Turbulent Combustion: Theory and Modelling
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Lecture – 45
Turbulence –Chemistry Interaction (contd…)

Welcome back. So, let us continue the discussion on this different combustion model, we have looked at the Eddy break up model and discussed about its issues, advantages and disadvantages, then the modification to the Eddy break up model also been discussed. Now, we will look at the Finite Rate Chemistry Model.

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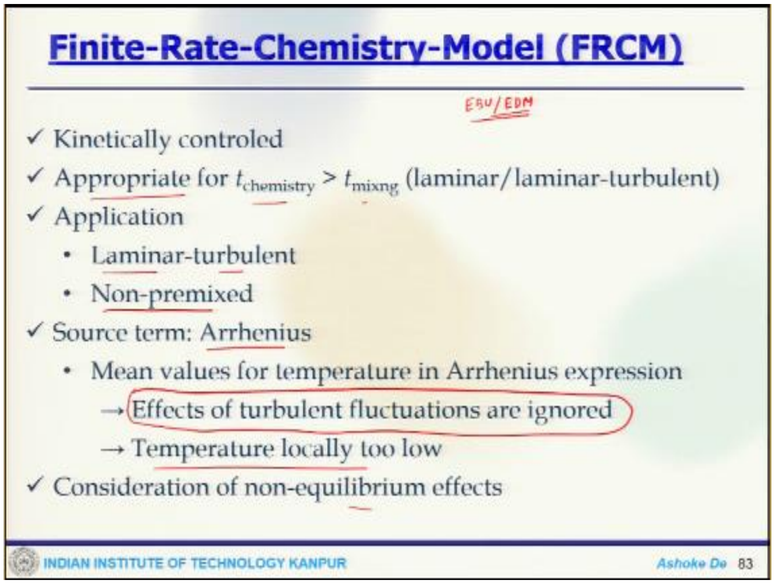

Finite-Rate-Chemistry-Model (FRCM)

EBU/EDM

- ✓ Kinetically controled
- ✓ Appropriate for $t_{chemistry} > t_{mixng}$ (laminar/laminar-turbulent)
- ✓ Application
  - Laminar-turbulent
  - Non-premixed
- ✓ Source term: Arrhenius
  - Mean values for temperature in Arrhenius expression
    - → Effects of turbulent fluctuations are ignored
    - → Temperature locally too low
- ✓ Consideration of non-equilibrium effects

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So, this is more or less detailed. So, this particular one important thing we have previously looked at when we talked about the EBU or EDM they are more or less mixing controlled, but this guy is kinetically controlled. So, it means the chemistry actually controls the whole physics. So, now, here there is approximate in the chemistry time is more than the mixing time.

So, that means it becomes a laminar or laminar-turbulent interaction kind of situation. So, one can think about the applicability. So, it can be used in non-premixed mode laminar case or the turbulent case either of the situations this is applicable and the source term it is kind of using the Arrhenius expression this is we use the mean values for the temperature in Arrhenius expression, but importantly here now, this case the effect of turbulent fluctuations are ignored. So, this is one thing which would be missing when we actually close the source term.

So, and also when you look at the local temperature that is also quite low. So, these are again I mean compared to the previous models, these are some of the issues that are going to come up here that it does not account for those things. And also I am in the consideration of the non-equilibrium effects and all these things, which are also sort of missing. So, we have looked at the issues of EBU and EDM and now, EDM is more mixing controlled. FRCM is kinetically controlled.

So, these 2 are sort of contradicting to each other, or if one actually combines these 2, that would be probably the best possible combination and then that can be used for the application.

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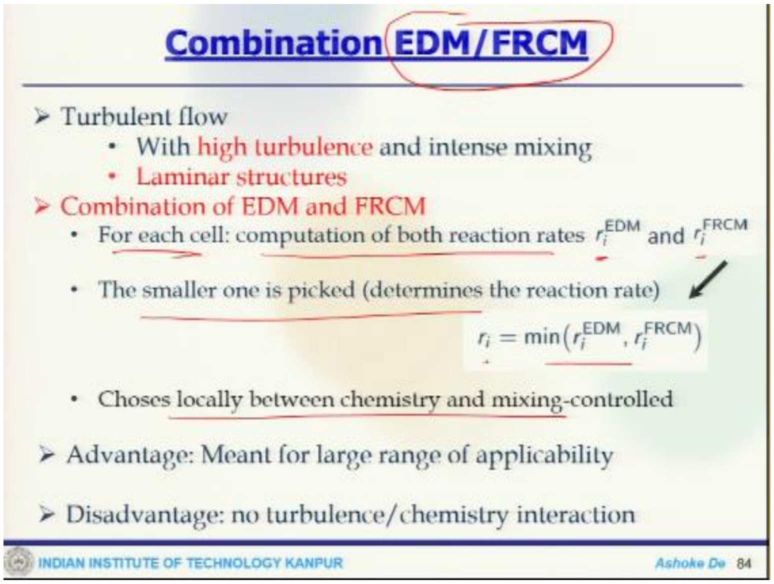

Combination EDM/FRCM

- Turbulent flow
  - With high turbulence and intense mixing
  - Laminar structures
- Combination of EDM and FRCM
  - For each cell: computation of both reaction rates r_i^{EDM} and r_i^{FRCM}
  - The smaller one is picked (determines the reaction rate)

$$r_i = \min\left(r_i^{EDM}, r_i^{FRCM}\right)$$

  - Choses locally between chemistry and mixing-controlled
- Advantage: Meant for large range of applicability
- Disadvantage: no turbulence/chemistry interaction

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So, that is where we talk about this combination of EDM and FRCM. So, then we can use it for turbulent flow with high turbulence and intense mixing and also if you have a laminar structure that can be handled easily because now, we are trying to take that advantage of both these 2 models. So, essentially the advantages of these 2 models are going to be used to somehow get these individuals 2, now when you combined these things.

So, for each cell, the computation of both the reaction rates is done that means, one is the reaction rate using EDM and the reaction rate using FRCM, then we look at the smaller one to determine the reaction rate. To determine the reaction rate, we pick the minimum of the smaller of between the EDM and FRCM. And then we look at the local chemistry and mixing controlled situation which allows to choose what is supposed to be added along with this reaction source term to take the advantage of whether it is a kinetically controlled situation or it is a mixing control situation. So, there you get some advantages, and obviously, you also pay some price. So, there is a large range of applicability, so this is one of the biggest advantages that one is the applicability range or application range increases that will be one of the best things one would expect to have.

But the other disadvantage is that there is no turbulence chemistry interaction. So, though we are coupling these 2 models, then taking the advantage of these 2, but there are still some issues.

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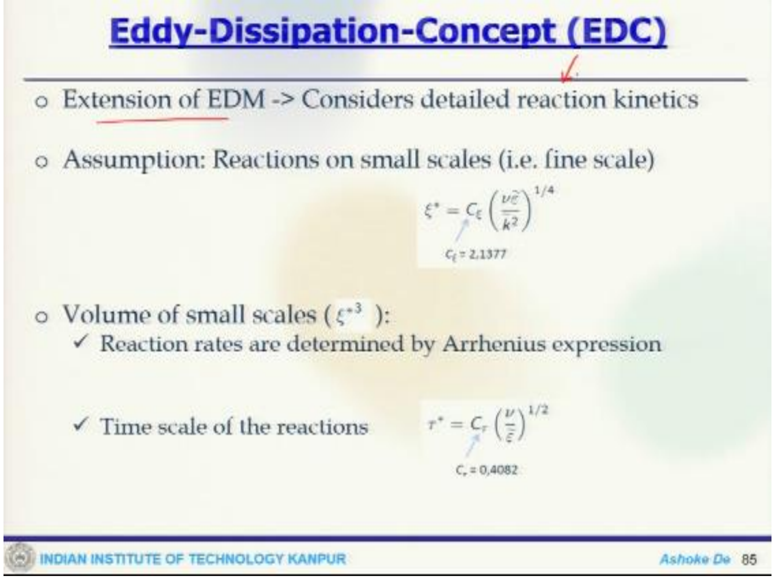

Eddy-Dissipation-Concept (EDC)

- Extension of EDM -> Considers detailed reaction kinetics
- Assumption: Reactions on small scales (i.e. fine scale)

$$\xi^* = C_\xi \left(\frac{\nu\tilde{\varepsilon}}{k^2}\right)^{1/4}$$

$C_\xi = 2{,}1377$

- Volume of small scales (ξ^{*3}):
  - ✓ Reaction rates are determined by Arrhenius expression
  - ✓ Time scale of the reactions $\tau^* = C_\tau \left(\frac{\nu}{\tilde{\varepsilon}}\right)^{1/2}$

$C_\tau = 0{,}4082$

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So, then the further modification which was proposed the Eddy Dissipation Concept, which is by extension of the EDM, where it does not take into account the detailed chemistry, but now, EDC can considers detailed reaction kinetics. So, that means, it can consider multi-step reaction chemistry. So, what it does that if you have a competition cell like this, then you divide that into a small section, this is your sort of a reaction zone and this is your mixing area.

So, the cell is divided into two segments, one is the reaction zone which is the fine-scale structure and these reactions happen on the small scale which is called the fine-scale and that is the estimated like this

$$\xi^* = C_\xi \left(\frac{\nu\tilde{\varepsilon}}{\tilde{k}^2}\right)^{1/4}$$

And the volume of the cell would be ξ^{*3}. So, reaction rates are determined by obviously Arrhenius reaction because that takes into account all the detailed chemistry and then the timescale of the reaction. It is also estimated as τ^*, which is

$$\tau^* = C_\tau \left(\frac{\upsilon}{\tilde{\varepsilon}}\right)^{1/2}$$

So, these are the constants which are default model constant which is proposed originally by the EDC model. But, later on, it has been shown by different researchers that this requires some tuning depending on the particular application. So, I mean more or less these constants work well for a large range of applications, but at the same time, this can fail for the small I mean the particular or rather specific application that you want has to delete.

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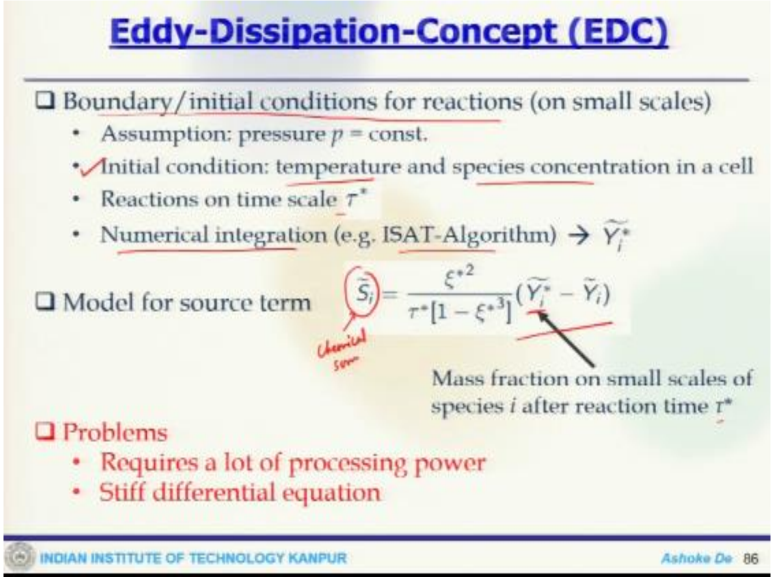

Eddy-Dissipation-Concept (EDC)

☐ Boundary/initial conditions for reactions (on small scales)
- Assumption: pressure p = const.
- ✓Initial condition: temperature and species concentration in a cell
- Reactions on time scale τ^*
- Numerical integration (e.g. ISAT-Algorithm) → $\widetilde{Y_i^*}$

☐ Model for source term $\tilde{S}_i = \frac{\xi^{*2}}{\tau^*[1-\xi^{*3}]}(\widetilde{Y_i^*} - \tilde{Y}_i)$

Chemical Source

Mass fraction on small scales of species i after reaction time τ^*

☐ Problems
- Requires a lot of processing power
- Stiff differential equation

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Now, once you have this, so, you need the boundary and initial condition for the reactions. So, one of the assumptions is that you have a pressure constant situation that means, it is sort of isobaric combustion and then you need some initial condition which is quite important that is for temperature and the species mass fraction or molar concentration whatever it is, then we need a reaction time scale and then the numerical integration that means one of the algorithms which were proposed by Pope is that I said algorithm which is quite efficient.

Then you get these numerical, then we close the source term the reaction system this is my chemical source term. So, this is for individual species here, since, we are solving individual species mass fraction equation. So, each mass species will have a source terms in terms of a chemical source term and that is closed like

$$\widetilde{S_\iota} = \frac{\xi^{*2}}{\tau^{*}[1 - \xi^{*3}]} (\widetilde{Y_\iota^{*}} - \widetilde{Y_\iota})$$

So, this is a mass fraction on a small scale of species after having a reaction over τ. So, that means, the mass fraction one has to find out that these things still this is quite.

I mean, if you look at globally, this is a huge advantage from the application point of view, it can be applied to a premixed case or non-premixed case or partially premixed case, but it has problems if someone applies for using detailed kinetics and all these things. So, when you use the more detailed kinetics, your computation power will go up. So, the resource requirement becomes quite high and at the same time, this integration of the reaction source term or there that will lead to some stiff differential equation, when we try to integrate these species mass fraction.

So, these are the things but there are ways to handle it because these days the computational power are quite handy due to the advancement of the architecture and all these things, but the differential equation solver, which is another area of concern where the ISAT-Algorithm has been found to be quite effective.

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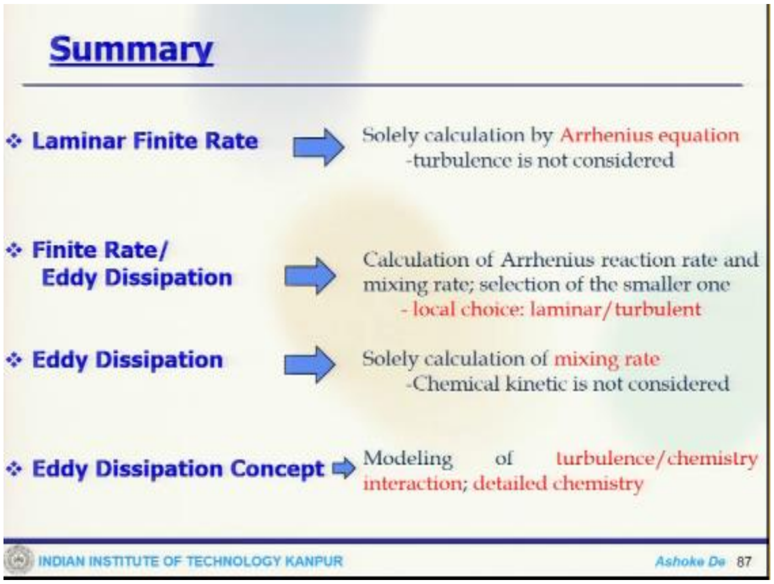

Summary

- **Laminar Finite Rate** ⇨ Solely calculation by Arrhenius equation -turbulence is not considered
- **Finite Rate/ Eddy Dissipation** ⇨ Calculation of Arrhenius reaction rate and mixing rate; selection of the smaller one - local choice: laminar/turbulent
- **Eddy Dissipation** ⇨ Solely calculation of mixing rate -Chemical kinetic is not considered
- **Eddy Dissipation Concept** ⇨ Modeling of turbulence/chemistry interaction; detailed chemistry

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Now if we pull up the discussion of this fast part where we first look at the laminar finite rate. This is where the issue here is that bigger issues that turbulence is not considered and the reaction source term, the calculation is made by the Arrhenius equation and if you go to finite rate of eddy dissipation. So, there again we use the Arrhenius expression to the calculation of the source term and we calculate the mixing rate and this is a local choice with a laminar or turbulent depending on what is used.

That means primarily there is in now the eddy dissipation. This is solely calculation of mixing rate here the kinetics is not considered that means, it is more or less, so this case is mixing control and then finally we get eddy dissipation concept for the actual interaction between turbulence and chemistry these are taken into consideration and then detailed chemistry can be used.

So, all said and done this looks and quite advantages in that way, and the applicability is also quite high because one can use this particular model to irrespective of mode of combustion, the reason is, it solves for individual mass transport equation. So, that gives you the simple models.

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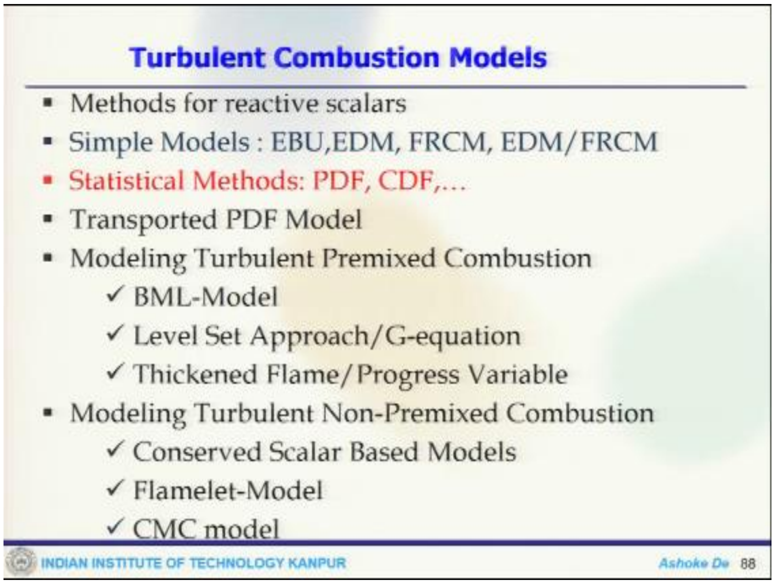

Turbulent Combustion Models

- Methods for reactive scalars
- Simple Models : EBU,EDM, FRCM, EDM/FRCM
- Statistical Methods: PDF, CDF,…
- Transported PDF Model
- Modeling Turbulent Premixed Combustion
  - ✓ BML-Model
  - ✓ Level Set Approach/G-equation
  - ✓ Thickened Flame/Progress Variable
- Modeling Turbulent Non-Premixed Combustion
  - ✓ Conserved Scalar Based Models
  - ✓ Flamelet-Model
  - ✓ CMC model

Now, then we can look at a slightly advanced model that is based on statistical methods so that would be also quite handy. See, so this set of models, what we discussed here can be theoretically applied to any mode of combustion, but obviously, with some advantages and disadvantages, and then these are the ones which are very specific to this particular mode of combustion.

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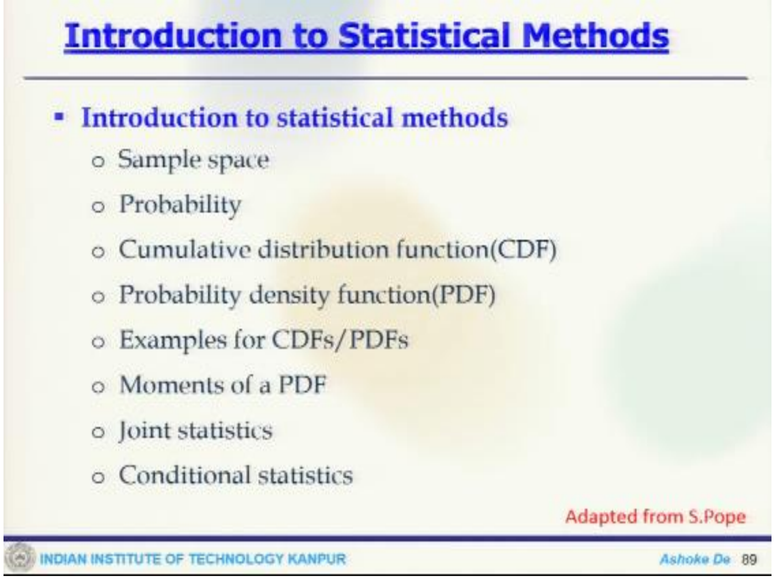

Introduction to Statistical Methods

- **Introduction to statistical methods**
  - Sample space
  - Probability
  - Cumulative distribution function(CDF)
  - Probability density function(PDF)
  - Examples for CDFs/PDFs
  - Moments of a PDF
  - Joint statistics
  - Conditional statistics

Adapted from S.Pope

Now we move to the statistical methods where we can see what are the sample spaces. What are going to be the probability, cumulative distribution function, probability density function, then moments of a PDF, joint statistics, conditional statistics? So, some of these terminologies, these things are required for a statistical-based model and this is primarily adapted from Pope.

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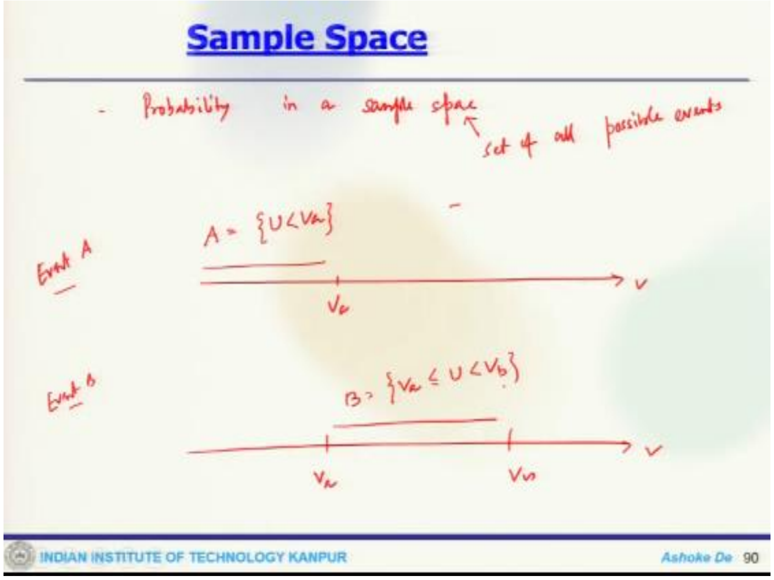

Sample Space

- Probability in a sample space ← set of all possible events

Event A

$A = \{U < V_a\}$

Event B

$B = \{V_a \le U < V_b\}$

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So, now we can look at the probability of an event. So, the probability of an event probability in a sample space. So, what is sample space? Sample space is nothing but a set of all possible events. Now, for the velocity field, you think about there will be a random variable of U and then the sample space variable V which is independent of the variable. Now, for example, if you take this is my sample variable V and this is let us say event a then this is where you can say that

$$A = \{U < V_a\}$$

Similarly, one can look at the event B where again in the sample space, this could be

$$B = \{V_a \le U < V_b\}$$

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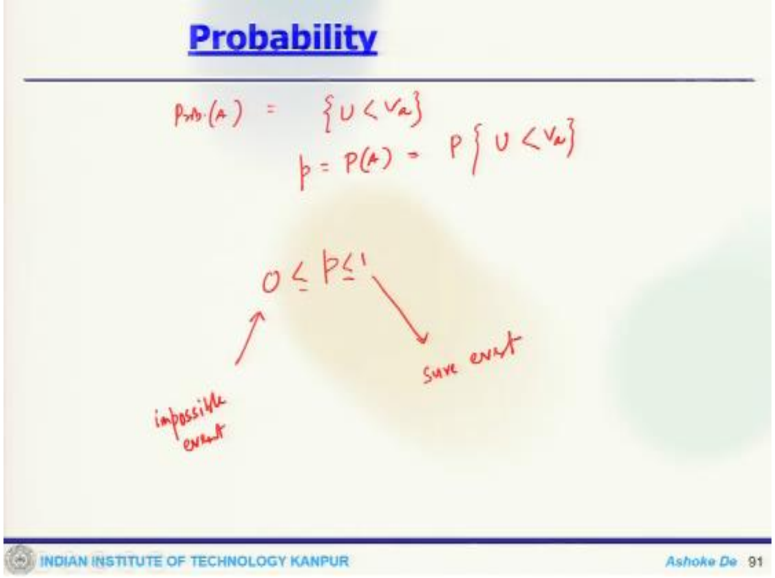

Probability

$Prob.(A) = \{U < V_a\}$

$p = P(A) = P\{U < V_a\}$

$0 \le p \le 1$

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Now, the probability of the event A would be U when it is less than V$_a$ .So, that means

$$p = p(A) = p\{U < V_a\}$$

and the probability P which is lies between 0 to 1 when it is 0 which means, it is an impossible event and when it is 1, it is a sure event.

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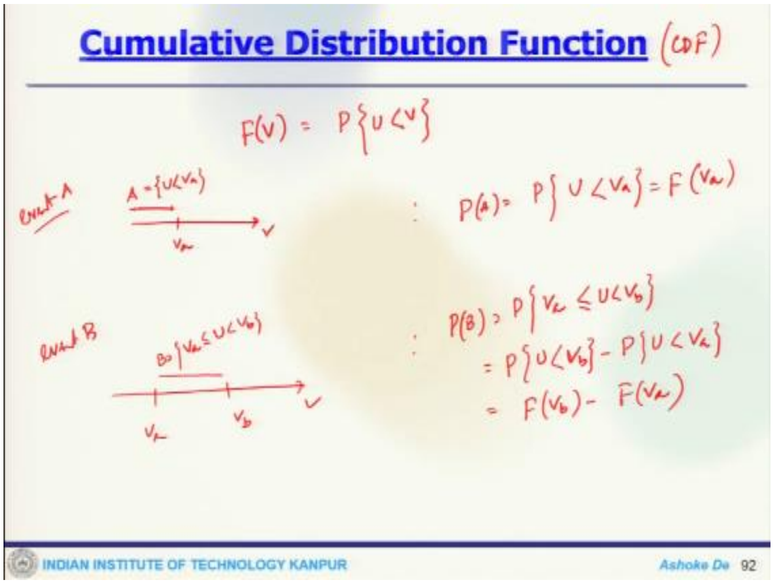

Cumulative Distribution Function (CDF)

$F(V) = P\{U < V\}$

event A

$A = \{U < V_a\}$

$P(A) = P\{U < V_a\} = F(V_a)$

event B

$B = \{V_a \leq U < V_b\}$

$P(B) = P\{V_a \leq U < V_b\}$

$= P\{U < V_b\} - P\{U < V_a\}$

$= F(V_b) - F(V_a)$

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Now we look at the CDF or cumulative distribution function. Now, one can look at the probability of any event which can be determined from the CDF. So, let us say

$$F(V) = P\{U < V\}$$

This is my A where U<V$_a$ then

$$P(A) = P\{U < V_a\} = F(V_a)$$

For event B ,

$$P(B) = P\{V_a \leq U \leq V_b\}$$

$$= P\{U < V_b\} - P\{U < V_a\}$$

$$= F(V_b) - F(V_a)$$

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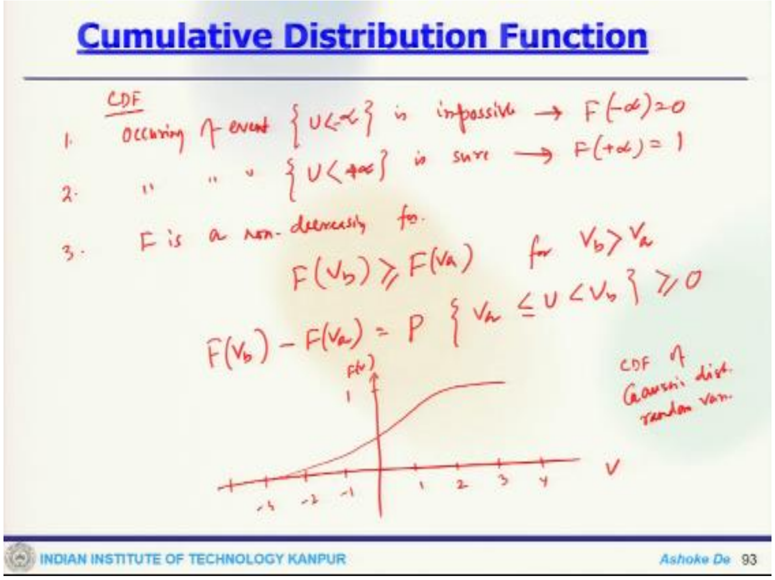

Cumulative Distribution Function

CDF

1. occurring of event $\{U < -\infty\}$ is impossible $\rightarrow F(-\infty) = 0$
2. " " " $\{U < +\infty\}$ is sure $\rightarrow F(+\infty) = 1$
3. F is a non-decreasing fn.

$F(V_b) \geq F(V_a)$ for $V_b > V_a$

$F(V_b) - F(V_a) = P\{V_a \leq U < V_b\} \geq 0$

CDF of Gaussian dist. random var.

So, there are some basic properties of CDF. So, let us say occurring of an event which is U less than -∞ is impossible. For which one can say if -∞ is 0 then occurring of event either U less than +∞ is sure for which one can write this is 1 and third F is a non-decreasing function for which one can write F(V_b) greater than equals to F(V_a) for V_b greater than V_a and one can write

$$F(V_b) - F(V_a) = P\{V_a \leq U \leq V_b\} \geq 0$$

So, I can look at this is let us say 1, 2, 3, 4 this is V and let us say this is F(V) -1, -2, -3 -1, -2, -3. So, this is how this guy will vary. So, this is the same CDF of Gaussian distributed random variable.

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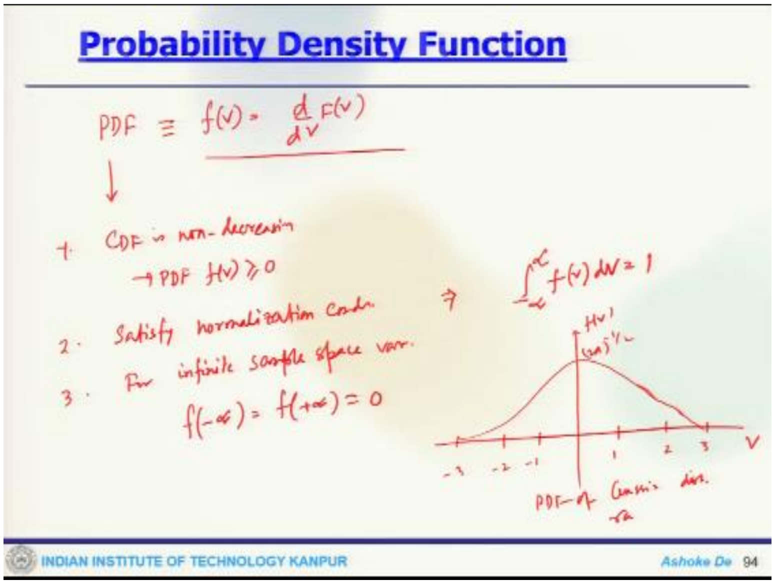

Probability Density Function

PDF $\equiv f(v) = \frac{d}{dV} F(v)$

↓

1. CDF is non-decreasing

$\rightarrow$ PDF $f(v) \geq 0$

2. Satisfy normalization condn. $\Rightarrow \int_{-\infty}^{\infty} f(v)\, dV = 1$
3. For infinite sample space var.

$f(-\infty) = f(+\infty) = 0$

PDF of Gaussian dist. rv

Now, if we take the derivative of CDF that will give you the probability density function. So, that means

$$PDF \equiv f(v) = \frac{dF(v)}{dx}$$

If that is what this is my probability density function which is represented the derivative of my CDF now also PDF will have some properties one of the properties is that CDF when the CDF is non decreasing. The PDF that is f(v) would be greater than 0 then it also satisfies the normalization condition that means, which is

$$\int_{-\infty}^{+\infty} f(v)dv = 1$$

Third for the infinite sample space variable you get

$$f(-\infty) = f(+\infty) = 0$$

So, one can look at this 1, 2, 3 -1, -2, -3. So, this will go between like this. This is my v this is my F(v) $(2\pi)^{-1/2}$, so again the PDF of Gaussian distributed random variable.

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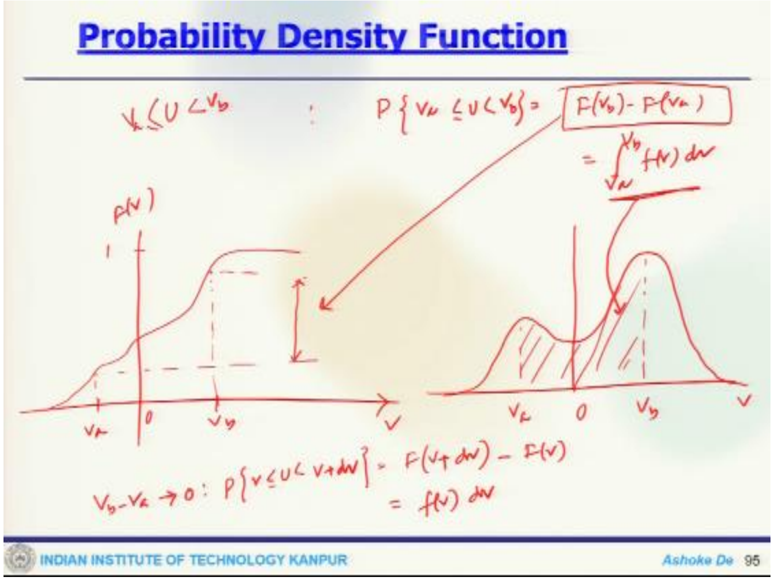

Probability Density Function

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So, these are the function often now one can look at more specifically, let us say in the particular event for our event V which was occurring there in the sample space. So

$$P\{V_a \leq U \leq V_b\} = F(V_b) - F(V_a)$$

So, if I schematically look at it, this is 0 let us say V_a, V_b and so the curve goes like that. That is one this is my F(V).

So this is my distribution of this guy and the same thing when I put it back 0. This is my space V, this is V_b, this is V_a, so this is the part which corresponds to, so the interval where V_b - V_a tends to 0 the probability will be

$$\begin{aligned} P\{V \leq U \leq V + dV\} &= F(V + dV) - F(V) \\ &= F(V)dV \end{aligned}$$

So that is how you get for the PDF.

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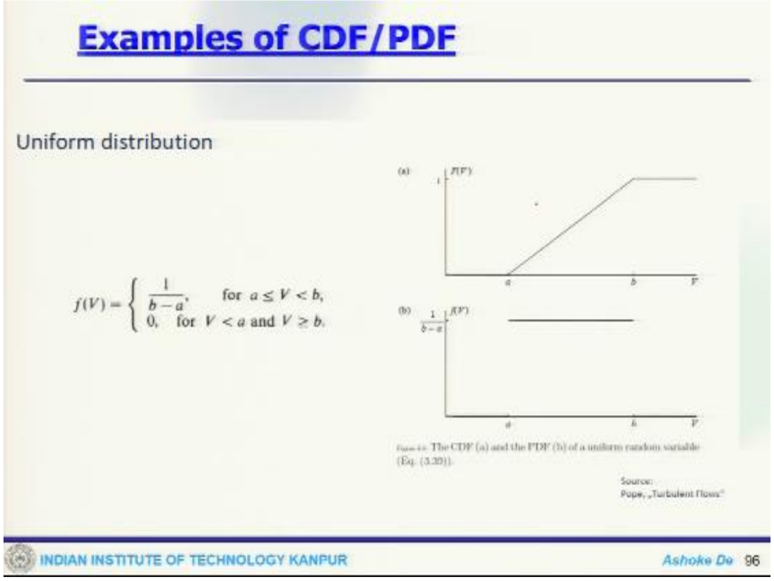

Examples of CDF/PDF

Uniform distribution

$$f(V) = \begin{cases} \dfrac{1}{b-a}, & \text{for } a \leq V < b, \\ 0, & \text{for } V < a \text{ and } V \geq b. \end{cases}$$

[illegible] The CDF (a) and the PDF (b) of a uniform random variable (Eq. (3.30)).

Source:
Pope, „Turbulent Flows"

Now, we can take some examples like this is a distribution of CDF and this is the probability distribution function. So, this is a uniform distribution where probability distribution will be between a to b to 1 by b - a otherwise 0. So, this is how it looks like this is how the CDF variation is there.

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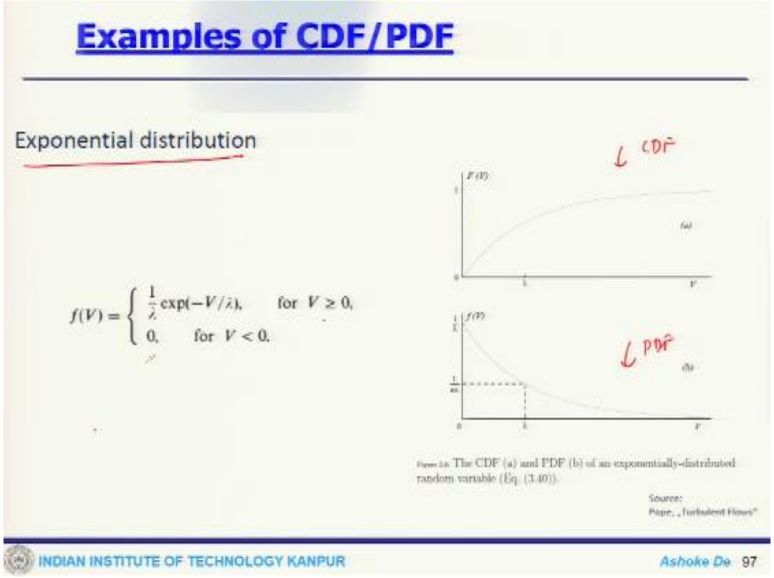

Examples of CDF/PDF

Exponential distribution

$$f(V) = \begin{cases} \frac{1}{\lambda}\exp(-V/\lambda), & \text{for } V \geq 0, \\ 0, & \text{for } V < 0. \end{cases}$$

Figure 3.6 The CDF (a) and PDF (b) of an exponentially-distributed random variable (Eq. (3.40)).

Source:
Pope, „Turbulent Flows"

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So, this is a uniform distribution, you can take an exponential distribution or this is how CDF looks like and this is how the PDF looks like. And when V is greater than 0, this is $\frac{1}{\lambda}\exp\left(-\frac{V}{\lambda}\right)$.

So, that is to give you an idea from CDF and all this.

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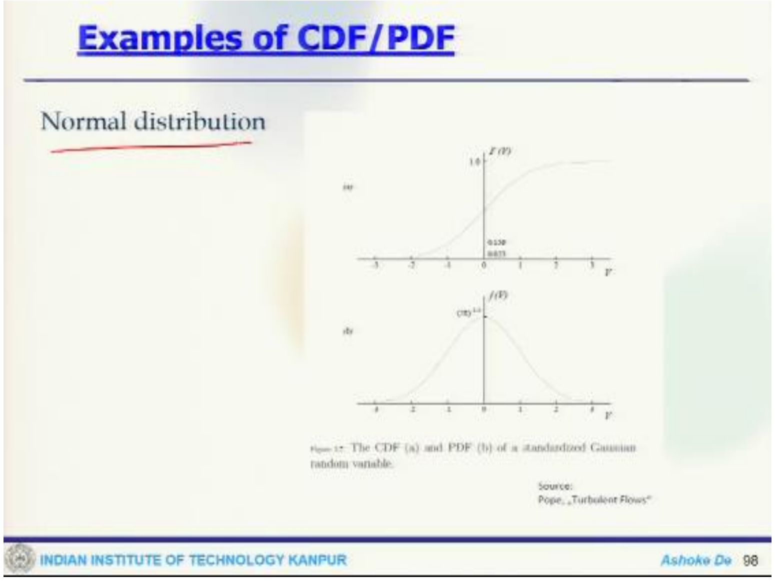

Examples of CDF/PDF

Normal distribution

Figure 3.7 The CDF (a) and PDF (b) of a standardized Gaussian random variable.

Source:
Pope, „Turbulent Flows"

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Now, this is a normal distribution, which already we have seen. This is the CDF variation and this you get.

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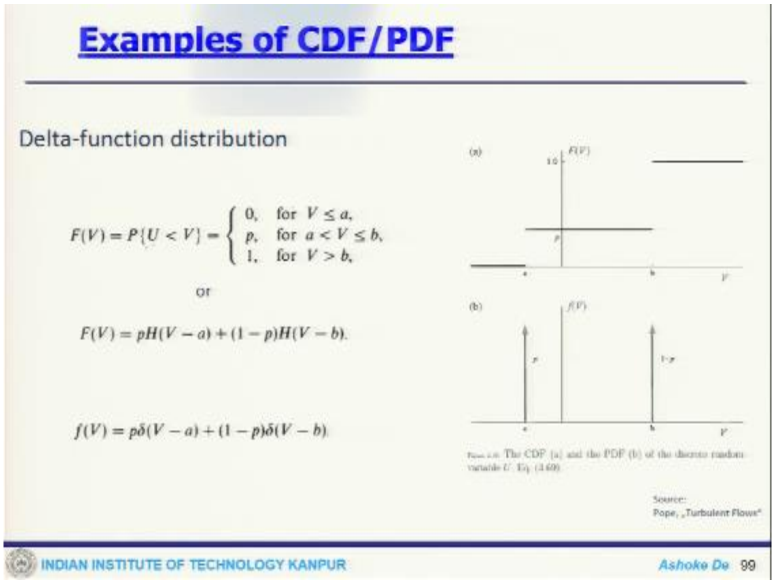

Examples of CDF/PDF

Delta-function distribution

$$F(V) = P\{U < V\} = \begin{cases} 0, & \text{for } V \le a, \\ p, & \text{for } a < V \le b, \\ 1, & \text{for } V > b, \end{cases}$$

or

$$F(V) = pH(V-a) + (1-p)H(V-b).$$

$$f(V) = p\delta(V-a) + (1-p)\delta(V-b).$$

The CDF (a) and the PDF (b) of the discrete random variable U. Eq. (3.60)

Source:
Pope, „Turbulent Flows"

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And now, if you have, for example, δ function distribution that means the CDF is here applicable they are so, that means V less than a, 0; it would be p for a<V<b. So, that is my CDF. So, this can be written like a function. Now the probability distribution at this point there will be the peak. So, this is my probability distribution function of that.

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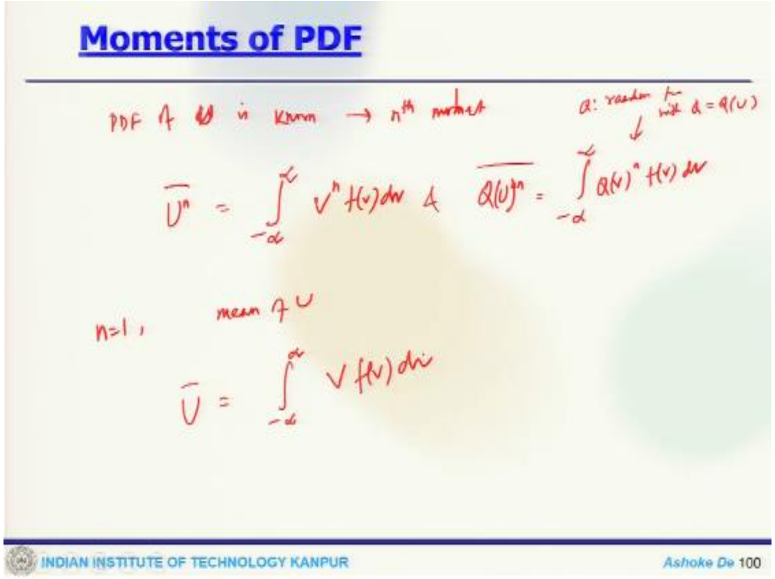

Moments of PDF

PDF of U is known → n^{th} moment

Q: random fn with $Q = Q(U)$

$$\overline{U^n} = \int_{-\propto}^{\propto} V^n f(v)\,dv \;\; \& \;\; \overline{Q(U)^n} = \int_{-\propto}^{\propto} Q(V)^n f(v)\,dv$$

n=1, mean of U

$$\overline{U} = \int_{-\propto}^{\propto} V f(V)\,dv$$

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Because now we can take the let us say PDF of U is known then we can find that n^{th} moment. How do you find that n^{th} moment would be

$$\overline{U^n} = \int_{-\propto}^{\propto} V^n f(v)\,dv$$

And

$$\overline{Q(U^n)} = \int_{-\propto}^{\propto} Q(V)^n f(v)dv$$

. Now, you can take the first moment if n =1, then this will be

$$\bar{U} = \int_{-\propto}^{\propto} Vf(v)dv$$

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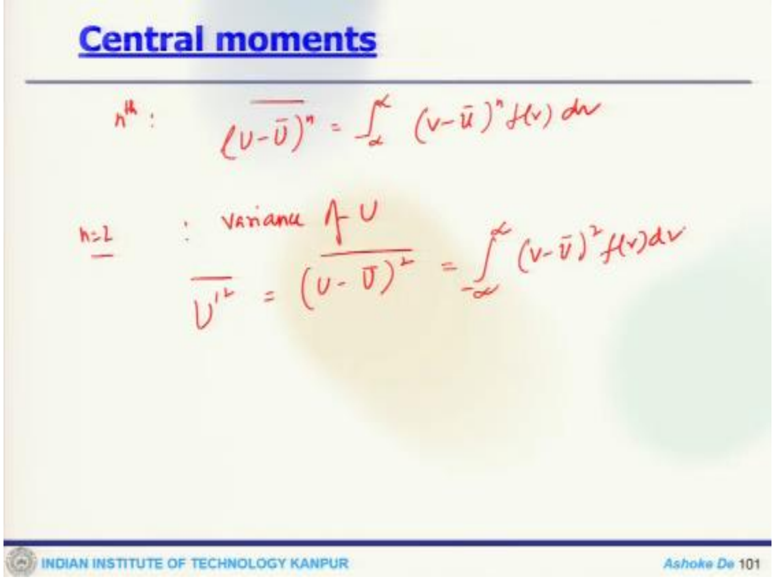

Central moments

n^{th} : $\overline{(U-\bar{U})^n} = \int_{\infty}^{\infty} (v-\bar{u})^n f(v)\, dv$

$n=2$: variance of U

$\overline{U'^2} = \overline{(U-\bar{U})^2} = \int_{-\infty}^{\infty} (v-\bar{v})^2 f(v) dv$

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Similarly, you can find the nth central moment, which is let us say

$$\overline{(U-\bar{U})^n} = \int_{-\propto}^{\propto} (v-\bar{u}) f(v)dv$$

So, the n equals 2, which will give you the second central moment, which is essentially the variance of U, which give you

$$\overline{U'^2} = \overline{(U-\bar{U})^2} = \int_{-\propto}^{\propto} (v-\bar{u})^2 f(v)dv$$

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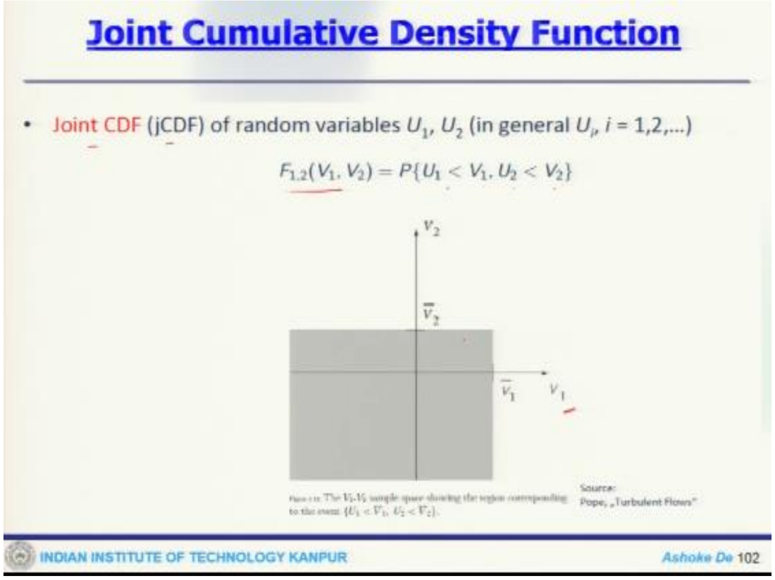

Joint Cumulative Density Function

- Joint CDF (jCDF) of random variables U_1, U_2 (in general U_i, $i = 1,2,\ldots$)

$$F_{1,2}(V_1, V_2) = P\{U_1 < V_1, U_2 < V_2\}$$

[illegible] The V_1-V_2 sample space showing the region corresponding to the event $\{U_1 < V_1, U_2 < V_2\}$.

Source:
Pope, „Turbulent Flows"

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So, from the PDF you can find out now, we can look at the joint cumulative density function. So, that is the joint CDF of random variable U_1, U_2 in general. So, the joint CDF would be written that

$$F_{1,2}(V_1, V_2) = P\{U_1 < V_1, U_2 < V_2\}$$

So, this is a distribution of V_1, this is a distribution of V_2. So, the joint CDF will belong in this particular space because this is more than V_1 more than V_2. So, this is the idea for this that means it is dependent on 2 spaces.

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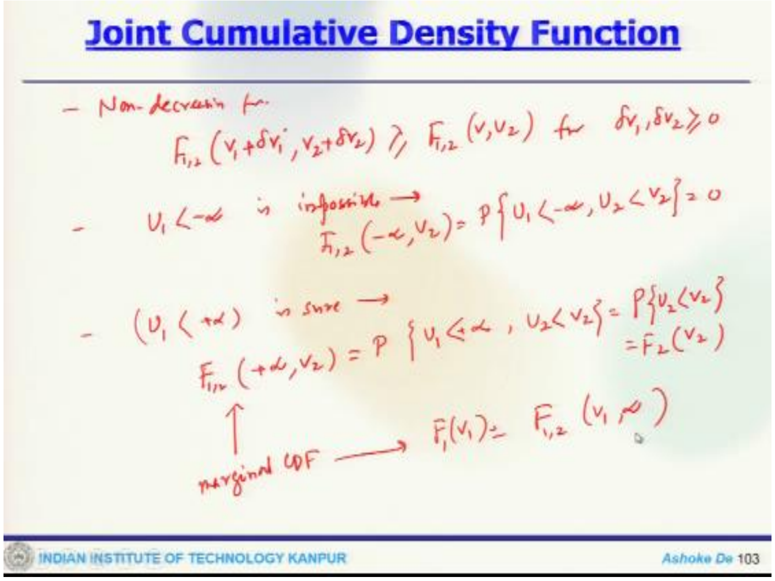

Joint Cumulative Density Function

- Non-decreasin fn.

$$F_{1,2}(v_1+\delta v_1, v_2+\delta v_2) \geq F_{1,2}(v_1, v_2) \text{ for } \delta v_1, \delta v_2 \geq 0$$

- $U_1 < -\infty$ is impossible $\rightarrow$

$$F_{1,2}(-\infty, V_2) = P\{U_1 < -\infty, U_2 < V_2\} = 0$$

- $(U_1 < +\infty)$ is sure $\rightarrow$

$$F_{1,2}(+\infty, V_2) = P\{U_1 < +\infty, U_2 < V_2\} = P\{U_2 < V_2\} = F_2(V_2)$$

$\uparrow$

marginal CDF $\longrightarrow$ $F_1(V_1) = F_{1,2}(V_1, \infty)$

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Now some properties of that this is non-decreasing function that means,

$$F_{1,2}(V_1 + \delta V_1, V_2 + \delta V_2) \geq F_{1,2}(V_1, V_2) \;\; for \; \delta V_1, \delta V_2 \geq 0$$

Now since $U_1 < -\infty$ is impossible, which gets you

$$F_{1,2}(+\infty, V_2) = P\{U_1 < +\infty, U_2 < V_2 \} = 0$$

Also $U_1 < +\infty$ is sure you get

$$F_{1,2}(-\infty, V_2) = P\{U_1 < -\infty, U_2 < V_2 \} = P\{U_2 < V_2\} = F_2(V_2)$$

So, this is one can think about a marginal CDF which means,

$$F_1(V_1) = F_{1,2}(V_1, \infty)$$

So, these are some of the properties of the joint CDF. Now, we look at the other properties in the next class we will stop here today.