V} \rangle \langle \phi \rangle) = \nabla \cdot \left(\Gamma \nabla \langle \phi \rangle - \langle \mathbf{u} \phi' \rangle \right)$$

- *Gradient diffusion* hypotesis models the unknown term $\langle \mathbf{u} \phi' \rangle$ as:

$$\langle \mathbf{u} \phi' \rangle = -\Gamma_{\mathsf{T}} \nabla \langle \phi \rangle$$

It this way the effective diffusivity is: $\Gamma_{\mathsf{eff}}(\mathbf{x}, t) = \Gamma + \Gamma_{\mathsf{T}}(\mathbf{x}, t)$

Turbulent viscosity hypotesis — I

- In the same way, *turbulent viscosity* hypotesis models the deviatoric part of the RST $-\rho\langle u_i u_j\rangle$ by assuming linear dependence from the tensor $\bar{S}_{ij}$ (Boussinesq, 1877)

$$\langle u_i u_j\rangle - \frac{2}{3}k\delta_{ij} = -2\nu_{\mathsf{T}}\left(\mathbf{x}, t\right)\bar{S}_{ij}$$

  ν_{T} is the *turbulent viscosity*.

- Boussinesq hypotesis can be expressed in a more compact way as:

$$a_{ij} = -2\nu_{\mathsf{T}}\bar{S}_{ij}$$

  in analogy with the deviatoric part of the stress tensor:

$$\tau_{ij}^{\mathsf{d}} = -2\mu S_{ij}$$

Turbulent viscosity hypotesis — II

- Effective viscosity is::

$$\nu_{\text{eff}} = \nu_{\text{T}}\left(\mathbf{x}, t\right) + \nu$$

- Mean momentum equation reads:

$$\frac{\partial \langle U_j \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle U_j \rangle}{\partial x_i} = -\frac{1}{\rho}\frac{\partial}{\partial x_j}\left(\langle p \rangle + \frac{2}{3}\rho k\right) + \frac{\partial}{\partial x_i}\left[\nu_{\text{eff}}\left(\mathbf{x}, t\right)\left(\frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\partial \langle U_j \rangle}{\partial x_i}\right)\right]$$

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Turbulent viscosity hypotesis: remarks — I

The specification of $\Gamma_{\mathsf{T}}(\mathbf{x}, t)$ and $\nu_{\mathsf{T}}(\mathbf{x}, t)$ overcomes the *closure problem* of Reynolds equations. Some remarks are however made:

- $\Gamma_{\mathsf{T}}(\mathbf{x}, t)$ and $\nu_{\mathsf{T}}(\mathbf{x}, t)$ are in general functions of space and time. Their specification requires the solution of *ad hoc* equations (differential or algebraic)

- Closure problem actually remains. We have simplified the problem in the sense that we passed from the specification of six functions (simmetric tensor $\langle u_i u_j \rangle$ components) to the specification of a single function (ν_{T}).

Turbulent viscosity hypotesis: remarks — II

- *Turbulent diffusivity* hypotesis is rigorously valid if passive scalar flux due to turbulent motion is aligned with the gradient of the mean scalar field

- In the same way, *turbulent viscosity* hypotesis is rigorously valid if principal axes of the deviatoric part of the RST are aligned with symmetric part of the mean velocity gradient

In both cases these assumption are generally incorrect and experimentally not always verified!

Turbulent viscosity hypotesis: shear flows

- For 2D parallel shear flows RST has a unique non null component, which is the term $\langle uv \rangle$. Turbulent viscosity hypotesis becomes:

$$\langle uv \rangle = -\nu_{\mathsf{T}}\left(\mathbf{x}, t\right) \frac{\partial \langle U \rangle}{\partial y}$$

- In this case Boussinesq hypotesis can be seen as a *definition* of turbulent viscosity

Mixing length — I

- By analogy with kinetic theory for ideal gases, Prandtl proposed the following expression for turbulent viscosity:

$$\mu = \frac{1}{2}\rho\bar{u}\lambda \qquad \longrightarrow \qquad \mu_{\mathsf{T}} = \frac{1}{2}\rho v_{\mathsf{m}}\ell_{\mathsf{m}}$$

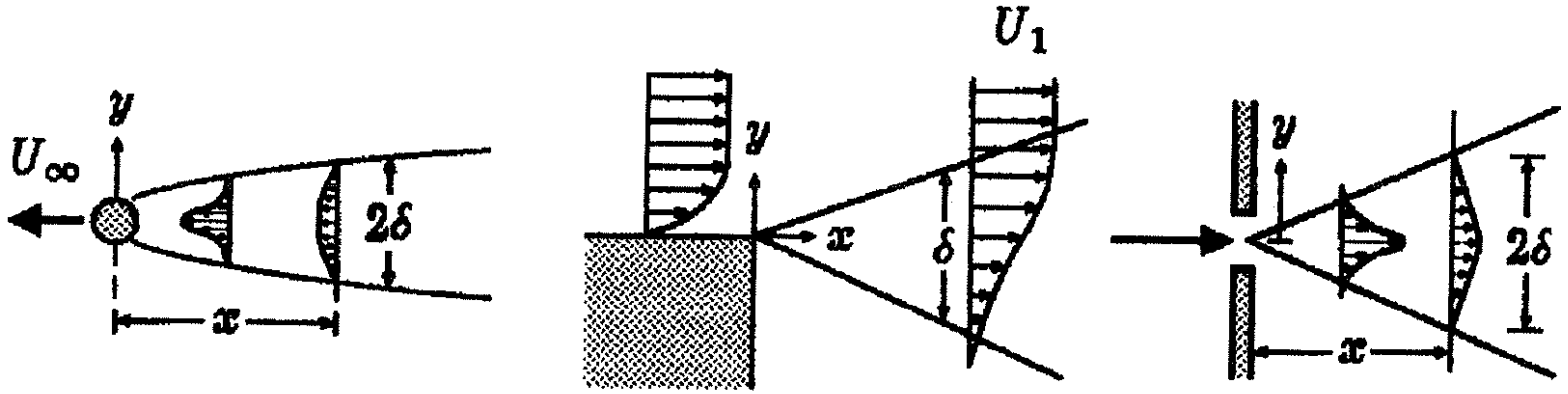
  where v_{m} and ℓ_{m} are respectively the *mixing velocity* and the *mixing length* (Prandtl, 1925)

- For the mixing velocity Prandtl made the hypotesis

$$v_{\mathsf{m}} \sim \ell_{\mathsf{m}} \left|\frac{d\langle U\rangle}{dy}\right|$$

  and hence turbulent viscosity is given by: $\nu_{\mathsf{T}} = \ell_{\mathsf{m}}^2 \left|\frac{d\langle U\rangle}{dy}\right|$

Mixing length: free shear flows — I



- For simple shear flows, mixing length is assumed as:

$$\ell_{\mathsf{m}} = \alpha\delta(x)$$

- the parameters α and $\delta(x)$ are determined *ad hoc* for each particular flow by making *similarity* considerations and by reference with *experimental data*

Mixing length: free shear flows — II

For simple cases the one has the following values (Wilcox, 1993):

- *Far wake* $\delta(x) \approx 0.805\sqrt{\frac{Dx}{\rho U_\infty^2}}$ $\alpha = 0.180$
- *Mixing layer* $\delta(x) \approx 0.247x$ $\alpha = 0.071$
- *Round jet* $\delta(x) \approx 0.233x$ $\alpha = 0.080$
- *Plane jet* $\delta(x) \approx 0.246x$ $\alpha = 0.098$

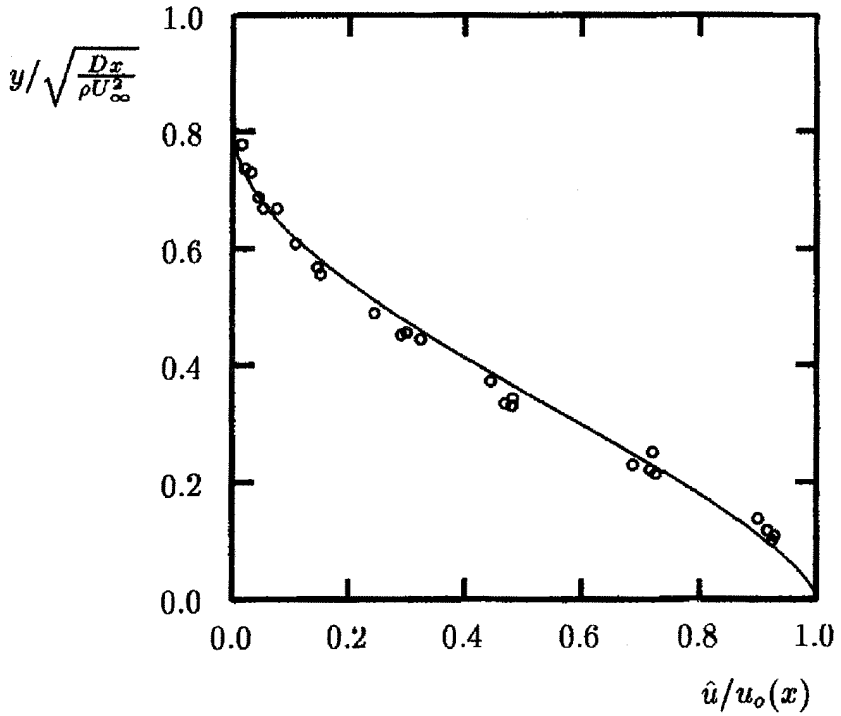


Figure 3.3: Comparison of computed and measured velocity profiles for the far wake; —— Mixing length; o Fage and Falkner.

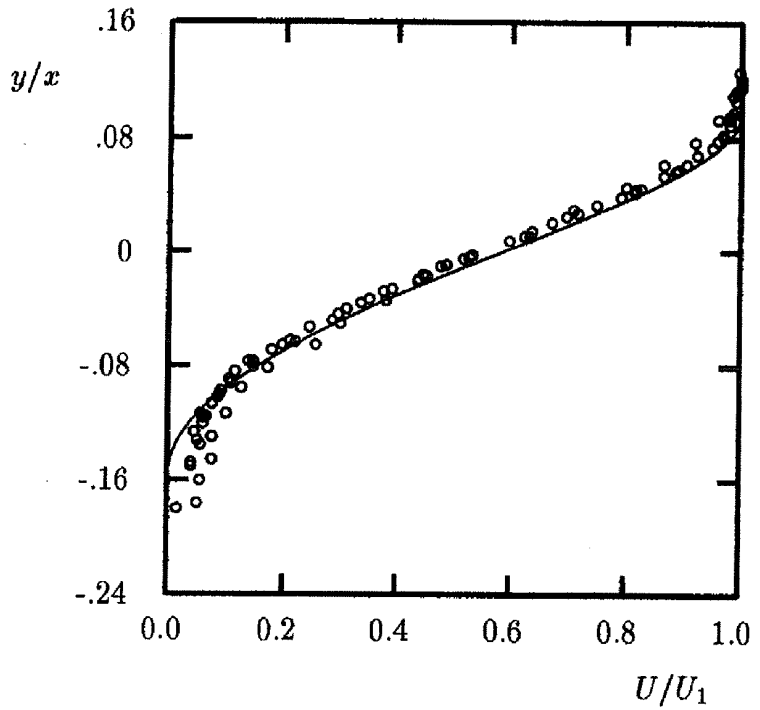


Figure 3.4: Comparison of computed and measured velocity profiles for mixing layer; —— Mixing length; o Liepmann and Laufer.

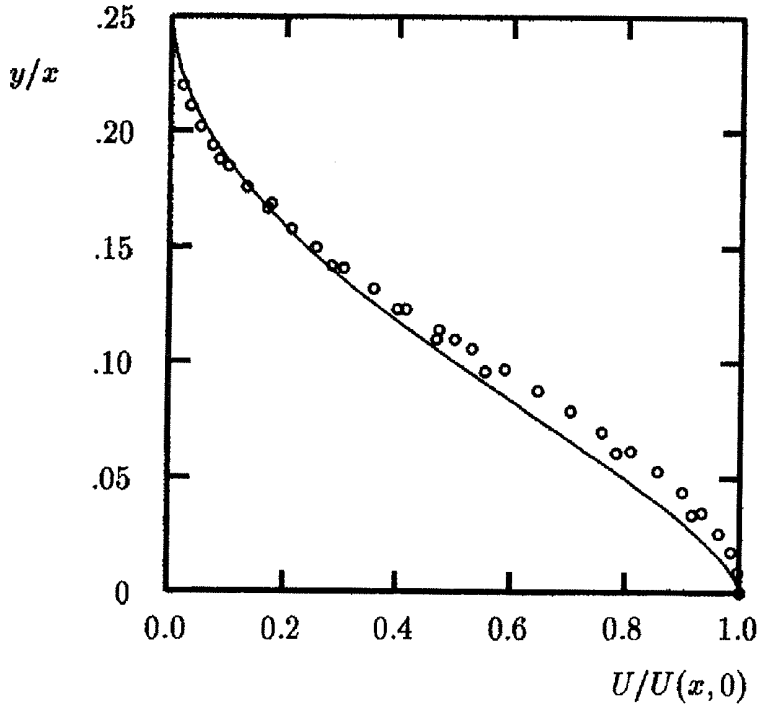


Figure 3.5: Comparison of computed and measured velocity profiles for the plane jet; —— Mixing length; o Wygnanski and Fiedler.

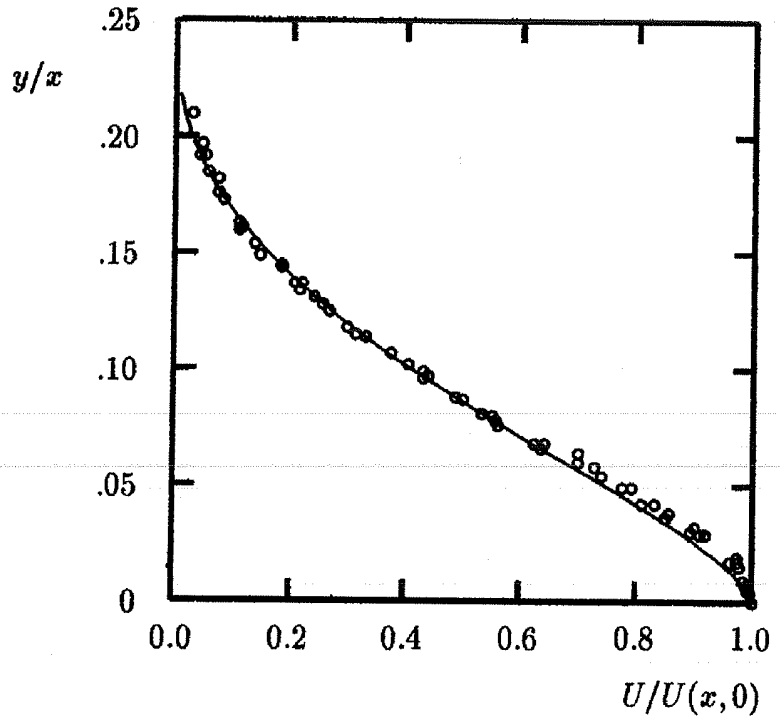


Figure 3.6: Comparison of computed and measured velocity profiles for tl round jet; —— Mixing length; o Bradbury.

Mixing length: wall bounded flows— I

- For wall bounded flows Prandtl assumption is that ℓ_{m} is linearly related to the distance from the wall:

$$\ell_{\mathsf{m}} = \kappa y$$

- This assumption is consistent with the *logaritmic law of the wall* (von Karman, 1930):

$$\langle U \rangle^{+} = \frac{1}{\kappa} \ln y^{+} + B$$

with $\kappa \approx 0.41$ (Karman constant) and $B \approx 5.0$

Mixing length: wall bounded flows— II

Mostly used variants are:

- Cebeci-Smith (1967) model
- Baldwin-Lomax (1978) model

These models incorporate the effects of the so-called *external intermittency*

One-equation models— I
Turbulent-kinetic-energy model

- *Turbulent-kinetic-energy* model is based on the specification of ν_T given by (Prandtl, 1945):

$$\nu_\mathsf{T} = ck^{1/2}\ell_\mathsf{m}$$

  based on dimensional analysis arguments

- It is obtained by assuming $ck^{1/2}$ as velocity scale for the definition of ν_T, instead of $\ell_\mathsf{m}|\partial\langle U\rangle/\partial y|$

- For the definition of the model, one needs an equation for k, and a specification for ℓ_m (incomplete model)

One-equation models— II
Turbulent-kinetic-energy model

- The balance equation for k is:

$$\frac{\bar{D}k}{\bar{D}t} + \nabla \cdot \mathbf{T} = \mathcal{P} - \varepsilon$$

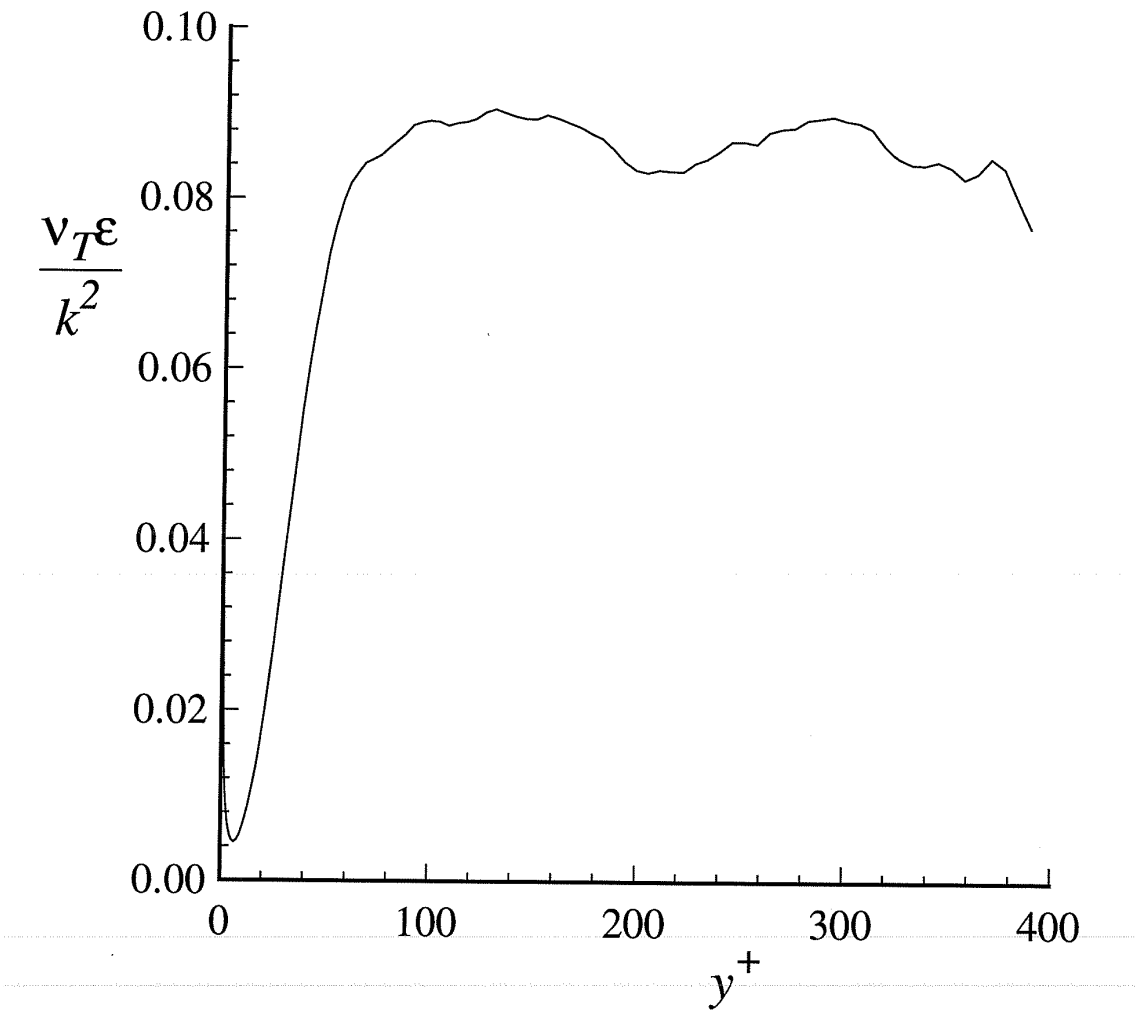
  where $\mathbf{T}$ and ε requires a specification

- A model for ε is given by employing a velocity scale derived from turbulent kinetic energy k and a length scale given by the mixing length:

$$\varepsilon = Ck^{3/2}/\ell_{\mathsf{m}}$$

- This assumption, together with the specification for ν_{T}, implicitely implies the assumption:

$$\frac{\nu_{\mathsf{T}}\varepsilon}{k^2} = cC$$



DNS, channel flow (Kim *et al.* 1987)

One-equation models— III
Turbulent-kinetic-energy model

- For $\mathbf{T}$ one assumes (gradient diffusion hypothesis):

$$\mathbf{T} = -\left(\nu + \frac{\nu_{\mathsf{T}}}{\sigma_k}\right)\nabla k$$

- The final equation for k is:

$$\frac{\bar{D}k}{\bar{D}t} = \nabla \cdot \left(\left(\nu + \frac{ck^{1/2}\ell_{\mathsf{m}}}{\sigma_k}\right)\nabla k\right) + \mathcal{P} - Ck^{3/2}/\ell_{\mathsf{m}}$$

Where the unknown (to be specified) is ℓ_{m}

Two equations models: k-ε

$k - \varepsilon$ models are based on the specification of turbulent viscosity:

$$\nu_T = C_\mu k^2/\varepsilon$$

- k is determined by the equation already seen for the Turbulent-kinetic-energy model

- ε is determined by an *ad hoc* equation

$k - \varepsilon$ model is **complete**

"standard" k-ε model

Jones e Launder (1972)

- k is determined with the exact equation, with the assumptions employed for the Turbulent-kinetic-energy model:

$$\frac{\bar{D}k}{\bar{D}t} = \underbrace{\nabla \cdot \left(\left(\nu + \frac{\nu_\mathrm{T}}{\sigma_k} \right) \nabla k \right)}_{\nabla \cdot \mathbf{T}} \underbrace{-\langle \mathbf{uu} \rangle \nabla \langle \mathbf{U} \rangle}_{\mathcal{P}} - \varepsilon$$

- ε si determined with an *empirical* equation based on physical considerations:

$$\frac{\bar{D}\varepsilon}{\bar{D}t} = \nabla \cdot \left(\left(\nu + \frac{\nu_\mathrm{T}}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \mathcal{P} \frac{\varepsilon}{k} - C_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

- Constants are given by:

$$C_\mu = 0.09, \quad C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3$$

k-ε model: conclusions

- $k - \varepsilon$ is the simplest *complete* model
- Is quite accurate for simple flows, but inaccurate for complex flows
- Sources of uncertainity are:
  1. Turbulent viscosity hypotesis
  2. The equation for ε

Two equations models: k-ω

- In principle, other two-equations model can be proposed. Hystorically, the first equation has usually been for k while different choiches are possible for the second variable.

- Since 1942 Kolmogorov proposed as a second parameter the function ω, which is defined as the dissipation per unit turbulent kinetic energy:

$$\omega = \frac{\varepsilon}{k}$$

- To the term ω various physical interpretations can be given. Each of them is at the basis of the empirical equation written for it

"standard" k-ω model

Wilcox (1988)

- Eddy viscosity is given by:

$$\nu_T = \frac{k}{\omega}$$

- Equation for k:

$$\frac{\bar{D}k}{\bar{D}t} = \nabla \cdot \left(\left(\nu + \frac{\nu_\mathsf{T}}{\sigma_k} \right) \nabla k \right) - \mathcal{P} - C_1 k\omega$$

- Equation for ω:

$$\frac{\bar{D}\omega}{\bar{D}t} = \nabla \cdot \left(\left(\nu + \frac{\nu_\mathsf{T}}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_2 \mathcal{P} \frac{\omega}{k} - C_3 \omega^2$$

- Constants are given by:

$$C_1 = 0.09, \quad C_2 = 5/9, \quad C_3 = 3/40, \quad \sigma_k = 2.0, \quad \sigma_\varepsilon = 2.0$$

k-ω model: conclusions

- Various implementations of the model are available in literature, depending on the flow to be calculated

- For boundary layer flows it is more accurate than k-ε in the treatment of viscous near wall regions

- The treatment of non turbulent free stream boundaries is problematic

Discretization of the balance equations

The three principal methodologies for the numerical discretization of balance equations are:

- Finite Differences (FD)
- Finite Element Method (FEM)
- Finite Volume Methods (FVM)

Finite Volume Methods: basic concepts — I

In the FVM technique an *integral formulation* of the balance equations is discretized directly in the physical space.

Main features of the technique are:

- It is based on cell-averaged values
- Once a grid is generated, one has to associate control volumes
- It permits a straightforward implementation of a conservative discretization
- It is easly implemented on arbitrary grids

Finite Volume Methods: basic concepts — II

Flow equations are the expression of conservation (balance) laws.

For a scalar quantity U the balance equation can be recast in the conservative form

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = Q$$

where $\mathbf{F}$ is the *flux* of U.

For example, for the passive scalar balance equation $\frac{\partial \phi}{\partial t} + \mathbf{V} \cdot \nabla \phi - \Gamma \nabla^2 \phi = 0$ the conservative form of the equation is:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{F}(\phi) = 0$$

with $\mathbf{F}(\phi) = \mathbf{V}\phi - \Gamma \nabla \phi$

Finite Volume Methods: basic concepts — III

Differential equations are derived from integral balance equation (on arbitrary volumes). Integrating in space over a subdomain D_j one obtains the integral form of the equations:

$$\frac{d}{dt}\int_{\mathcal{D}_j} U\, d\mathcal{D}_j = -\int_{\mathcal{S}_j} \mathbf{F}\cdot\mathbf{n}\, d\mathcal{S}_j + \int_{\mathcal{D}_j} Q\, d\mathcal{D}_j$$

which can be discretized by expressing volume integrals by means of the averaged values over the volume:

$$\frac{d\overline{U_j}}{dt} = -\frac{1}{\mu(\mathcal{D}_j)}\int_{\mathcal{S}_j} \mathbf{F}\cdot\mathbf{n}\, d\mathcal{S}_j + \overline{Q_j}$$

where $\overline{g} = \dfrac{1}{\mu(\mathcal{D}_j)}\int_{\mathcal{D}_j} g\, d\mathcal{D}_j$

Finite Volume Methods: basic concepts — IV

The most general integral conservation form reads:

$$\int_{\mathcal{D}_j} U \, d\mathcal{D}_j \Big|^{n+1} = \int_{\mathcal{D}_j} U \, d\mathcal{D}_j \Big|^{n} - \int_n^{n+1} \int_{\mathcal{S}_j} \mathbf{F} \cdot \mathbf{n} \, d\mathcal{S}_j \, d\tau + \int_n^{n+1} \int_{\mathcal{D}_j} Q \, d\mathcal{D}_j \, d\tau$$

which leads to the exact discretized equation

$$\overline{U_j} \Big|^{n+1} = \overline{U_j} \Big|^{n} - \frac{\Delta t}{\mu(\mathcal{D}_j)} \int_{\mathcal{S}_j} \mathbf{F}^* \cdot \mathbf{n} \, d\mathcal{S}_j + \Delta t \overline{Q_j^*}$$

where $\mathbf{F}^* = \frac{1}{\Delta t} \int_n^{n+1} \mathbf{F} \, d\tau$ is the *numerical flux*

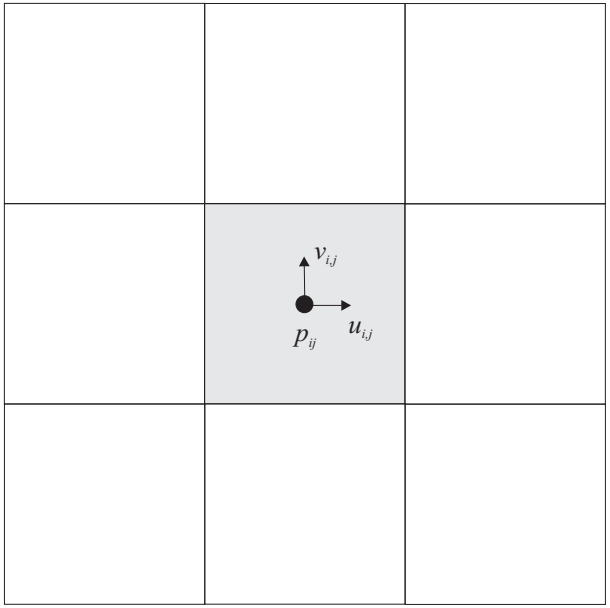
Variables arrangement on the grid

- NS equations have four scalar unknowns. In a FVM one has to generate a grid and to associate to each variable a set of Control Volumes.

- The basic distinction is between colocated and staggered arrangements.

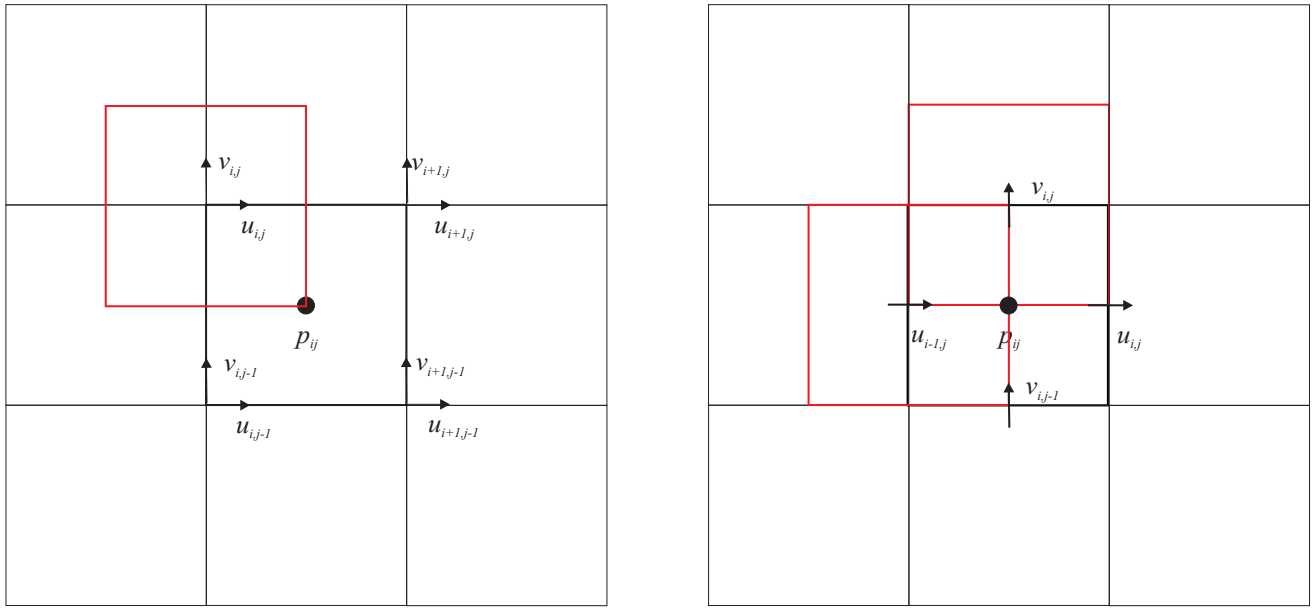
- Among staggered grids one can further choose between various configurations

Variables arrangement on the grid: Colocated arrangement



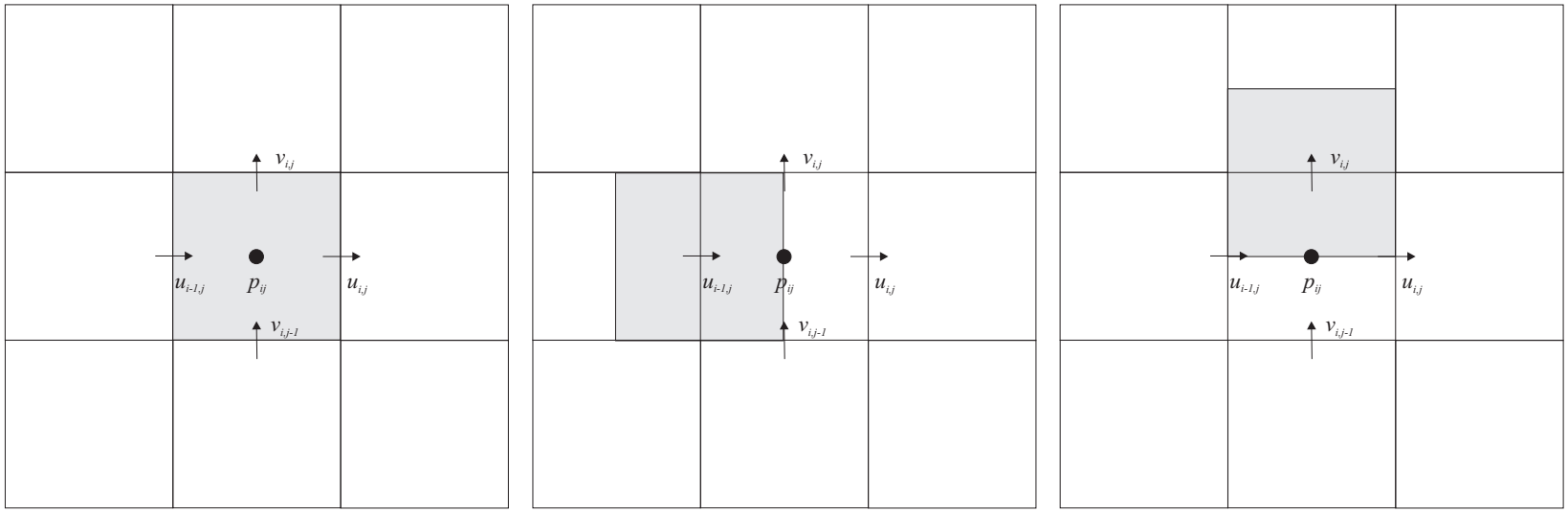
- Colocated arrangement is the obvious choiche in order to store the variables. The same CV is shared by all the variables
- Programming and storing of variables is simplified
- It was out of favour for incompressible flow calculation due to difficulties with pressure-velocity coupling

Variables arrangement on the grid: Staggered arrangement — I



- There is no need for all the variables to share the same grid
- Several terms can be calculated without interpolation
- It can improve the coupling between velocities and pressure

Variables arrangement on the grid: MAC staggered arrangements (Harlow Welch (1965))



MAC arrangement by Harlow and Welch is the most used variable arrangement. It has several advantages.

- Evaluation of mass fluxes in the continuity equation are straightforward
- Pressure and diffusion gradients can be naturally approximated without interpolation
- The biggest advantage is that it has a strong coupling between velocities and pressure

Numerical solution of NS equations: Projection methods – I

Recall the NS equations:

$$\begin{cases} \nabla \cdot \mathbf{V} = 0 \\ \\ \dfrac{\partial \mathbf{V}}{\partial t} = -\mathbf{V} \cdot \nabla \mathbf{V} - \dfrac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{V} \end{cases} \qquad (\mathbf{NS})$$

There is not an evolution equation for p and a kinematic constraint has to be enforced at each time step.
The fundamental approach is to decouple pressure field form velocity field

- An intermediate velocity field $\mathbf{V}^*$ is calculated with a tentative pressure field. The resulting field has correct curl and non correct div
- This field is corrected with a gradient field (affects only div and not curl)
- The potential field for correction is determined in such a way that continuity is enforced (it *projects* $\mathbf{V}^*$ onto the space of div-free fields)

Numerical solution of NS equations: Projection methods – II

- The equation for the intermediate field $\mathbf{V}^*$ is:

$$\mathbf{V}^* = \mathbf{V}^n + \mathbf{r}(\mathbf{V}^n)\Delta t$$

where $\mathbf{r}(\mathbf{V}) = -\nabla \cdot (\mathbf{V}\mathbf{V}) + \nu\nabla^2\mathbf{V}$

(tentative gradient pressure field is taken zero here)

- The *projection* step is made with a gradient field, which does not affect the (correct) curl

$$\mathbf{V}^{n+1} = \mathbf{V}^* - \nabla p \Delta t$$

- The requirement $\nabla \cdot \mathbf{V}^{n+1} = 0$ is satisfied by a pressure gradient satisfying:

$$\nabla^2 p = \frac{1}{\Delta t}\nabla \cdot \mathbf{V}^*$$

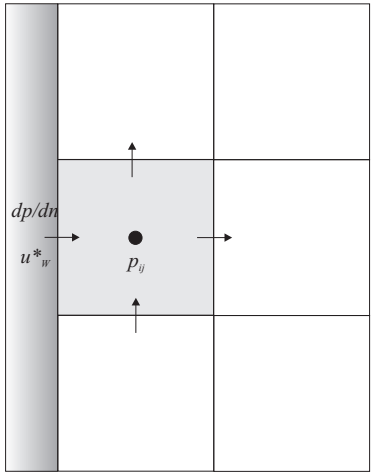
Numerical solution of NS equations: Projection methods – III

- Pressure Poisson Equation (PPE) is equipped with a Neumann BC obtained from projection of NS on the boundary normal. For impermeable walls one has:

$$\frac{\partial p}{\partial n} = \frac{1}{\Delta t}\mathbf{V}^* \cdot \mathbf{n}$$

- The upgrade of $\mathbf{V}^*$ has been computed on internal points. There is an indetermination in the value of $\mathbf{V}^* \cdot \mathbf{n}$. The same indetermination arise in the evaluation of the RHS of PPE near the boundary.

- The two indeterminations cancel in the implementation. Any value for $\partial p/\partial n$ can be given if the source term in the PPE is suitably modified near the boundary



Numerical solution of NS equations: stability requirements

Explicit stability constraints

- From linear diffusion equation a stability constraint for explicit calculations for 2D centered diffusion:

$$\frac{\nu \Delta t}{h^2} \leq \frac{1}{4}$$

  h is the smallest grid spacing

- From linear advection equation a *necessary* condition for stability of explicit discretizations is the CFL condition (Courant, Friedrichs, Lewy, 1928):

$$\frac{u_{max} \Delta t}{h} \leq p$$

  where the stencil extends p nodes to the left of the collocation node ($u \geq 0$)

Numerical solution of NS equations: Implicit methods – I

- When implicit integration is needed, a different procedure for the determination of $\mathbf{V}^{n+1}$ and $\mathbf{P}^{n+1}$ has to be implemented, since the RHS of Poisson equation depends non linearly on $\mathbf{V}^{n+1}$

- An implicit discretization of NS equations can be symbolically written in the form:

$$\begin{aligned} \mathcal{A}\left(\mathbf{V}^{n+1}\right)\mathbf{V}^{n+1} + \mathcal{G}\mathbf{p}^{n+1} &= \mathbf{q} \\ \mathcal{D}\mathbf{V}^{n+1} &= 0 \end{aligned}$$

  where $\mathcal{A}$ is a representation of a suitable discretization of non stationary and convection diffusion operators, while $\mathcal{G}$ and $\mathcal{D}$ are discretizations of gradient and divergence operator respectively

Numerical solution of NS equations: Implicit methods – II

The classical SIMPLE (Semi Implicit Method for Pressure Linked Equations) method proceeds as follows:

1. Linearize around velocity field $\mathbf{V}^n$

$$\mathcal{A}(\mathbf{V}^n)\,\mathbf{V}^{n+1} + \mathcal{G}\mathbf{p}^{n+1} = \mathbf{q}$$

2. Compute a tentative velocity field $\mathbf{V}^*$ corresponding to a tentative pressure field $\mathbf{p}^*$ (solve a linear system)

$$\mathcal{A}(\mathbf{V}^n)\,\mathbf{V}^* + \mathcal{G}\mathbf{p}^* = \mathbf{q}$$

3. Defined $\delta\mathbf{p} = \mathbf{p}^{n+1} - \mathbf{p}^*$ and $\delta\mathbf{V} = \mathbf{V}^{n+1} - \mathbf{V}^*$ momentum equation furnishes the link between $\delta\mathbf{p}$ and $\delta\mathbf{V}$:

$$\mathcal{A}(\mathbf{V}^n)\,\delta\mathbf{V} + \mathcal{G}\delta\mathbf{p} = 0$$

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Numerical solution of NS equations: Implicit methods – III

4. Substitute this relation with the approximate relation (Patankar, Spalding)

$$\Sigma\delta\mathbf{V} + \mathcal{G}\delta\mathbf{p} = 0 \tag{1}$$

(with $\Sigma = \text{diag}\mathcal{A}$) which is easily inverted: $\delta\mathbf{V} = -\Sigma^{-1}\mathcal{G}\delta\mathbf{p}$

5. Pressure correction is obtained by employing continuity:

$$\mathcal{D}\mathbf{V}^{n+1} = \mathcal{D}\mathbf{V}^{*} + \mathcal{D}\delta\mathbf{V} = 0$$

and hence:

$$\mathcal{D}\left(\Sigma^{-1}\mathcal{G}\delta\mathbf{p}\right) = \mathcal{D}\mathbf{V}^{*}$$

6. Since equation (2) is not exact, pressure and velocity corrections are not exact. An internal iteration is needed re-starting from step 3.

Numerical solution of NS equations: Implicit methods – III

4. Substitute this relation with the approximate relation (Patankar, Spalding)

$$\Sigma\delta\mathbf{V} + \mathcal{G}\delta\mathbf{p} = 0 \tag{2}$$

   (with $\Sigma = \mathrm{diag}\mathcal{A}$) which is easily inverted: $\delta\mathbf{V} = -\Sigma^{-1}\mathcal{G}\delta\mathbf{p}$

5. Pressure correction is obtained by employing continuity:

$$\mathcal{D}\mathbf{V}^{n+1} = \mathcal{D}\mathbf{V}^{*} + \mathcal{D}\delta\mathbf{V} = 0$$

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