15 Curricular Unit

Advanced Physics Topics 1

Module

Computational Physics (CP)

Type

Lecture course

Contact hours

18

Professor/Researcher in charge

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Summary of Contents

Part 1
Monte Carlo Methods in Statistical Physics
Markov Chains: Chapman-Kolmogorov equation; Transient and stationary regimes; Detailed balance.
Monte-Carlo Integration: Hit or Miss Monte-Carlo; integration as an average calculation; random Sampling; importance sampling; Markov Chain Monte-Carlo; Metropolis algorithm
Applications to Statistical Physics: ergodicity; detailed balance; equilibration; estimating errors.
Part 2
Parallel Programming
Introduction; motivations and actual state of development; advantages and disadvantages; parallel computation models; message passing; shared memory; combination of different models; present status and future trends
MPI: introduction and basic concepts; MPI functions; Point-to-point communication; datatypes; compiling and running programs; collective communication; communicators; parallel libraries; implementations.

Part 3
Monte-Carlo method in radiation transport (9h)
Context and relevance of MC methods for both light and ionizing radiation modelling
transport mechanism: phase space, random walks, sampling, interactions, particle creation and destruction, tallies.
computational geometry and boundaries definition
physics: interaction cross sections, attenuation reference to Monte-Carlo packages.

References

Understanding Molecular Simulations, Daan Frenkel and Berend Smit
Computer Simulation of Liquids, M P Allen and D J Tildesley
Monte Carlo Methods in Statistical Physics, by Mark Newman, G T Barkema
Parallel Programming in C with MPI and OpenMP", Michel J. Quinn, 2004, McGraw-Hill.
Parallel Programming with MPI, Peter S. Pacheco, 1997, Morgan Kaufmann.
Using MPI – second edition, W. Gropp, E. Lusk, A. Skjellum, 1999, MIT Press.
Monte Carlo Techniques in Radiation Therapy, CRC Press, Joao Seco e Frank Verhaegen eds., 2013
Fundamentals of Monte Carlo Transport for neutral and Charged particles; Alex F Bielajew, University of Michigan, 1998-2001

Evaluation

Exam with computational exercise
Essay and written report on practical exercises.

Jury

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