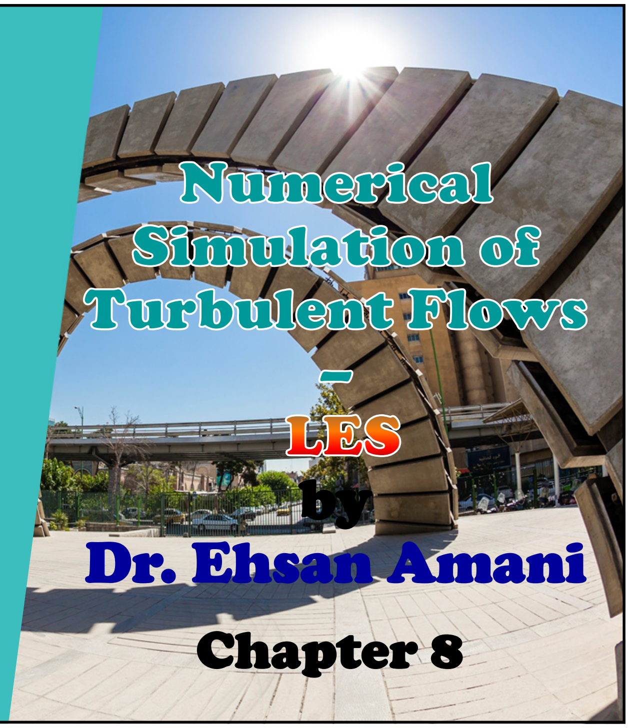


Numerical Simulation of Turbulent Flows – LES

by

Dr. Ehsan Amani

Chapter 8

VIII.1 The statistical description

The random nature of turbulence

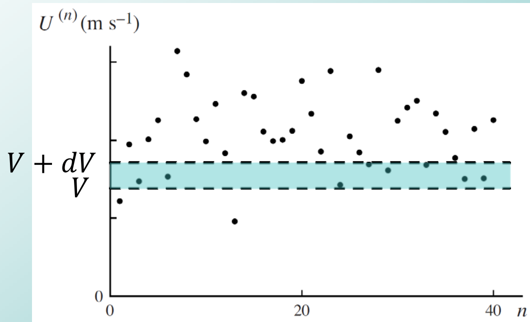
- Consistent with deterministic Navier-Stokes (NS) equations?
- Turbulent flow: Chaotic behavior of NS + perturbations in the state
- Random nature of turbulence: Every flow property $U(\vec{x}_0, t_0)$ can be regarded as a random variable.

Chap 8 By E. Amani

VIII.1 The statistical description

Random variables

- Consider a random variable U, e.g. $U = U_1(\vec{x}_0, t_0)$:



- The Probability Density Function (PDF) of U is defined as:

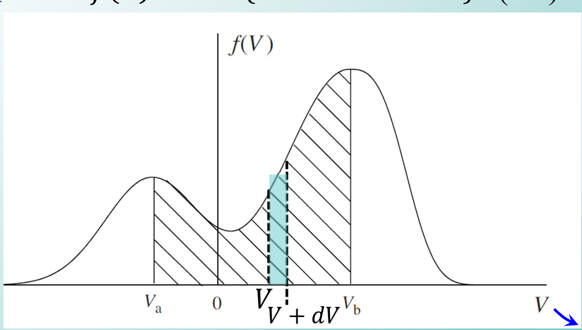
$$f(V)dV \equiv \underset{\text{Probability}}{P}\underbrace{\{V < U < V + dV\}}_{\text{event}} \qquad (8.1)$$

Chap 8 By E. Amani

VIII.1 The statistical description

Random variables

- PDF $\quad f(V)dV \equiv P\{V < U < V + dV\} \quad (8.1)$



Sample space, i.e., the probable values of U

- Therefore;

$$P\{V_a < U < V_b\} = \int_{V_a}^{V_b} f(V)dV \qquad (8.2)$$

$$\int_{-\infty}^{+\infty} f(V)dV = 1 \qquad (8.3) \text{ (Normalization condition)}$$

Chap 8 By E. Amani

VIII.1 The statistical description

Random variables

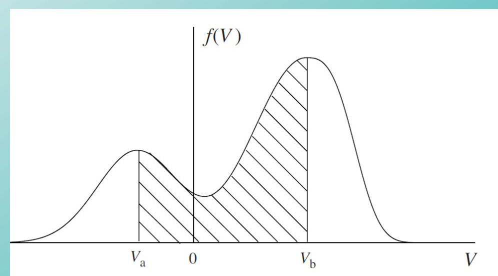
- The Cumulative Distribution Function (CFD):

$$F(V) = \int_{-\infty}^{V} f(V')dV' = P\{U < V\} \qquad (8.2)'$$

- Therefore,

$$f(V) = \frac{dF(V)}{dV} \qquad (8.2)''$$

$$P\{V_a < U < V_b\} = \int_{V_a}^{V_b} f(V)dV = \int_{0}^{V_b} f(V)dV - \int_{0}^{V_a} f(V)dV = F(V_b) - F(V_a) \qquad (8.2)'''$$



Chap 8 By E. Amani

VIII.1 The statistical description

Random variables

- PDF
  - contains a large amount of information: all one-point statistics (mean and moments)
- The mean (or expectation) of the random variable U:

$$\mu = \langle U \rangle = \int_{-\infty}^{+\infty} V \underbrace{f(V)dV}_{\text{Probability of } U \text{ being in } V < U < V + dV} \qquad (8.4)$$

  - Simple example:

$$\langle U \rangle = \frac{3+5+5+6}{4} = \frac{1}{4}\times 3 + \frac{2}{4}\times 5 + \frac{1}{4}\times 6 = \sum_i \overbrace{P(V_i)}^{f(V_i)dV_i;\ i\to\infty} V_i$$

Chap 8 By E. Amani

VIII.1 The statistical description

Random variables

- Corollary: If $Q = Q(U)$

$$\langle Q(U)\rangle = \int_{-\infty}^{+\infty} Q(V) f(V) dV \qquad (8.4)'$$

- The fluctuation of the random variable U is defined by:

$$u = U - \langle U\rangle \qquad (8.5)$$

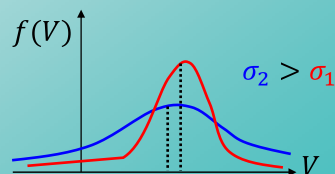
- The one-point statistics of the random variable U:

variance

$$\mu_2 = \sigma^2 = \int (V - \langle U\rangle)^2 f(V) dV = \langle (V - \langle U\rangle)^2\rangle = \langle u^2\rangle \qquad (8.6)$$

Standard deviation or Root-Mean-Square (RMS)

$$\sigma = u' = \langle u^2\rangle^{1/2} \quad (8.7)$$



VIII.1 The statistical description

Random variables

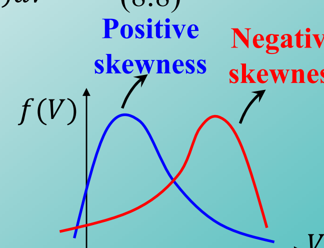
- The one-point statistics of the random variable U:

$\mathrm{n^{th}}$ central moment

$$\mu_n = \langle u^n\rangle = \int (V - \langle U\rangle)^n f(V) dV \qquad (8.8)$$

$\mathrm{n^{th}}$ standardized moment

$$\hat{\mu}_n \equiv \frac{\mu_n}{\sigma^n}; n \geq 3 \qquad (8.9)$$



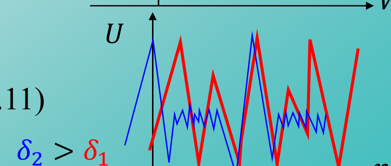
  - Examples:

skewness

$$\hat{\mu}_3 = S = \frac{\mu_3}{\sigma^3} = \frac{\langle u^3\rangle}{\langle u^2\rangle^{3/2}} \qquad (8.10)$$

flatness or kurtosis

$$\hat{\mu}_4 = \delta = \frac{\mu_4}{\sigma^4} = \frac{\langle u^4\rangle}{\langle u^2\rangle^2} \qquad (8.11)$$

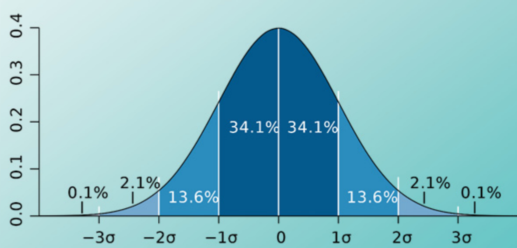


VIII.1 The statistical description

Random variables

- Analytical PDFs
  - Gaussian (or Normal) PDF

$$f(V) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(V-\mu)^2}{2\sigma^2}\right) \qquad (8.12)$$



  - Exercise: For the Gaussian PDF, $S = 0$ and $\delta = 3$.

Chap 8 By E. Amani

VIII.1 The statistical description

Joint random variables

- Joint statistical properties, e.g. $\langle uv \rangle$
- Consider two random variables U_1 and U_2, e.g. $U_1 = U_1(\vec{x}_0, t_0)$ and $U_2 = U_2(\vec{x}_0, t_0)$, the joint PDF of U_1 and U_2 is defined:

$$f_{12}(V_1, V_2)dV_1 dV_2 \equiv P\{V_1 < U_1 < V_1 + dV_1, V_2 < U_2 < V_2 + dV_2\} \qquad (8.13)$$

- The normalization condition:

$$\iint f_{12}(V_1, V_2)dV_1 dV_2 = 1 \qquad (8.14)$$

- The relation with PDF of U_1 (marginal PDF):

$$\int f_{12}(V_1, V_2)dV_2 = P\{V_1 < U_1 < V_1 + dV_1, \overbrace{-\infty < U_2 < +\infty}^{\text{sure event}}\}/dV_1$$
$$= P\{V_1 < U_1 < V_1 + dV_1\}/dV_1 = f_1(V_1) \qquad (8.15)$$

Chap 8 By E. Amani

VIII.1 The statistical description

Joint random variables

- $f_1(V_1)$ is only a part of information contained in $f_{12}(V_1, V_2)$
- The one-point joint statistics of $U_1$and U_2:

$$\langle Q(U_1, U_2)\rangle = \int\int Q(V_1, V_2) f_{12}(V_1, V_2) dV_1 dV_2 \quad (8.16)$$

$$\text{cov}(U_1, U_2) = \langle u_1 u_2 \rangle = \int\int (V_1 - \langle U_1\rangle)(V_2 - \langle U_2\rangle) f_{12}(V_1, V_2) dV_1 dV_2 \quad (8.18)$$

covariance

$$CC(U_1, U_2) = \frac{\langle u_1 u_2\rangle}{(\langle u_1^2\rangle\langle u_2^2\rangle)^{1/2}} \quad (8.18)'$$

Correlation coefficient

- Exercise: Show that for $Q(U_1, U_2) = Q(U_1)$, Eq. (8.16) is simplified to Eq. (8.4)'.
- Exercise: Show that (Cauchy-Schwarz inequality):

$$|\langle u_1 u_2\rangle| \le \left(\langle u_1^2\rangle\langle u_2^2\rangle\right)^{1/2} \quad (8.19)$$

$$-1 \le CC \le 1$$

Chap 8 By E. Amani

VIII.1 The statistical description

Joint random variables

- Joint CDF:

$$F_{12}(V_1, V_2) = \int_{-\infty}^{V_2}\int_{-\infty}^{V_1} f_{12}(V_1', V_2') dV_1' dV_2' = P\{U_1 < V_1, U_2 < V_2\} \quad (8.15)'$$

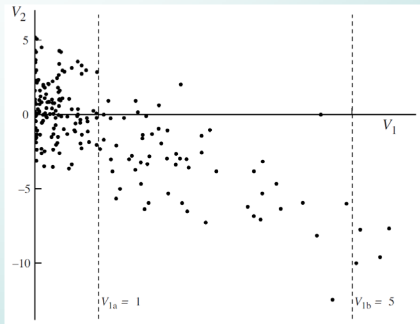
$$f_{12}(V_1, V_2) = \frac{\partial^2}{\partial V_1 \partial V_2} F_{12}(V_1, V_2) \quad (8.15)''$$

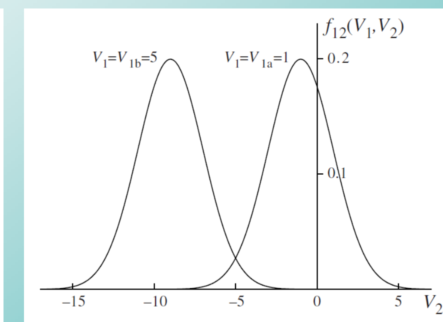
Chap 8 By E. Amani

VIII.1 The statistical description

Joint random variables

- Conditional PDF:





$$f_{2|1}(V_2|V_1)dV_2 \equiv P\{V_2 < U_2 < V_2 + dV_2 | U_1 = V_1\}$$

$$= \frac{P\{V_1 < U_1 < V_1 + dV_1, V_2 < U_2 < V_2 + dV_2\}}{P\{V_1 < U_1 < V_1 + dV_1\}} = \frac{f_{12}(V_1,V_2)dV_1 dV_2}{f_1(V_1)dV_1}$$

$$= \frac{f_{12}(V_1,V_2)}{f_1(V_1)} dV_2$$

VIII.1 The statistical description

Joint random variables

- Conditional PDF:

$$f_{2|1}(V_2|V_1) = \frac{f_{12}(V_1,V_2)}{f_1(V_1)} \qquad (8.20)$$

- Exercise: Show that

$$\int_{-\infty}^{+\infty} f_{2|1}(V_2|V_1)dV_2 = 1 \qquad (8.21)$$

- Conditional mean:

$$\langle Q(U_1,U_2)|U_1 = V_1\rangle = \langle Q(U_1,U_2)|V_1\rangle \equiv \int Q(V_1,V_2) f_{2|1}(V_2|V_1)dV_2 \quad (8.22)$$

- Exercise: Show that

$$\langle Q(U_1)|U_1 = V_1\rangle = Q(V_1) \qquad (8.23)$$

$$\langle Q(U_1,U_2)\rangle = \int \langle Q(U_1,U_2)|V_1\rangle f_1(V_1)dV_1 \qquad (8.24)$$

VIII.1 The statistical description

Joint random variables

- Independent random variables:

$$f_{2|1}(V_2|V_1) = f_2(V_2) \qquad (8.25)$$

- Exercise: Show that for independent random variables

$$f_{12}(V_1, V_2) = f_1(V_1)f_2(V_2) \qquad (8.26)$$

- If $\langle u_1 u_2 \rangle = 0$, U_1 and U_2 are said to be uncorrelated.
- Exercise: Independence vs. zero-correlation: Which property is followed given the other?

Chap 8 By E. Amani

VIII.1 The statistical description

Random processes and random fields

- Extensions:

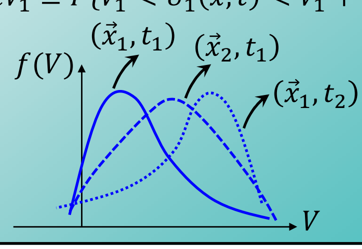
Random variable ← $U_1 = U_1(\vec{x}_0, t_0)$

→ $U_1(t) = U_1(\vec{x}_0, t)$ → Random process

→ $U_1(\vec{x}, t) = U_1(\vec{x}, t)$ → Random field

- All definitions can be extended straightforwardly, e.g.

$$f_1(V_1; \vec{x}, t)dV_1 \equiv P\{V_1 < U_1(\vec{x}, t) < V_1 + dV_1\} \qquad (8.27)$$



Chap 8 By E. Amani

VIII.1 The statistical description

Random processes and random fields

- Example of one-point statistics:

$$U_1 = U_1(\vec{x},t) \quad \Big\} \quad \langle u_1(\vec{x},t)u_1(\vec{x},t)\rangle \rightarrow \textbf{variance}$$

- Example of one-point joint statistics:

$$\left.\begin{matrix} U_1 = U_1(\vec{x},t) \\ U_2 = U_2(\vec{x},t) \end{matrix}\right\} \quad \langle u_1(\vec{x},t)u_2(\vec{x},t)\rangle \rightarrow \textbf{covariance}$$

- Example of two-point or two-time joint statistics:

$$\left.\begin{matrix} U_1 = U_i(\vec{x},t) \\ U_2 = U_j(\vec{x}+\vec{r},t) \end{matrix}\right\} \quad \langle u_i(\vec{x},t)u_j(\vec{x}+\vec{r},t)\rangle \rightarrow \textbf{(spatial) autocovariance}$$

$$\left.\begin{matrix} U_1 = U_i(\vec{x},t) \\ U_2 = U_j(\vec{x},t+s) \end{matrix}\right\} \quad \langle u_i(\vec{x},t)u_j(\vec{x},t+s)\rangle \rightarrow \textbf{(temporal) autocovariance}$$

VIII.2 PDF methods

Joint PDF of velocity

- State (or internal) space: 3 components of the fluid velocity field

$$U_i(\vec{x},t) \quad \Big\} \xrightarrow{\textbf{Joint PDF}} f(\vec{V};\vec{x},t) \qquad \vec{V} = \{V_1, V_2, V_3\}$$

$f(\vec{V};\vec{x},t) \rightarrow$ **Eulerian PDF of velocity**

- One-point velocity statistics:

$$\langle U_i(\vec{x},t)\rangle = \int V_i f(\vec{V};\vec{x},t)d\vec{V} \qquad \int(\ \ )d\vec{V} \rightarrow \iiint(\ \ )dV_1dV_2dV_3$$

$$\langle u_i u_j\rangle = \iiint (V_i - \langle U_i\rangle)(V_j - \langle U_j\rangle) f(\vec{V};\vec{x},t)d\vec{V}$$

...

VIII.2 PDF methods

PDF transport equation

- See appendix H of reference [1] for the details of derivation.
- Mathematics:

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} = -\frac{\partial}{\partial V_i}\left[f \left\langle \frac{\mathrm{D}U_i}{\mathrm{D}t} \middle| \boldsymbol{V} \right\rangle \right] \qquad (8.28)$$

- Expressing the material derivative of the sate variables Using Navier-Stokes equations:

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} = \frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i}\frac{\partial f}{\partial V_i} - \frac{\partial}{\partial V_i}\left[f \left\langle \nu \nabla^2 U_i - \frac{1}{\rho}\frac{\partial p'}{\partial x_i} \middle| \boldsymbol{V} \right\rangle \right] \qquad (8.29)$$

- or

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} = \nu \nabla^2 f + \frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i}\frac{\partial f}{\partial V_i} + \frac{\partial^2}{\partial x_i \partial V_i}\left(f \left\langle \frac{p'}{\rho} \middle| \boldsymbol{V} \right\rangle \right) + \frac{1}{2}\frac{\partial^2}{\partial V_i \partial V_j}\left[f \left\langle \frac{p'}{\rho}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - 2\nu \frac{\partial U_i}{\partial x_k}\frac{\partial U_j}{\partial x_k} \middle| \boldsymbol{V} \right\rangle \right]. \qquad (8.30)$$

Chap 8 By E. Amani

VIII.2 PDF methods

PDF transport equation

- Closure problem: The conditional means including the two-point velocity gradients or pressure fluctuation

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} = \frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i}\frac{\partial f}{\partial V_i} - \frac{\partial}{\partial V_i}\left[f \boxed{\left\langle \nu \nabla^2 U_i - \frac{1}{\rho}\frac{\partial p'}{\partial x_i} \middle| \boldsymbol{V} \right\rangle} \right] \qquad (8.29)$$

$$\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} = \nu \nabla^2 f + \frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_i}\frac{\partial f}{\partial V_i} + \frac{\partial^2}{\partial x_i \partial V_i}\left(f \boxed{\left\langle \frac{p'}{\rho} \middle| \boldsymbol{V} \right\rangle} \right) + \frac{1}{2}\frac{\partial^2}{\partial V_i \partial V_j}\left[f \boxed{\left\langle \frac{p'}{\rho}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - 2\nu \frac{\partial U_i}{\partial x_k}\frac{\partial U_j}{\partial x_k} \middle| \boldsymbol{V} \right\rangle} \right]. \qquad (8.30)$$

- Note the dimension of the equation: 4+3=7
- Modeling?
- Numerical solution? Monte Carlo (MC) method

Chap 8 By E. Amani

VIII.3 PDF modeling

Lagrangian point of view

- Lagrangian PDF

$$\left.\begin{array}{r}\vec{V}^{+}(t,\vec{Y})\\ \vec{X}^{+}(t,\vec{Y})\\ \vec{Y}=\vec{X}_0\end{array}\right\} \xrightarrow[\text{conditioned on } \vec{Y}]{\text{Joint PDF of } \vec{X}^{+} \text{ and } \vec{V}^{+}} f_L(\vec{V},\vec{x};t|\vec{Y})$$

Lagrangian PDF of fluid particle velocity

- Relation between f_L and f [1]:

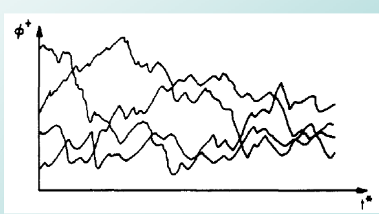
$$\int f_{\mathrm{L}}(\boldsymbol{V},\boldsymbol{x};t|\boldsymbol{Y})\,\mathrm{d}\boldsymbol{Y} = f(\boldsymbol{V};\boldsymbol{x},t). \qquad (8.31)$$

Chap 8 **By E. Amani**

VIII.3 PDF modeling

Lagrangian point of view

- Stochastic Processes (SPs) and Stochastic Differential Equations (SDEs) are suitable candidates for modeling Lagrangian fluid particle properties ($\phi^{+}(t,\vec{Y})$) .
- Fluid particle ($\phi^{+}(t,\vec{Y})$) vs. stochastic particle ($\phi^{*}(t,\vec{Y})$):



- For PDF methods, the consistency is assured at the level of PDF

Chap 8 **By E. Amani**

VIII.4 Stochastic processes and calculus

The need to extend the ordinary calculus

- SDE vs. ODE and SP vs. deterministic function:

$$\mathrm{d}U(t) = a[U(t),t]\,\mathrm{d}t + b[U(t),t]\,\mathrm{d}W(t),$$

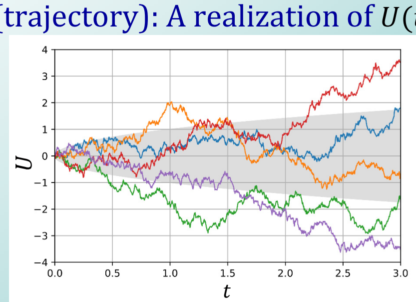
- If $b \neq 0$, the above equation is a SDE and the solution, $U(t)$, is a SP.
- The second term requires special treatment with the knowledge of stochastic calculus

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Properties of SPs

- Sample path (trajectory): A realization of $U(t)$ vs. t



- N-point PDFs
- Increment:

Positive time interval

$$\Delta_h U(t) \equiv U(t+h) - U(t). \qquad (8.32)$$

- Infinitesimal parameters:

$$B_n(V,t) \equiv \lim_{h\downarrow 0} \frac{1}{h}\langle[\Delta_h U(t)]^n\,|U(t)=V\rangle, \qquad (8.33)$$

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Classification of SPs

- Markov vs. non-Markov process:
  - N-point conditional PDF satisfies:

$$f_{N-1}(V_N;t_N|V_{N-1},t_{N-1},V_{N-2},t_{N-2},\ldots,V_1,t_1) = f_1(V_N;t_N|V_{N-1},t_{N-1}). \quad (8.34)$$

  - Interpretation: The present is enough to predict the future (the information of the past is included in the present)
- Continuous-time vs. discrete-time processes.

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- A branch of continuous-time Markov processes
- Properties:
  - Continuous trajectory

$$\lim_{h\downarrow 0}\frac{1}{h}P\{|\Delta_h U(t)| > \epsilon | U(t)=V\} = 0. \quad (8.35)$$

  - The drift coefficient exists:

$$a(V,t) \equiv B_1(V,t), \quad (8.36)$$

  - The diffusion coefficient exists:

$$b(V,t)^2 \equiv B_2(V,t), \quad (8.37)$$

$$\langle [\Delta_h U(t)]^2 / h \rangle$$

$$\langle [\Delta_h U(t)/h]^2 \rangle \to \infty$$

Not differentiable anywhere

  - Other infinitesimal parameters are:

$$B_n(V,t) = 0, \quad \text{for } n \geq 3. \quad (8.38)$$

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- It can be shown that
  - The diffusion SP is the solution of the following SDE called the generalized Langevin equation:

$$\mathrm{d}U(t) = a[U(t),t]\,\mathrm{d}t + b[U(t),t]\,\mathrm{d}W(t), \qquad (8.39)$$

The Wiener SP: The elementary diffusion SP

  - The conditional PDF evolves with the Fokker-Planck or forward Kolmogorov equation

$$\frac{\partial}{\partial t} f_1(V;t|V_1,t_1) = -\frac{\partial}{\partial V}[a(V,t) f_1(V;t|V_1,t_1)] + \frac{1}{2}\frac{\partial^2}{\partial V^2}[b(V,t)^2 f_1(V;t|V_1,t_1)]. \qquad (8.40)$$

  - The marginal PDF evolves with:

$$\frac{\partial}{\partial t} f(V;t) = -\frac{\partial}{\partial V}[a(V,t) f(V;t)] + \frac{1}{2}\frac{\partial^2}{\partial V^2}[b(V,t)^2 f(V;t)]. \qquad (8.41)$$

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- It can be shown that

$$\frac{\partial}{\partial t} f(V;t) = -\frac{\partial}{\partial V}[a(V,t) f(V;t)] + \frac{1}{2}\frac{\partial^2}{\partial V^2}[b(V,t)^2 f(V;t)]. \qquad (8.41)$$

  - The diffusion term interpretation:

$$\frac{\partial f}{\partial t} = \frac{\partial^2}{\partial v^2}(Df)$$

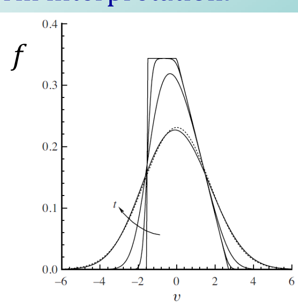


Fig. 12.1. The effect of diffusion on the shape of the PDF: the solutions to Eq. (12.29) for $\mathcal{D}t = 0$, 0.02, 0.2, and 1. The dashed line is the Gaussian with the same mean (0) and variance (3) as those of the PDF at $\mathcal{D}t = 1$.

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- It can be shown that

$$\frac{\partial}{\partial t}f(V;t) = -\frac{\partial}{\partial V}[a(V,t)f(V;t)] + \frac{1}{2}\frac{\partial^2}{\partial V^2}[b(V,t)^2 f(V;t)]. \quad (8.41)$$

  - The drift term interpretation:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial v}\left(\frac{v}{T_L}f\right)$$

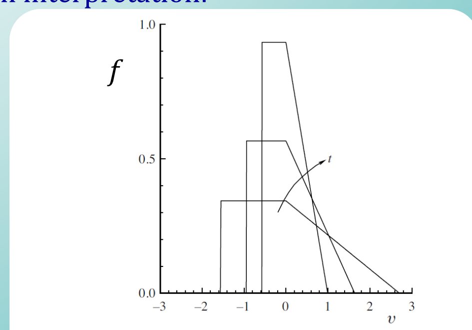


Fig. 12.2. Solutions (Eq. (12.34)) to Eq. (12.32) for $t/T_L = 0, \frac{1}{2}, 1$.

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- It can be shown that
  - The moments evolve with:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle U(t)\rangle = \langle a[U(t),t]\rangle. \quad (8.42)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle U(t)^2\rangle = 2\langle U(t)a[U(t),t]\rangle + \langle b[U(t),t]^2\rangle. \quad (8.43)$$

Chap 8 By E. Amani

VIII.4 Stochastic processes and calculus

Diffusion process

- The Wiener process
  - The simplest diffusion process:

$$a(V,t) = 0, \quad b(V,t)^2 = 1. \qquad (8.44)$$

  - Some important properties:

$$f_1(V;t|V_1,t_1) = \frac{1}{\sqrt{2\pi(t-t_1)}} \exp\left(-\frac{\frac{1}{2}(V-V_1)^2}{t-t_1}\right), \qquad (8.45)$$

$$\Delta_h W(t) \stackrel{\mathrm{D}}{=} \mathcal{N}(0,h). \qquad (8.46)$$

$$\begin{aligned} &\text{(i)} \ \langle W(t_2) - W(t_1) \rangle = 0, \\ &\text{(ii)} \ \langle [W(t_2) - W(t_1)]^2 \rangle = \operatorname{var}[W(t_2) - W(t_1)] = t_2 - t_1, \\ &\text{(iii)} \ W(t_2) - W(t_1) \stackrel{\mathrm{D}}{=} \mathcal{N}(0, t_2 - t_1), \end{aligned} \qquad (8.47)$$

…

VIII.4 Stochastic processes and calculus

Stochastic calculus

- Stochastic integral

$$dU(t) = a[t,U(t)]dt + b[t,U(t)]dW(t) \qquad (8.48)$$

$$U(t) - U(t_0) = \int_{t_0}^{t} a[t,U(t)]dt + \int_{t_0}^{t} b[t,U(t)]dW(t) \qquad (8.49)$$

?

$$I = \int_{t_0}^{t} b[t,U(t)]dW(t) \qquad (8.50)$$

- Ordinary calculus: Riemann-Stieltjes definition

$$I = \lim_{N\to\infty} I_N = \lim_{N\to\infty} \sum_{i=1}^{N} b[\tau_i, U(\tau_i)][W(t_{i+1}) - W(t_i)]\,;\tau_i \in [t_i, t_{i+1}] \qquad (8.51)$$

Converges but depends on the choice of τ_i in $[t_i, t_{i+1}]$

- Different choices are possible, the most commonly used one is called Ito calculus

VIII.4 Stochastic processes and calculus

Ito calculus

- Stochastic integral definition ($\tau_i = t_i$):

$$I = \lim_{N\to\infty} I_N = \lim_{N\to\infty} \sum_{i=1}^{N} b[t_i, U(t_i)][W(t_{i+1}) - W(t_i)] \quad (8.52)$$

  - Example: Using (8.47)(ii) ($(dW)^2 \sim dt$), it can be shown that

$$\int_0^t W(t)dW(t) = \frac{1}{2}W^2(t) - \underbrace{\frac{1}{2}t}_{\text{extra term}} \quad (8.53)$$

- Ito lemma (extended chain rule): If $dU = adt + bdW$ and $g(t,x)$ is a differentiable function

$$dg(t,U(t)) = \frac{\partial g}{\partial t}dt + \left(\frac{\partial g}{\partial x}\right)(adt + bdW) + \underbrace{\frac{1}{2}\frac{\partial^2 g}{\partial x^2}b^2 dt}_{\text{extra term}} \quad (8.54)$$

Chap 8 By E. Amani

VII.5 Modeling

Stationary isotropic turbulence

- $\langle U_i \rangle = 0$ and U_1^+, U_2^+, and U_3^+ are independent and evolve with the same model, i.e. the Langevin model:

$$\frac{dX^*(t)}{dt} = U^*(t). \qquad dU^*(t) = -U^*(t)\frac{dt}{T_L} + \left(\frac{2\sigma^2}{T_L}\right)^{1/2} dW(t), \quad (8.55)$$

- The simplest stationary diffusion process called Ornstein-Uhlenbeck (OU) process with

$$dU(t) = a[U(t),t]\,dt + b[U(t),t]\,dW(t),$$

$$a(V,t) = -\frac{V}{T_L},$$

$$b(V,t)^2 = \frac{2\sigma^2}{T_L},$$

$$U(0) \stackrel{D}{=} \mathcal{N}(0,\sigma^2),$$

Chap 8 By E. Amani

VII.5 Modeling

Stationary isotropic turbulence

- It can be shown that appendix J [1]:
  - The solution to its Fokker-Planck equation:

$$\frac{\partial f_L^*}{\partial t} = \frac{1}{T_L}\frac{\partial}{\partial V}(V f_L^*) + \frac{\sigma^2}{T_L}\frac{\partial^2 f_L^*}{\partial V^2}. \quad f_L^*(V;t_1|V_1,t_1) = \delta(V - V_1). \quad (8.56)$$

  - is:

$$f_L(V;t|V_1,t_1) = \mathcal{N}\left[V_1 e^{-(t-t_1)/T_L},\ \sigma^2\left(1 - e^{-2(t-t_1)/T_L}\right)\right], \quad (8.57)$$

$$\rho(s) = e^{-|s|/T_L}. \quad (8.58)$$

$$T_L \equiv \int_0^\infty \rho(s)\,\mathrm{d}s. \quad (8.59)$$

$$D_L^*(s) \equiv \langle [U^*(t+s) - U^*(t)]^2 \rangle \quad = \frac{2\sigma^2}{T_L}s, \quad \text{for } s \ll T_L, \quad (8.60)$$

Chap 8 By E. Amani

VII.5 Modeling

Stationary isotropic turbulence

- Expressing T_L in terms of k and ε:
  - According to Kolmogorov 2nd-hypothesis:

$$D_L(s) = \mathcal{C}_0\varepsilon s, \quad \text{for } \tau_\eta \ll s \ll T_L, \quad (8.61)$$

  - From Eqs. (8.60) and (8.61)

$$T_L^{-1} = \frac{C_0\varepsilon}{2\sigma^2} = \tfrac{3}{4}C_0\frac{\varepsilon}{k}. \quad \sigma^2 = \tfrac{2}{3}k \quad (8.62)$$

$$\mathrm{d}U^*(t) = -\tfrac{3}{4}C_0\frac{\varepsilon}{k}U^*(t)\,\mathrm{d}t + (C_0\varepsilon)^{1/2}\,\mathrm{d}W(t). \quad (8.63)$$

- Exercise: Using Eq. (8.43) show that

$$\frac{dk}{dt} = 0$$

Chap 8 By E. Amani

VII.5 Modeling

More general models

- The Simplified Langevin Model (SLM)
  - Extending Eq. (8.63) to 3D inhomogeneous flow

Mean pressure gradient effect

To have $\frac{dk}{dt} = \varepsilon$ instead of $\frac{dk}{dt} = 0$

$$\mathrm{d}U_i^*(t) = \underbrace{-\frac{1}{\rho}\frac{\partial\langle p\rangle}{\partial x_i}}\,\mathrm{d}t - \left(\tfrac{1}{2} + \tfrac{3}{4}C_0\right)\frac{\varepsilon}{k}\left(U_i^*(t) - \langle U_i\rangle\right)\mathrm{d}t + (C_0\varepsilon)^{1/2}\,\mathrm{d}W_i(t), \quad (8.64)$$

$\langle U_i\rangle \neq 0$

- Exercise: Using Eq. (8.42) and (8.43) show that

$$\frac{dk}{dt} = \varepsilon$$

VII.5 Modeling

More general models

- The Generalized Langevin Models (GLMs)
  - Extending the drift term in Eq. (8.64)

$$\mathrm{d}U_i^*(t) = -\frac{1}{\rho}\frac{\partial\langle p\rangle}{\partial x_i}\mathrm{d}t + G_{ij}(U_j^*(t) - \langle U_j\rangle)\,\mathrm{d}t + (C_0\varepsilon)^{1/2}\,\mathrm{d}W_i(t), \quad (8.65)$$

$$\frac{\mathrm{d}\boldsymbol{X}^*(t)}{\mathrm{d}t} = \boldsymbol{U}^*(t). \quad (8.65)'$$

  - For SLM:

$$G_{ij} = -\left(\tfrac{1}{2} + \tfrac{3}{4}C_0\right)\frac{\varepsilon}{k}\delta_{ij}, \quad (8.66)$$

  - The corresponding Fokker-Planck equations

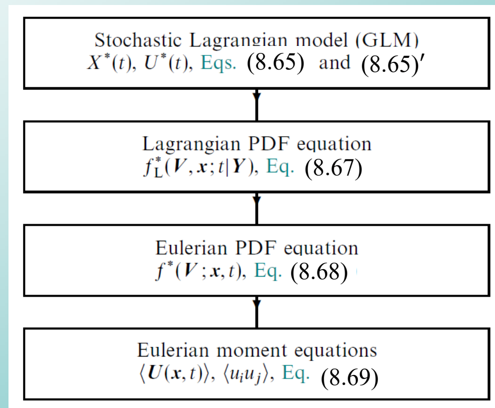
$$\frac{\partial f_{\mathrm{L}}^*}{\partial t} = -V_i\frac{\partial f_{\mathrm{L}}^*}{\partial x_i} + \frac{1}{\rho}\frac{\partial f_{\mathrm{L}}^*}{\partial V_i}\frac{\partial\langle p\rangle}{\partial x_i} - G_{ij}\frac{\partial}{\partial V_i}\left[f_{\mathrm{L}}^*\left(V_j - \langle U_j\rangle\right)\right] + \tfrac{1}{2}C_0\varepsilon\frac{\partial^2 f_{\mathrm{L}}^*}{\partial V_i\,\partial V_i}, \quad (8.67)$$

$$\frac{\partial f^*}{\partial t} + V_i\frac{\partial f^*}{\partial x_i} - \frac{1}{\rho}\frac{\partial f^*}{\partial V_i}\frac{\partial\langle p\rangle}{\partial x_i} = -G_{ij}\frac{\partial}{\partial V_i}[f^*(V_j - \langle U_j\rangle)] + \tfrac{1}{2}C_0\varepsilon\frac{\partial^2 f^*}{\partial V_i\,\partial V_i}. \quad (8.68)$$

VII.5 Modeling

More general models

- The Generalized Langevin Models (GLMs)
  - Realizable Reynolds stress models can be derived starting from the SDE or PDF transport equations



Chap 8 By E. Amani

VII.5 Modeling

More general models

- The Generalized Langevin Models (GLMs)
  - Realizable Reynolds stress models can be derived starting from the SDE or PDF transport equations

$$\frac{\bar{\mathrm{D}}}{\bar{\mathrm{D}}t}\langle u_i u_j\rangle + \frac{\partial}{\partial x_k}\langle u_i u_j u_k\rangle = \mathcal{P}_{ij} + G_{ik}\langle u_j u_k\rangle + G_{jk}\langle u_i u_k\rangle + C_0\varepsilon\delta_{ij}. \qquad (8.69)$$

Chap 8 By E. Amani

VII.5 Numerical solution

Monte Carlo (MC) method

- Given a particle property U at time t_i
- The particle property at time $t_{i+1} = t_i + \Delta t_i$ is computed by integrating a SDE of the general form:

$$\mathrm{d}U(t) = a[U(t), t]\,\mathrm{d}t + b[U(t), t]\,\mathrm{d}W(t), \qquad (8.70)$$

- Different discretized form of this SDE can be proposed using Ito-Taylor expansion [Sauer,6]
- For detailed derivation see reference [7]
- Knowing U of all particles at time t_{i+1}, the Eulerian statistics of U including its one-point Eulerian PDF can be computed on an Eulerian grid

Chap 8 By E. Amani

VII.5 Numerical solution

SDE discretization $\mathrm{d}U(t) = a[U(t), t]\,\mathrm{d}t + b[U(t), t]\,\mathrm{d}W(t),$

- Euler-Maruyama Method:

$$U(t_{i+1}) = U(t_i) + a[t_i, U(t_i)]\Delta t_i + b[t_i, U(t_i)]\Delta W_i \qquad (8.71)$$

$$\Delta W_i = W(t_{i+1}) - W(t_i) = \zeta_i\sqrt{\Delta t_i};\, \zeta_i \in \mathcal{N}(0,1) \qquad (8.72)$$

- Simplified to explicit Euler for ODEs
- The order of convergence:
  - Strong: 0.5 (or 1 if $b[t_i, U] = b(t)$)
  - Weak: 1
- convergence of order m:
  - Strong:

$$\lim_{\Delta t \to 0} \langle |U(t) - U_{\Delta t}(t)| \rangle = \lim_{\Delta t \to 0} \mathcal{O}(\Delta t^m) = 0 \qquad (8.73)$$

  - Weak: (for all polynomials $f(x)$)

$$\lim_{\Delta t \to 0} |\langle f[U(t)] \rangle - \langle f[U_{\Delta t}(t)] \rangle| = \lim_{\Delta t \to 0} \mathcal{O}(\Delta t^m) = 0 \qquad (8.74)$$

Chap 8 By E. Amani

VII.5 Numerical solution

SDE discretization

- Weak 2[nd]-Order Runge-Kutta:

$$U(t_{i+1}) = U(t_i) + \tfrac{1}{2}\{a[U^1(t_{i+1})] + a[U(t_i)]\}\Delta t_i + \tfrac{1}{4}\{b[U^+(t_{i+1})] + b[U^-(t_{i+1})] + 2b[U(t_i)]\}\Delta W_i + \tfrac{1}{4}\{b[U^+(t_{i+1})] - b[U^-(t_{i+1})]\}\left(\Delta W_i^{\,2} - \Delta t_i\right)/\sqrt{\Delta t_i} \qquad (8.75)$$

$$U^1(t_{i+1}) = U(t_i) + a[U(t_i)]\Delta t_i + b[U(t_i)]\Delta W_i$$

$$U^+(t_{i+1}) = U(t_i) + a[U(t_i)]\Delta t_i + b[U(t_i)]\sqrt{\Delta t_i} \qquad (8.76)$$

$$U^-(t_{i+1}) = U(t_i) + a[U(t_i)]\Delta t_i - b[U(t_i)]\sqrt{\Delta t_i}$$

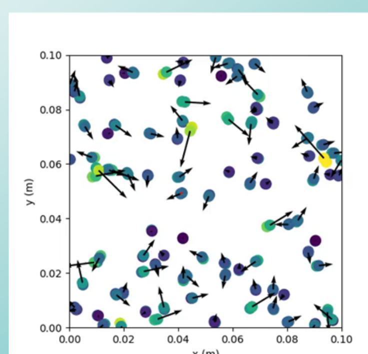
Chap 8 By E. Amani

Hands-on practice

- **HW#6:**
  - Using "pyPDF.py" for 2D stationary isotropic turbulence
  - SDE integration

$$\frac{\mathrm{d}\boldsymbol{X}^*(t)}{\mathrm{d}t} = \boldsymbol{U}^*(t). \qquad \mathrm{d}U^*(t) = -U^*(t)\frac{\mathrm{d}t}{T_\mathrm{L}} + \left(\frac{2\sigma^2}{T_\mathrm{L}}\right)^{1/2}\mathrm{d}W(t), \qquad (8.55)$$

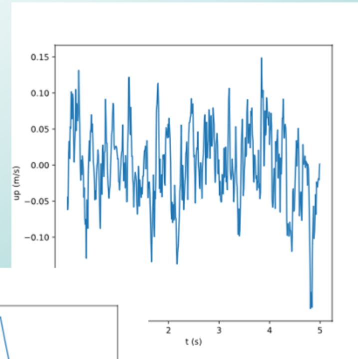
  - MC computation for one grid cell with N_p particles per cell



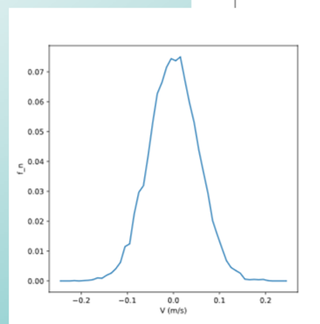
Chap 8 By E. Amani

Hands-on practice

- **HW#6:**
  - Trajectory of $U(t)$ process



  - PDF of $U(t)$



  - **Isotropic decaying turbulence?**

Chap 8 By E. Amani

VII.6 Case study

Case study# 2

Applied Mathematical Modelling 34 (2010) 2223–2241

Contents lists available at ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

ELSEVIER

An efficient PDF calculation of flame temperature and major species in turbulent non-premixed flames

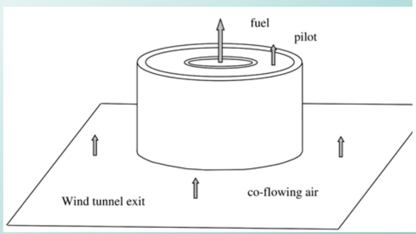
E. Amani, M.R.H. Nobari *

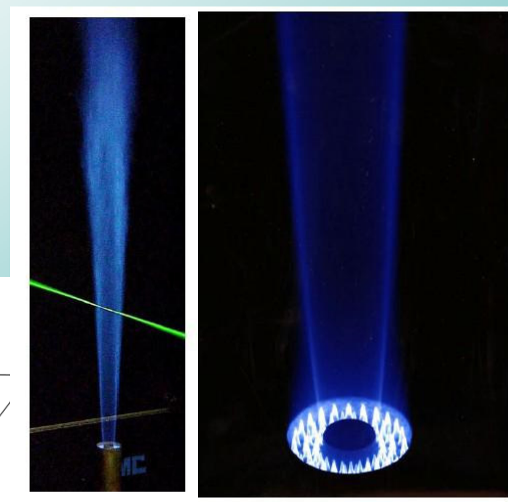
Mechanical Engineering Dept., Amirkabir University of Technology, 424 Hafez Avenue, P.O. Box 15875-4413, Tehran, Iran

Chap 8 By E. Amani

VII.6 Case study

Test case: Sandia Flame D

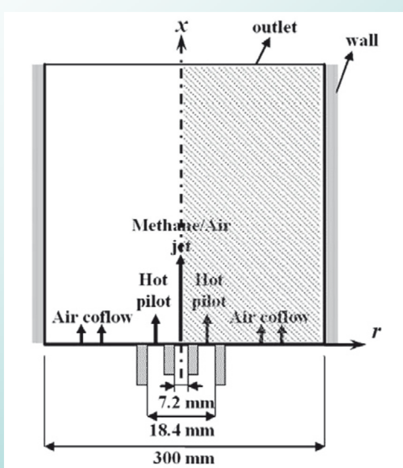


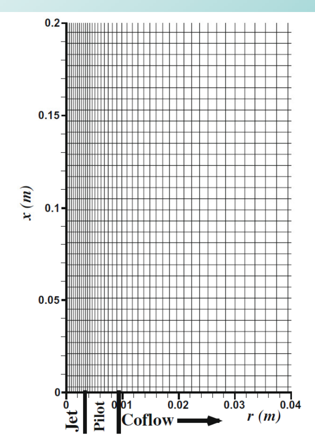


Chap 8 By E. Amani

VII.6 Case study

Computational geometry and grid





$120 \times 70\ (x - r)$

Chap 8 By E. Amani

VII.6 Case study

Modeling: RANS

- **Mass:**

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j}=0$$

- **Momentum (i =1, 2, 3):**

Reynolds stresses

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{u}_i}{\partial x_j}=-\frac{\partial \bar{\rho}\widetilde{u_i''u_j''}}{\partial x_j}+\frac{\partial \bar{\tau}_{ij}}{\partial x_j}$$

- **Species** (N species with k=1,..,N):

$$\frac{\partial \bar{\rho}\tilde{Y}_n}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Y}_n}{\partial x_j}=-\frac{\partial \bar{\rho}\widetilde{u_j''Y_n''}}{\partial x_j}-\frac{\partial \overline{J_j^n}}{\partial x_j}+\bar{\dot{\omega}}_n \qquad n=1,\ldots,N$$

- **Total enthalpy** ($h_t = h + u_i u_i/2$):

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{h}}{\partial x_j}=-\frac{\partial \bar{\rho}\widetilde{u_j''h''}}{\partial x_j}+\frac{\partial \overline{J_j^h}}{\partial x_j}-\sum_{n=1}^{N}h_{ref_n}\bar{\dot{\omega}}_n$$

Chap 8 By E. Amani

VII.6 Case study

Modeling: PDF

- Velocity-composition space

$$\underline{U}=(U_1,U_2,U_3)$$
$$\underline{\phi}=(Y_1,Y_2,\ldots,Y_N,T)$$

- State vector $\Rightarrow$ $(\underline{U}(\underline{x},t),\underline{\phi}(\underline{x},t))$
- State sample space: Velocity-Composition space $\Rightarrow (\underline{V},\underline{\psi})$
- One-point one-time joint PDF: $f_{\underline{u\phi}}(\underline{V},\underline{\psi})$

- Statistics:

$$<Q(\underline{U},\underline{\phi})>=\iint Q(\underline{V},\underline{\psi})f_{\underline{u\phi}}(\underline{V},\underline{\psi})d\underline{V}d\underline{\psi}$$
$$Q=<Q>+Q'$$

Chap 8 By E. Amani

VII.6 Case study

Modeling: PDF

$$\rho(\underline{\psi})\frac{\partial f}{\partial t}+\overbrace{\rho(\underline{\psi})V_j\frac{\partial f}{\partial x_j}}^{\text{Convection}}+\overbrace{(\rho(\underline{\psi})g_j-\frac{\partial <p>}{\partial x_j})\frac{\partial f}{\partial V_j}}^{\text{Mean pressure gradient and gravity}}+\overbrace{\frac{\partial}{\partial \psi_\alpha}[\rho(\underline{\psi})S_\alpha(\underline{\psi})f]}^{\text{Reaction}}$$

$$=\underbrace{\frac{\partial}{\partial V_j}\left[<-\frac{\partial \tau_{ij}}{\partial x_j}+\frac{\partial p'}{\partial x_j}|\underline{V},\underline{\psi}>f\right]}_{\text{Viscous stresses and fluctuating pressure gradient}}+\underbrace{\frac{\partial}{\partial \psi_\alpha}\left[<\frac{\partial J_i^\alpha}{\partial x_i}|\underline{V},\underline{\psi}>f\right]}_{\text{Molecular diffusion}}$$

- Mean pressure ⇒ Poisson equation

VII.6 Case study

Modeling: PDF

- Velocity-composition PDF

$$\rho(\underline{\psi})\frac{\partial f}{\partial t}+\rho(\underline{\psi})V_j\frac{\partial f}{\partial x_j}+(\rho(\underline{\psi})g_j-\frac{\partial <p>}{\partial x_j})\frac{\partial f}{\partial V_j}+\frac{\partial}{\partial \psi_\alpha}[\rho(\underline{\psi})S_\alpha(\underline{\psi})f]$$

$$=\frac{\partial}{\partial V_j}\left[<-\frac{\partial \tau_{ij}}{\partial x_j}+\frac{\partial p'}{\partial x_j}|\underline{V},\underline{\psi}>f\right]+\frac{\partial}{\partial \psi_\alpha}\left[<\frac{\partial J_i^\alpha}{\partial x_i}|\underline{V},\underline{\psi}>f\right]$$

- Exercise: What are the corresponding SDEs for $\vec{X}^*(t)$, $\vec{U}^*(t)$, and $\vec{\phi}^*(t)$? (Consult reference [1])

VII.6 Case study

Modeling: Composition PDF

- PDF for scaler variables
- State space $\Rightarrow \underline{\phi} = \left(Y_1, Y_2, \ldots, Y_N, T\right)$
- Statistics:

$$< Q(\underline{\phi}) > = \int_{-\infty}^{+\infty} Q(\underline{\psi})\, f_{\underline{\phi}}(\underline{\psi}; \vec{x}, t)\, d\underline{\psi}$$

$$< S_\alpha > \quad < \phi'_\alpha \phi'_\beta > \quad \checkmark$$

$$< u'_i \phi'_\alpha > \quad < u'_i u'_j > \quad \times$$

- Navier-Stokes equations for $\langle \vec{U} \rangle$ and $\langle p \rangle$
  - LES or RANS

VII.6 Case study

Modeling: Composition PDF

$$\langle \rho \rangle \langle u_i | \psi \rangle = -\frac{\Gamma_t}{\tilde{f}_\phi} \frac{\partial \tilde{f}_\phi}{\partial x_i}$$

$$\frac{\partial \tilde{f}_\phi}{\partial t} + \overbrace{\tilde{U}_i \frac{\partial \tilde{f}_\phi}{\partial x_i}}^{\text{Macro-mixing}} + \overbrace{\frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i}\left[\langle \rho \rangle \langle u_i | \psi \rangle \tilde{f}_\phi\right]}^{\text{Meso-mixing}} =$$

$$-\frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial J_i^\alpha}{\partial x_i} | \psi \right\rangle \tilde{f}_\phi\right] - \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}_\phi S_\alpha(\psi)\right]$$

Gradient diffusion

VII.6 Case study

Modeling: Composition PDF

$$\frac{\partial \tilde{f}_\phi}{\partial t} + \overbrace{\tilde{U}_i \frac{\partial \tilde{f}_\phi}{\partial x_i}}^{\text{Macro-mixing}} \overbrace{- \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial \tilde{f}_\phi}{\partial x_i}\right]}^{\text{Meso-mixing}} =$$

$$\underbrace{-\frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial J_i^\alpha}{\partial x_i} | \psi \right\rangle \tilde{f}_\phi\right]}_{\text{Micro-mixing}} - \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}_\phi S_\alpha(\psi)\right]$$

Curl's model

LIEM

, …

Chap 8 By E. Amani

VII.6 Case study

Modeling: Composition PDF

$$\frac{\partial \tilde{f}_\phi}{\partial t} + \overbrace{\tilde{U}_i \frac{\partial \tilde{f}_\phi}{\partial x_i}}^{\text{Macro-mixing}} \overbrace{- \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial \tilde{f}_\phi}{\partial x_i}\right]}^{\text{Meso-mixing}} =$$

$$\underbrace{E(\overline{\psi}; \overline{x}, t)}_{\text{Micro-mixing}} - \frac{\partial}{\partial \psi_\alpha}\underbrace{\left(\tilde{f}_\phi S_\alpha(\psi)\right)}_{\text{Reaction}}$$

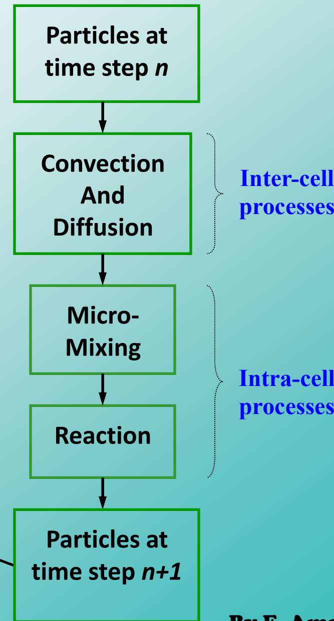
Chap 8 By E. Amani

VII.6 Case study

Numerics

- Fractional step algorithm
  - A grid of computational cells
  - There are N_ℓ particles in each cell $(\vec{x}_\ell, t)$
  - Each particle has a value $\underline{\phi}^{(n)}$
  - Statistics in each cell at each time are calculated from the particles presented in that cell at the given time

$$\langle\phi_\alpha\rangle(\vec{x}_\ell,t)=\frac{1}{N_\ell}\sum_{n=1}^{N_\ell}\phi_\alpha^{(n)}(\vec{x}_\ell,t)+\text{statistical error}$$

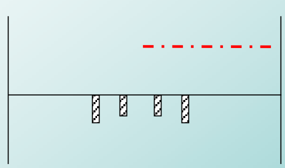


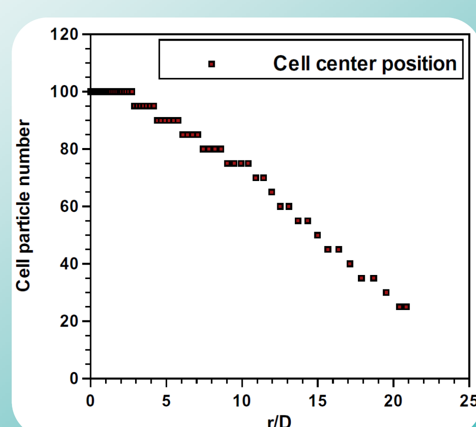
Chap 8 By E. Amani

VII.6 Case study

Numerics

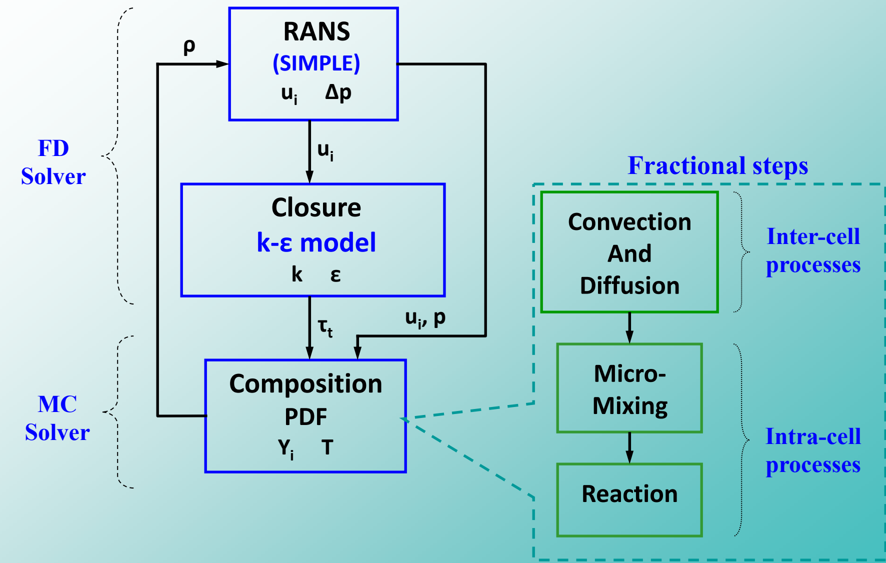
- Particles per cell





Chap 8 By E. Amani

VII.6 Case study

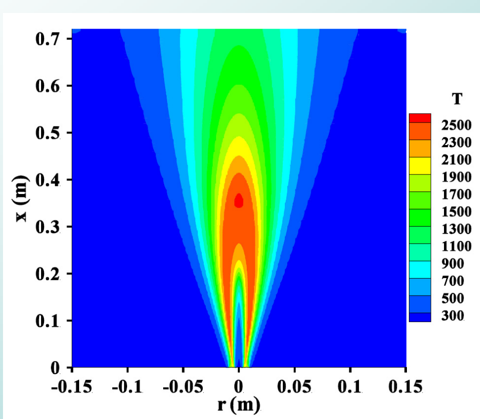


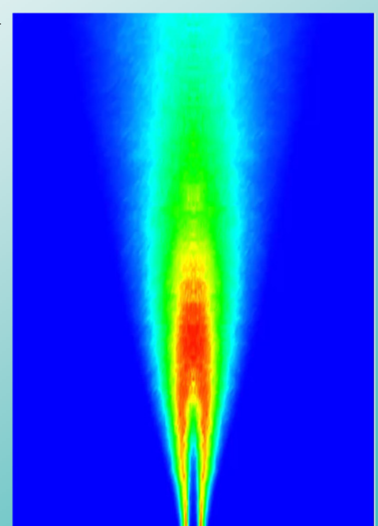
VII.6 Case study

Results

PDF ►

▼ RANS

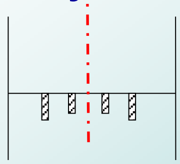


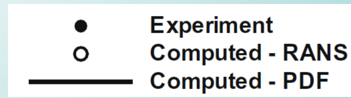


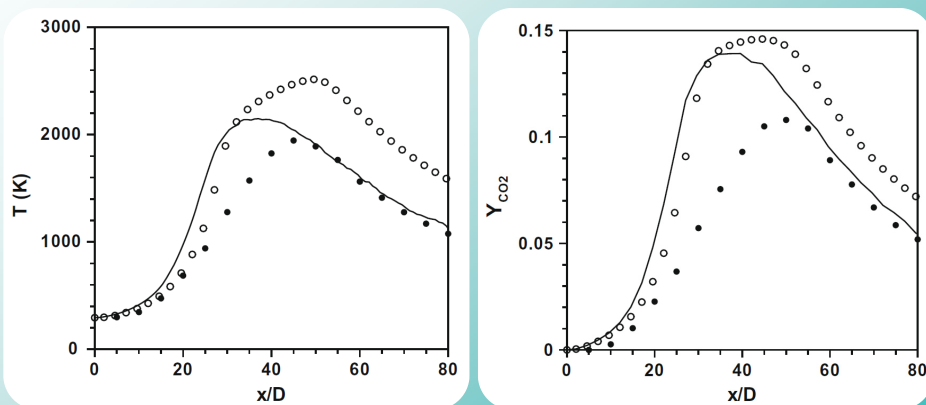
VII.6 Case study

Results

- Means







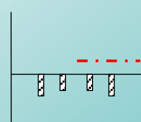
Chap 8 By E. Amani

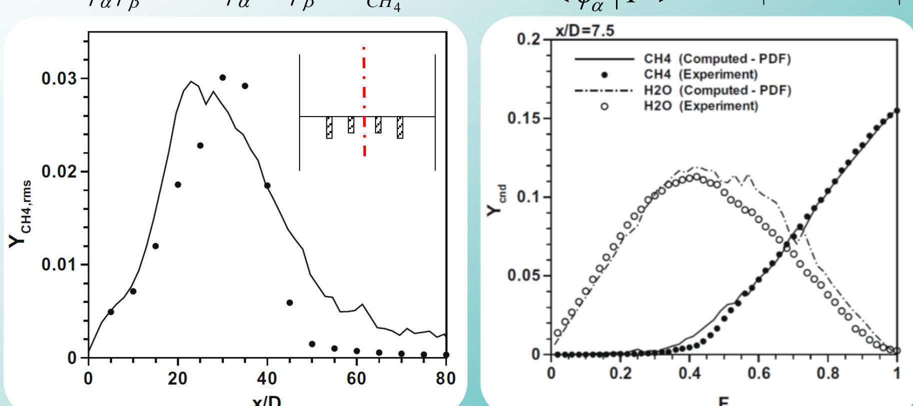
VII.6 Case study

Results

- Other statistics: RMSs and conditional means

$<\phi'_\alpha \phi'_\beta>^{1/2}: \ \phi_\alpha = \phi_\beta = Y_{CH_4}$ $<\phi_\alpha \mid F>$



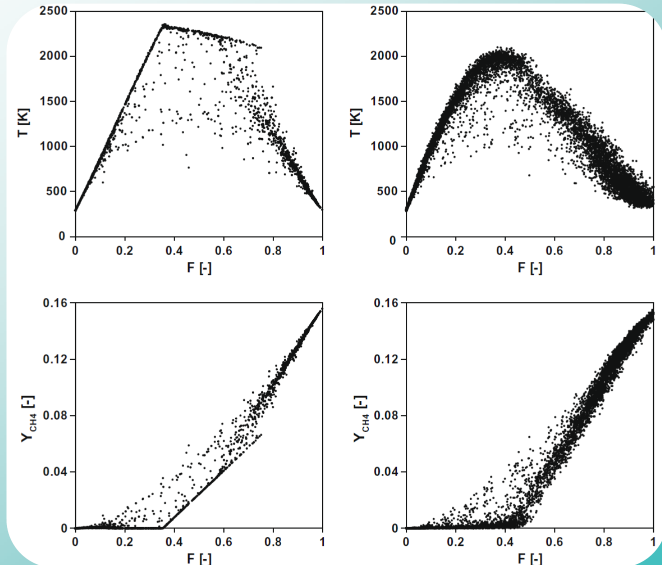


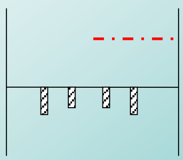
Chap 8 By E. Amani

VII.6 Case study

Results

- Scatter plots





Chap 8

By E. Amani