

## **Science 2 (PART 1)**

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### **Requirements:**

- Newtonian Mechanics
  - Lagrangian formulation /Classical Mechanics
  - Basics of Matrix
  - Statistical Mechanics
  - Matlab/Python/C++
  - Graphical Plot (Must)
  - Computational Complexity, Error calculation
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### **Module -1 a,b (prerequisite):**

- Basics of matrix
- Computational Knowledge
- Solving Linear Equations (Class 10 mode)

### **Module -1 a (Tools you will learn /or revisit):**

- Algebra of matrices
  - Singularity, condition of singularity, Symmetric, diagonal, Identity, upper triangular, zero, Hermitian, Vector Norm, Matrix norm, Matrix condition number, Error bounds,
  - Operation: Addition, Multiplication, Trace,
  - Naïve Gaussian elimination: Forward and backward elimination, pseudo code, computational complexity
  - Tridiagonal Systems, Diagonal Dominance, Tridiagonal Algorithm-importance, Examples, Gauss-Jordan Algorithm, LU decomposition in any linear equations, Cholesky decompositions , pseudo code
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**Module -1b (prerequisite):**

- Basics of matrix
- Module 1a
- Algebra of matrices

**Module -1 b (Tools you will learn /or revisit):**

- Linear Least square Problems :  $Ax \approx b$ ; data fitting, Existence and uniqueness, Normal Equations,
  - Orthogonality, Sensitivity, Normal Equations, QR factorization: Orthogonal transformation to triangular form,
  - Householder transformation, Gram-Schmidt Orthogonalization, Computational complexity
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**Overall Target:**

- Know how systems of linear equations can be compactly represented in terms of matrix-vector multiplication
  - Give examples of overdetermined and underdetermined systems, and systems with a unique solution
  - Application
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**Module -2 (prerequisite):**

- Basics of matrix
- Module 1
- Ordinary Differential Equations
- Newtonian Mechanics

**Module -2 (Tools you will learn):**

- Algebra of matrices

- Singular Value decomposition (used to solve linear least square problems in any rank)
  - Eigen Value Problems, Algorithm
  - Spring-mass systems, ecology
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### **Overall Targets:**

- Complete Idea about eigen value and eigen vector
  - Singular Value Decomposition
  - Application of eigen value and eigen vectors in real
    - spring-mass systems
    - Rabbit vs Sheep or Rabbit vs Lynx
    - Eigen value determines the stability of large eco systems
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### **Module -3 (prerequisite):**

- Module 1,2
- Ordinary Differential Equations
- Newtonian Mechanics

### **Module -3 (Learning outcome):**

- Learning of Non-linear Differential Equations
  - Predator-Prey interactions and SIR model
  - Numerical Methods-Euler, Runge-Kutta 4
  - Double Pendulum, Lorenz Oscillator
  - Chaos theory : A brief and general idea (sensitivity to IC)
  - Fractal
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### **Overall Target:**

- Numerical solution of nonlinear ordinary differential equations
  - Modelling disease, emergence of chaos, chaos in physical systems
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**Module -4 (prerequisite):**

- Random Numbers
- Numerical Integration
- Probability and Statistics (knowledge on distribution)

**Module -4 (Learning outcome):**

- Monte Carlo Method
  - Importance sampling
  - Random number generation techniques
  - Non-uniformly distributed Random Number Generator
  - Metropolis-Hastings algorithm
  - Application to numerical integration
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**Overall Targets:**

- Calculation of Pi
  - Random Walk
  - Multidimensional Integration
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**Module -5 (prerequisite):**

- Numerical techniques for ODE (Module 3)
- Module 4
- Brownian Motion

**Module -5 (Learning outcome):**

- SDE –Numerical solver
  - Brownian motion simulation/Langevin equation
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**Module -6 (prerequisite):**

- Differential Equation

**Module -6 (Learning outcome):**

- PDE –Numerical solver
  - Reaction-diffusion systems
  - Spiral/stripe pattern in reality
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## **Reference Material**

1. Introduction to Computational Physics, Lecture of Prof. H. J. Herrmann  
Swiss Federal Institute of Technology ETH, Zürich, Switzerland Script by  
Dr. H. M. Singer, Lorenz Müller and Marco - Andrea Buchmann  
Computational Physics, IfB, ETH Zürich **(Module 3, 4, and 6)**
  2. Nonlinear Dynamics –Steven Strogatz **(Module 2 and 3)**
  3. Scientific Computing, An Introductory Survey, Second Edition by Michael T.  
Heath **(Module 1-4,6)**
  4. Numerical Solution of Stochastic Differential Equations in Finance Timothy  
Sauer, Department of Mathematics, George Mason University, Fairfax, VA  
22030, tsauer@gmu.edu **(Module 5)**
  5. Books: Gilbert Strang **(Module 1 and 2)**
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