Methods of modeling and analysis of complex systems

7 lectures (2*7 = 14 hours)

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1. Course Description and Motivation

In this Course, we shall familiarise with the main computational tools which permit to simulate and analyse the dynamic behavior of a wide range of physical problems involving fluids, solids, soft matter and quantum systems, as well as the dynamics of (some) biological and social systems. Special attention will be paid to the data which result from simulations of the above systems, as well as to the techniques to analyse and extract physical knowledge from such datasets.

2. Learning goals

The main goal of the course is to make the student acquainted with major computational techniques for solving a broad range of complex problems involving fluids, solids, waves, as well as biological and social systems with internal degrees of freedom. Techniques to analyse the corresponding data will also be presented.

3. At the completion of the course, the student is expected to be able to:

- Employ and develop concepts and methods for the large scale simulations of the dynamic behavior of complex systems, as well as the corresponding data analysis techniques.
- Read the current literature and appreciate the various approaches to large-scale simulation of scientific and engineering applications
- Choose and code the most appropriate computational techniques for modelling and data-analysing complex problems in physics, engineering biology and also social sciences.
- Contribute to research projects involving the simulation and data analysis of complex natural and social systems.

4. Contents

I. Deterministic Methods

1) Numerical Differentiation. Finite Differences Finite Difference Derivatives. Numerical Integration. Rectangular Rule. Trapezoidal Rule. The SIMPSON Rule. The NEWTON-COTES Rules. GAUSS-LEGENDRE Quadrature. An Example.
2) Ordinary Differential Equations: Initial Value Problems. EULER AND RUNGE-KUTTA Methods. An Example: The KEPLER Problem. The Nonlinear Pendulum problem. The Lorenz system, numerical Analysis of Chaos. Molecular Dynamics.
3) Numeric Differential Equations: Boundary Value Problems. Finite Difference Approach. Shooting Methods. The One-Dimensional Stationary Heat Equation. The Time-Dependent Heat Equation.

II. Stochastic Methods

1) Some Basics of Stochastic Processes. Stochastic Processes. MARKOV Processes. MARKOV-Chains. Continuous-Time MARKOV-Chains.
2) A Brief Introduction to Monte-Carlo Methods. Monte-Carlo Integration.
3) The Random Walk and Diffusion Theory. The WIENER Process and Brownian Motion. Diffusion Models. MARKOV-Chain Monte Carlo Methods.
4) Brief introduction to Data Analysis. Statistical Analysis for Beginners. Calculation of Errors. Auto-Correlations. The Histogram Technique. Discrete Probability distributions: Uniform, Binomial, Poisson, Hyper-geometric, Empirical distribution. Hypothesis Testing. Regression: Simple and multiple linear regression techniques. Time series forecasting: moving average and exponential

Literature

1. Steven C. Chapra, Applied Numerical Methods with MATLAB® for Engineers and Scientists, Third Edition.
2. T. Pang, Computational Physics, Cambridge Univ. Press, (https://www.amazon.com/Introduction-Computational-Physics-Tao-Pang/dp/05...)
3. Mark Newman, Computational Physics, CreateSpace Independent Publishing Platform.
4. 3. A. Klein and A. Godunov, Introductory Computational Physics, Cambridge University.
5. Textbook: Numerical Recipes: The Art of Scientific Computing, William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery. (Free online), http://numerical.recipes/book.html.
6. Peck, R., Olsen, C. & Devore, J. (2019). Introduction to Statistics and Data Analysis. (6th ed.) Cengage Learning. ISBN 9781337793612.
7. Wasserman, L. (2004). A Concise Course in Statistical Inference. All of Statistics. New York, NY: Springer. URL: doi.org/10.1007/978-0-387-21736-9 ISBN 9781441923226. Weiss, N. A. (2016). Introductory Statistics. Pearson. ISBN 9780321989178.