



Universidade do Minho



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.

MAP-fis Physics Doctoral Program – mapfis@map.edu.pt – <http://www.map.edu.pt/fis>

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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.

Juri

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