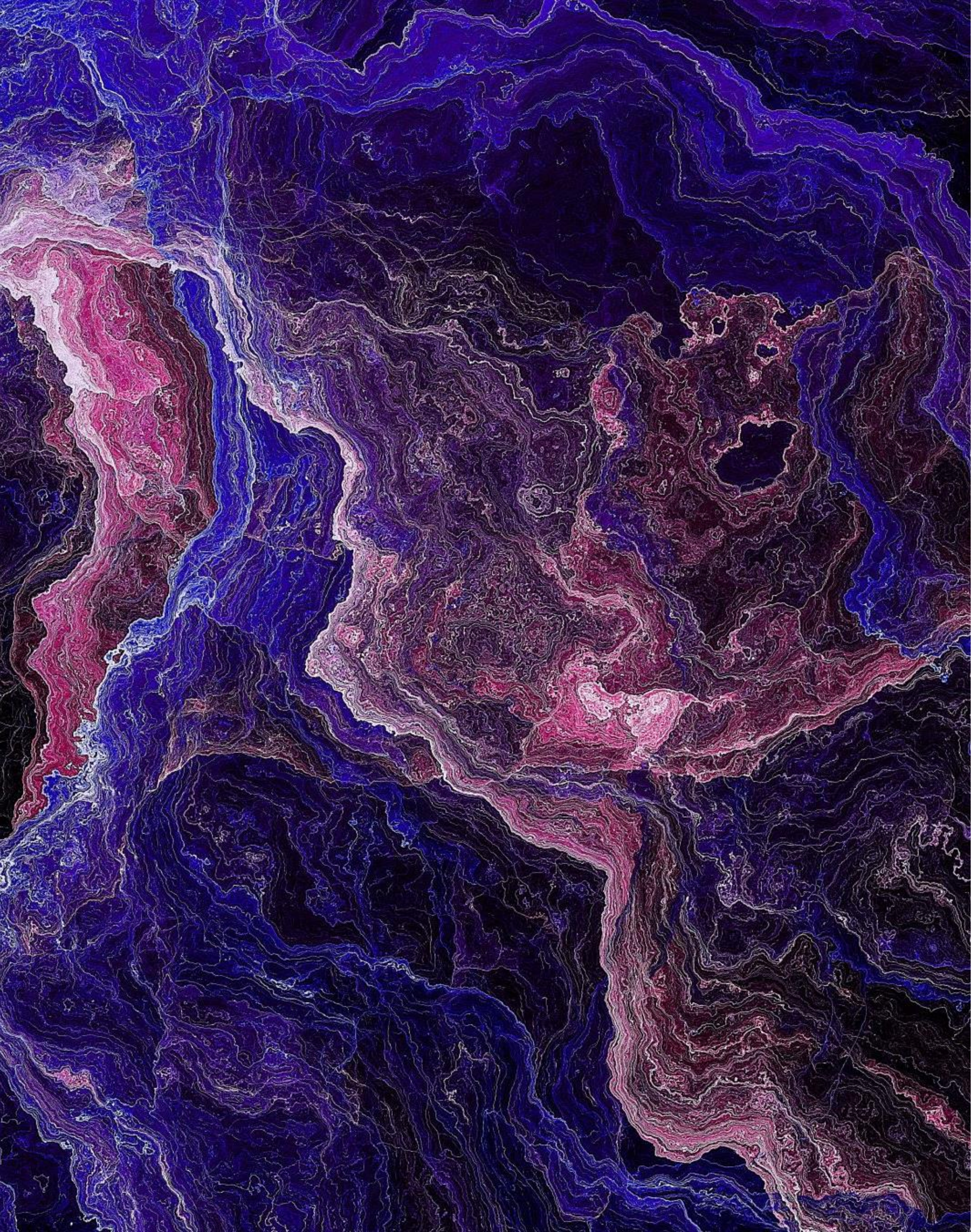
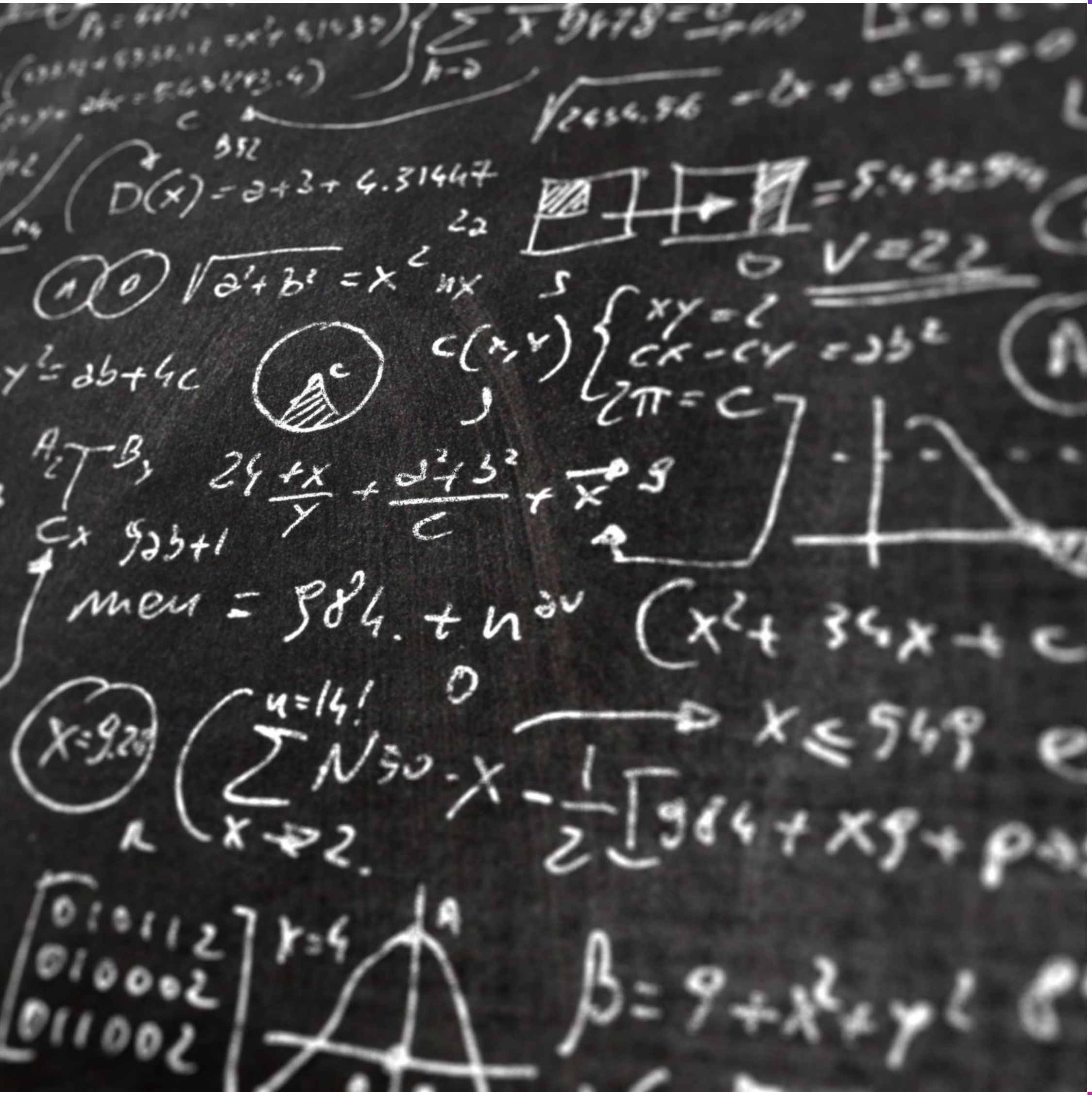


Computations in Chemical Engineering: Graphs and Monte Carlo

Chemineer's Project(Jan'24-May'24)

Mentors: Vaibhav & Samarth



PART 1: INTRODUCTION TO GRAPHS

-Vaibhav

Recursion and STL Basics

Introduction to recursion and its importance in problem-solving

List of problems for recursion practice:

- Reverse a String
- Valid Palindrome
- Tower Of Hanoi
- Subsets

Overview of C++ STL Basics focusing on vectors, stacks, and queues

- Reverse words in a given string
- Next Greater Element
- First Unique Character in a String

Structures, Linked Lists, and Trees

Introduction to structures in C++ and their significance

Standard problems on stacks, queues, and linked lists:

- Implement Stack using Queues
- Implement Queue using Stacks
- Problems related to linked lists such as reversing and deleting nodes

Overview of binary trees and standard tree traversal algorithms:

- Binary Tree Inorder, Preorder, and Postorder Traversals
- Level Order Traversal
- Symmetric Tree and Validate Binary Search Tree problems

Graphs and Additional Topics

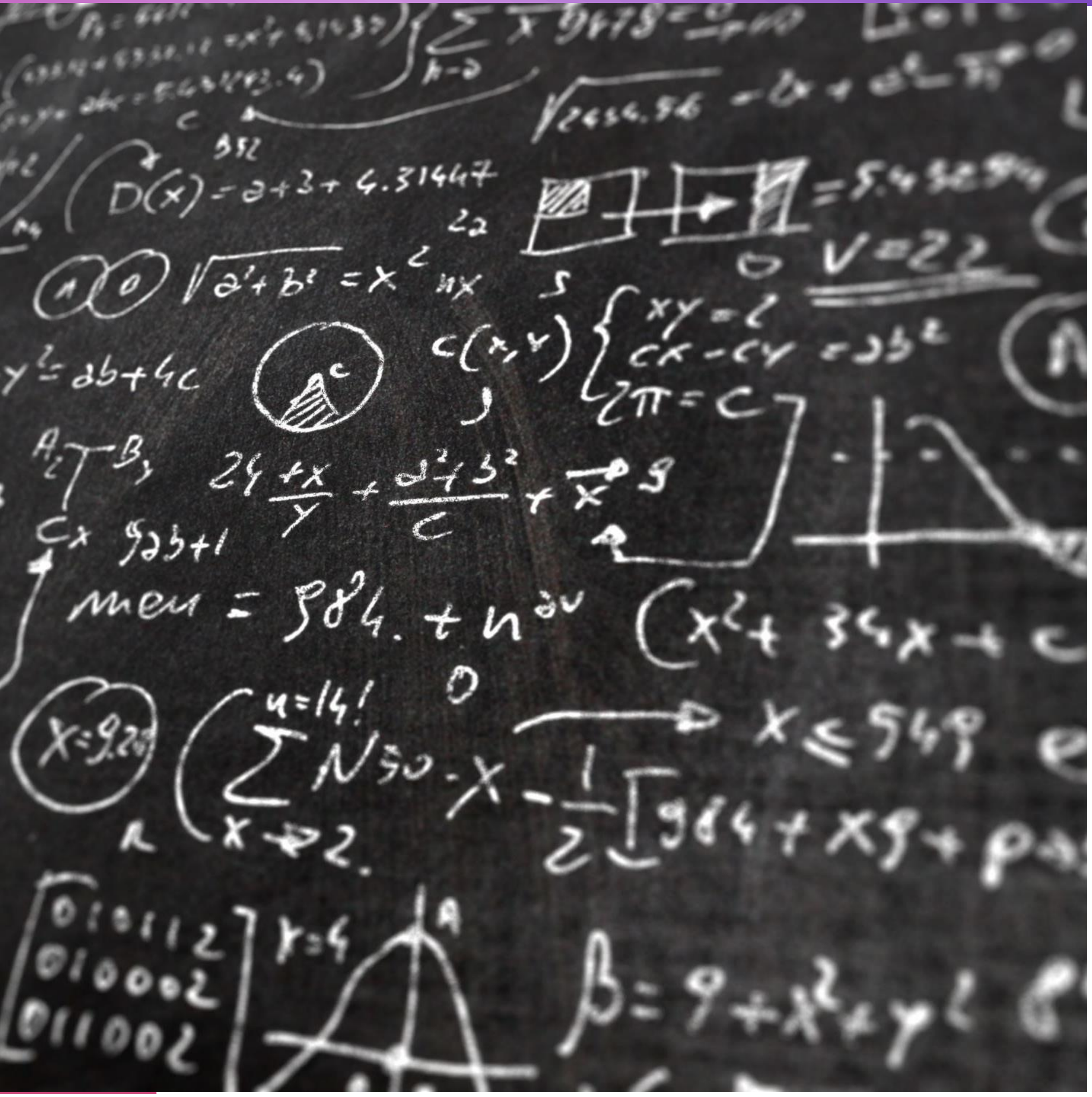
Introduction to graphs and their representation

Graph traversal algorithms: Breadth-First Search (BFS) and Depth-First Search (DFS)

- Is Graph Bipartite?
- Cycle Detection in Undirected and Directed Graphs

Brief overview of additional topics like Heaps, Priority Queues, and Grid DFS

- Graph traversal algorithms: Breadth-First Search (BFS) and Depth-First Search (DFS)



PART 2: MONTE CARLO

-Samarth

Understanding Random Variables and Statistical Distributions

1. Random Variables

Definition: Random variables map outcomes of random processes to numbers, quantifying the outcomes.

Distinction from algebra variables: Unlike algebra variables, random variables have a set of possible values and can randomly take any of those values.

Notation: Random variables are denoted by capital letters (e.g., $\boldsymbol{X}$).

2. Types of Random Variables

Discrete Random Variables: Have distinct, countable values obtained by counting.

- Example: Outcome of tossing a coin (1 for 'Head', 0 for 'Tail').

Continuous Random Variables: Have values obtained by measuring, within an interval.

- Example: Mass of a random human selected on Earth (any value between 0 and 200kg).

3. Statistical Distributions

Definition: Collections of data or scores on a variable, represented by functions giving probabilities of different outcomes.

Common Distributions:

- Bernoulli
- Binomial
- Poisson
- Uniform
- Normal (Gaussian)

4. Choosing the Right Distribution

Factors to consider:

- Discrete or continuous data
- Symmetry in data
- Presence of upper or lower limits
- Likelihood of observing extreme values

5. Common Distributions Explained

Bernoulli Distribution: Discrete distribution with only two outcomes.

Binomial Distribution: Collection of Bernoulli trials with the same probability throughout.

Poisson Distribution: Models the probability of many events occurring in a fixed interval.

Uniform Distribution: Equally likely outcomes within a range.

Normal Distribution: Symmetric distribution characterized by mean and standard deviation, suitable for central tendency analysis.

Conclusion: Understanding random variables and statistical distributions is crucial for interpreting data effectively in various domains, including data science and statistics.

Introduction to Monte Carlo Methods

1. Monte Carlo & its Methods

Overview: Monte Carlo methods are computational techniques based on random sampling to obtain numerical results.

Applications: Widely used in various fields, including physics, engineering, finance, and statistics.

2. Introduction to Monte Carlo

Monty Hall Problem: Famous probability problem illustrating counterintuitive results.

Example 1: Toy Collector Problem: Simulating random events to solve a practical scenario.

Example 2: Complicated Integral: Approximating complex integrals using random sampling.

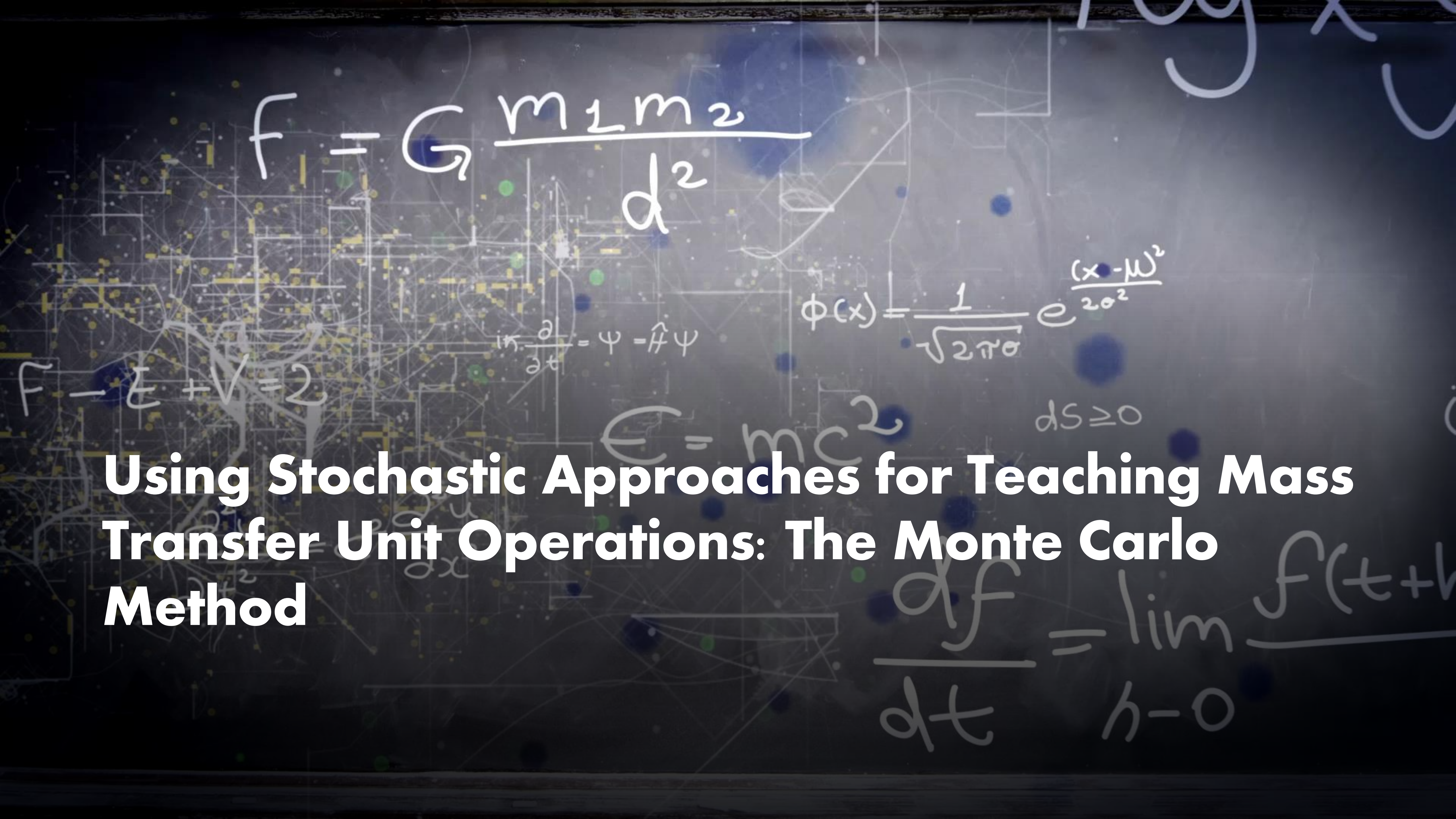
3. Discrete Inverse Transform

Generating Discrete Random Variables: Technique for generating random variables with discrete distributions.

Inverse Transform Method: Algorithm for transforming uniform random variables into desired distributions.

4. Discrete Accept Reject

The Acceptance-Rejection Technique: Method for generating random variables from a given distribution by accepting or rejecting samples.



Using Stochastic Approaches for Teaching Mass Transfer Unit Operations: The Monte Carlo Method

Introduction

- **Introduction:**
- Mass transfer separations are crucial in the chemical industry.
- Traditional teaching methods rely on deterministic models.
- Stochastic approaches, like Monte Carlo simulations, offer alternative perspectives.
- **Methodology:**
- **Software**: PTC Mathcad Prime used for easy implementation.
- **Algorithm**: Monte Carlo simulations applied to solve complex problems.

Application and Objectives

Application of Monte Carlo Method:

Case Studies:

- Batch distillation
- Gas membrane separation

Objectives and Limitations:

Objectives:

- Quantitative analysis without complex math.
- Utilization of statistical concepts.
- Enhancing computing skills.

Limitations:

- Suitable for advanced students.

Results and Conclusion

Results and Discussion:

Case Study 1: Batch Distillation

- Solution by deterministic equations vs. Monte Carlo stochastic approach.
- Implementation details and comparison of results.

Conclusion:

Monte Carlo simulations offer simpler and more versatile solutions.

Enhance students' understanding of mass transfer operations.

Promote integration of math, computing, and science in engineering education.

End Term Evaluation

- Using Stochastic approach, determine the ternary diagram for mixture of benzene, toluene, and cumene using Raoult's law with average relative volatilities as 2.4, 1, and 0.21 respectively. Given the initial mole fractions as 0.85, 0.12,and 0.03 respectively.
- Also, plot the curve showing how mole fraction of each compound is changing with each step.

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