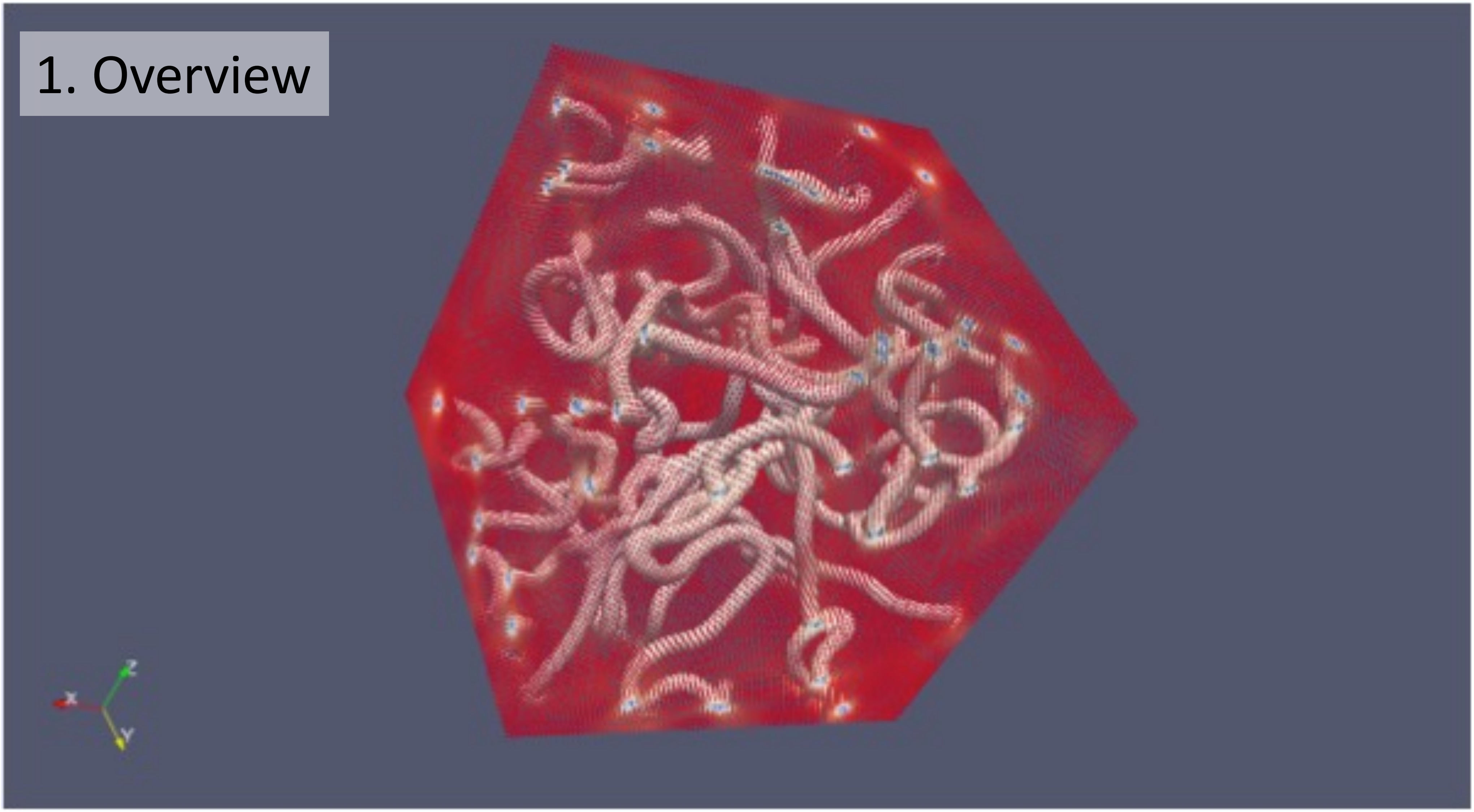
Computational Physics



PHYS 410/510

Information

- **lecture:**
  - Tuesdays and Thursdays , 9:30-10:45
  - no lectures on March 18th & 20th

- **homework:**
  - typically every other week
  - involves writing code
  - posted online

- **webpage:**
  http://www.aglatz.net/home/teaching/compphys_S2025/

- **office hours:**
  Virtual by appointment: aglatz@niu.edu
  Tue&Thu: 11:00-12:00

Exams & Grading

- **Exams/Presentations** *(tentative):*
  - *Midterm task:* March 25-27, 2025 (individualized, 48h)
  - final projects: April 24th, 2025 !

Final grade:

35%: homework percentage

15%: lecture attendance percentage

20%: midterm exam percentage

30%: final project percentage

→ total score between 0 and 1

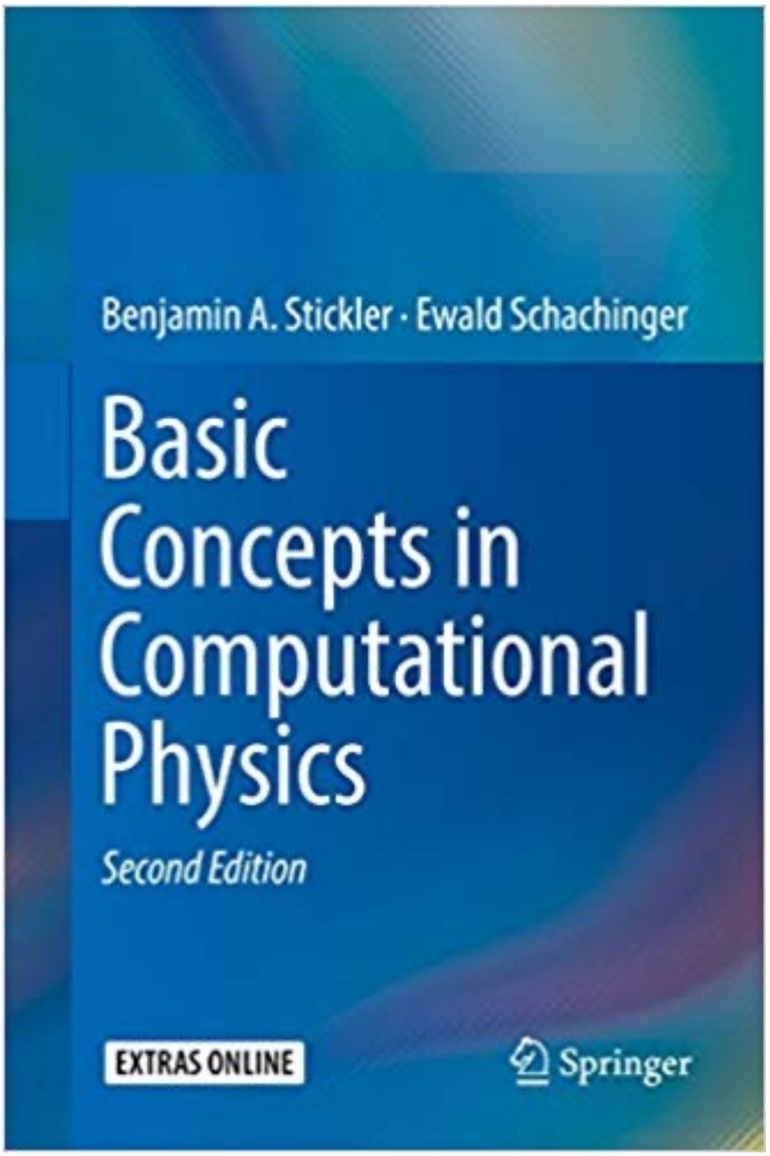
→ multiplied by 12

→ rounded to the closed integer

→ divided by 3, and finally graded according to →

A = 4.00
A- = 3.67
B+ = 3.33
B = 3.00
B- = 2.67
C+ = 2.33
C = 2.00
D = 1.00
F = 0.00

Required textbook



- Benjamin A. Stickler, Ewald Schachinger, *Basic Concepts in Computational Physics*, 2nd Edition, Springer 2016

  https://link.springer.com/content/pdf/10.1007%2F978-3-319-27265-8.pdf

Aim & format

The lecture should

- provide an overview of common deterministic and stochastic methods in computational (classical) physics
- teach the underlying methods and algorithms

→ ***The main aim is to serve as a base for possible future computational research projects.***

Format of the lecture:

- Partially classroom lecture and follows selected chapters of the required textbook
- Mostly hands-on practice in the computer lab [is needed] or on own laptop
- Homework is planned every other week involving writing & running codes plus data analysis.
- Again, attendance is essential, in particular the hands-on practice lectures in order to get started with the homework.

Topics

1. Introduction/Basic Remarks

a. Motivation
b. Floating-point numbers and numerical accuracy: round-off errors
c. Methodological Errors
d. Numerical stability

Based on Chapter 1 + details & examples

2. Numerical Differentiation & Integration

a. Finite Differences
b. Integration/summation rules: Rectangular, trapezoidal, Simpson, Newton-Cotes, Gauss-Legendre

Chapters 2 & 3

Deterministic methods

Chapter 4: The Kepler problem

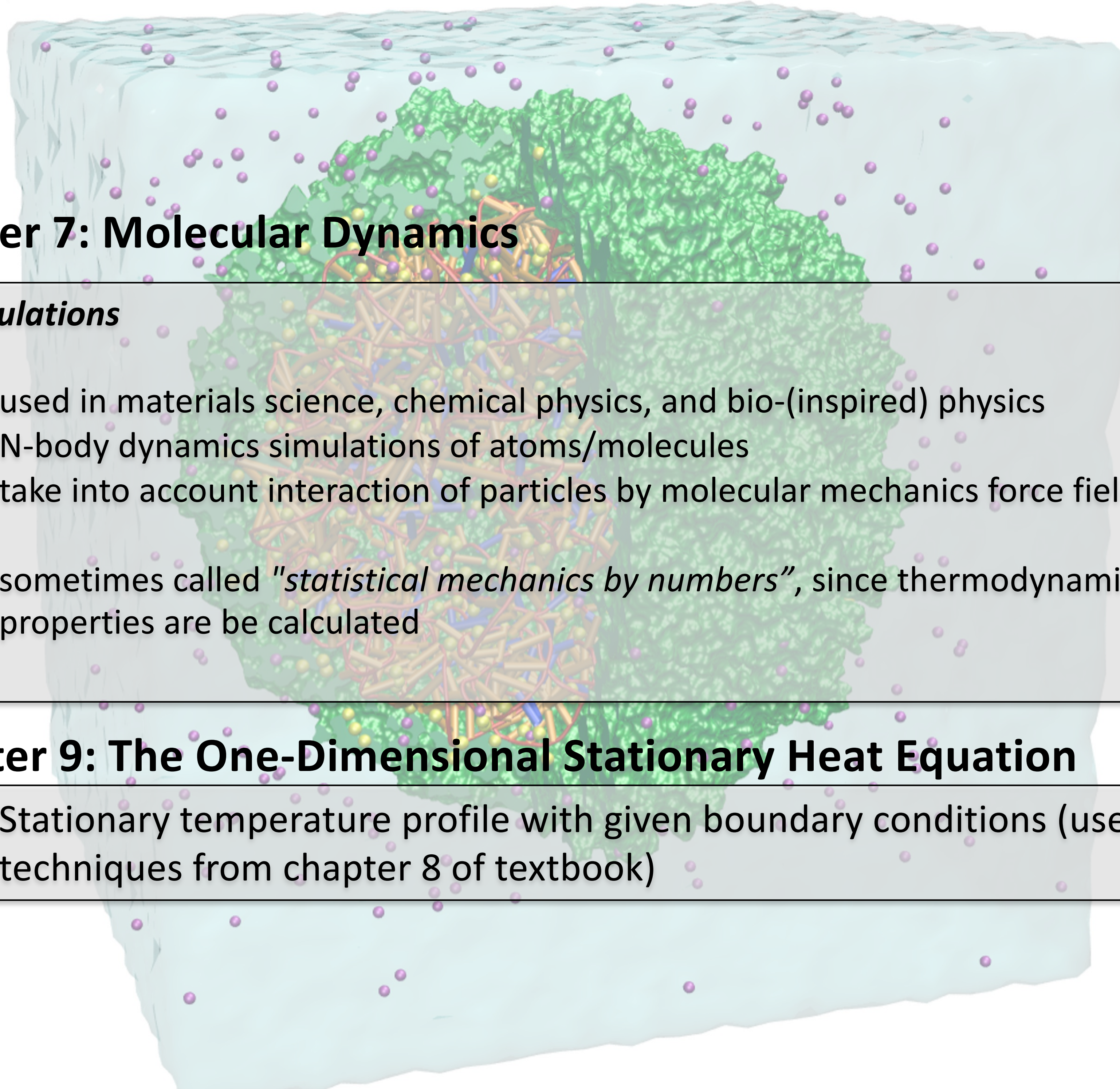
- Special case of the two-body problem
- Application of the Euler method

Chapter 5: ODEs: Initial value problems

- Simple Integration methods
- Runge-Kutta method

Chapter 6: The Double Pendulum

- Hamilton Equation
- Visualization



Chapter 7: Molecular Dynamics

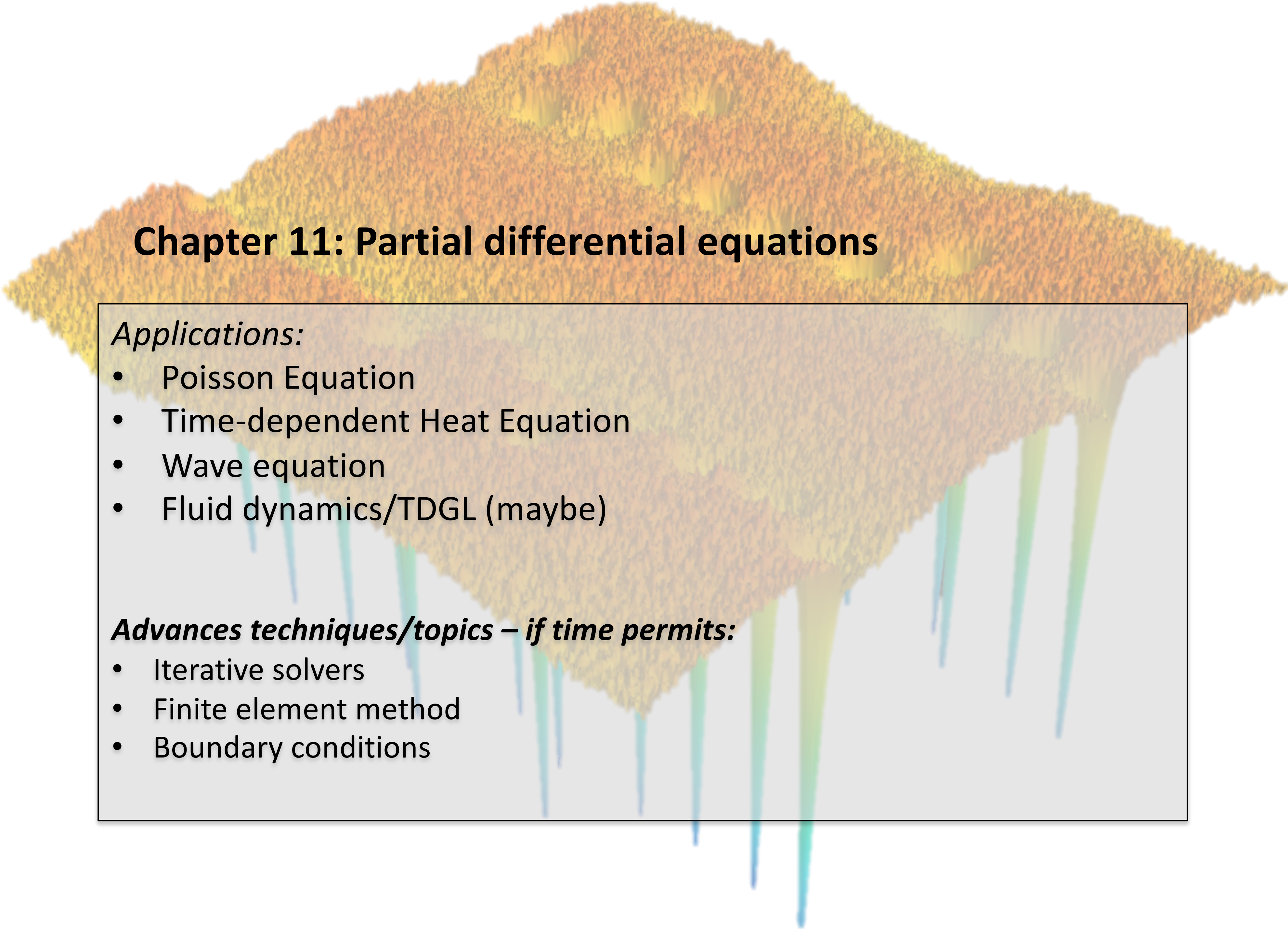
MD simulations

- used in materials science, chemical physics, and bio-(inspired) physics
- N-body dynamics simulations of atoms/molecules
- take into account interaction of particles by molecular mechanics force fields

- sometimes called *"statistical mechanics by numbers"*, since thermodynamics properties are be calculated

Chapter 9: The One-Dimensional Stationary Heat Equation

- Stationary temperature profile with given boundary conditions (use techniques from chapter 8 of textbook)



Chapter 11: Partial differential equations

Applications:

- Poisson Equation
- Time-dependent Heat Equation
- Wave equation
- Fluid dynamics/TDGL (maybe)

Advances techniques/topics – if time permits:

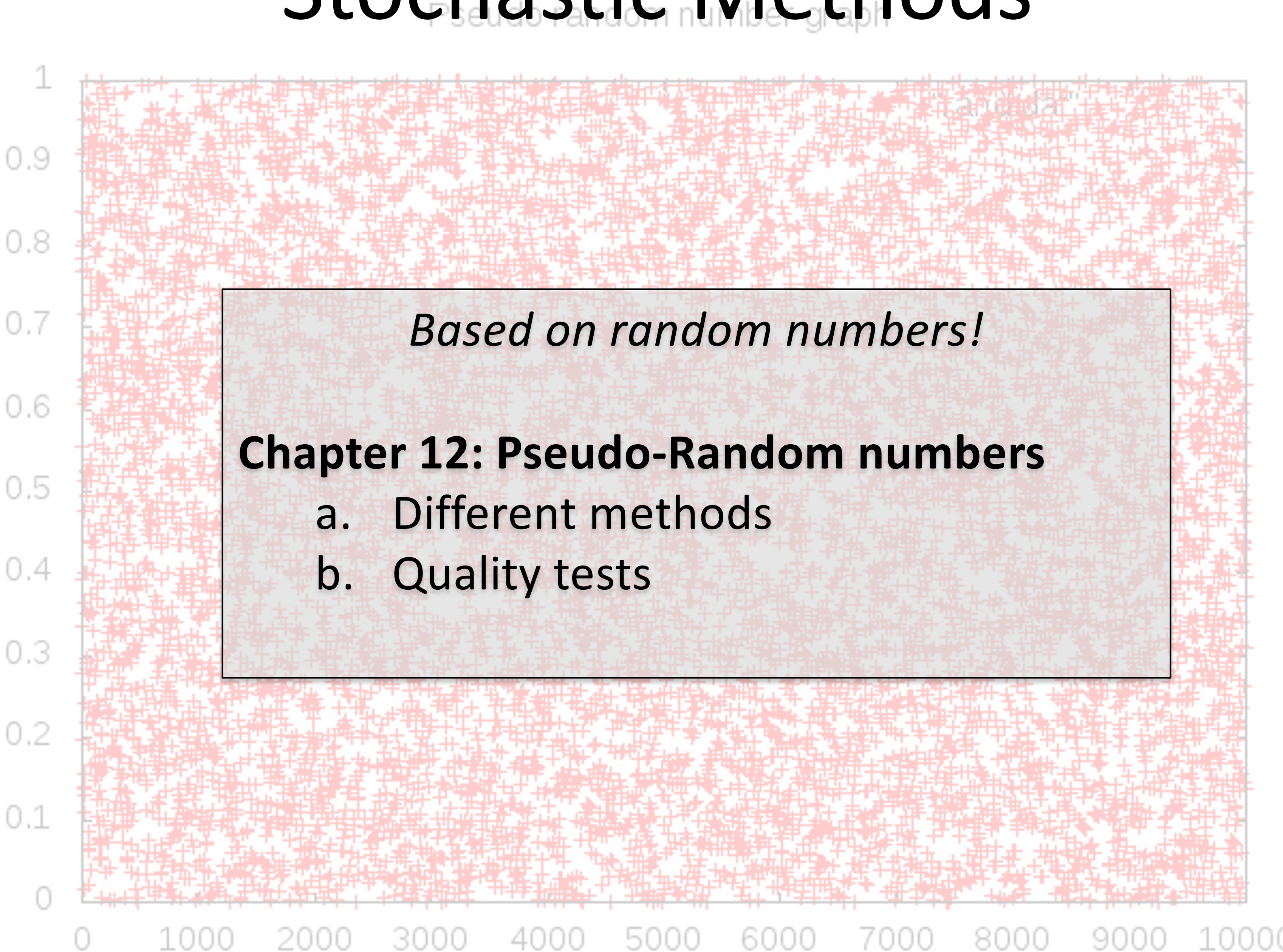
- Iterative solvers
- Finite element method
- Boundary conditions

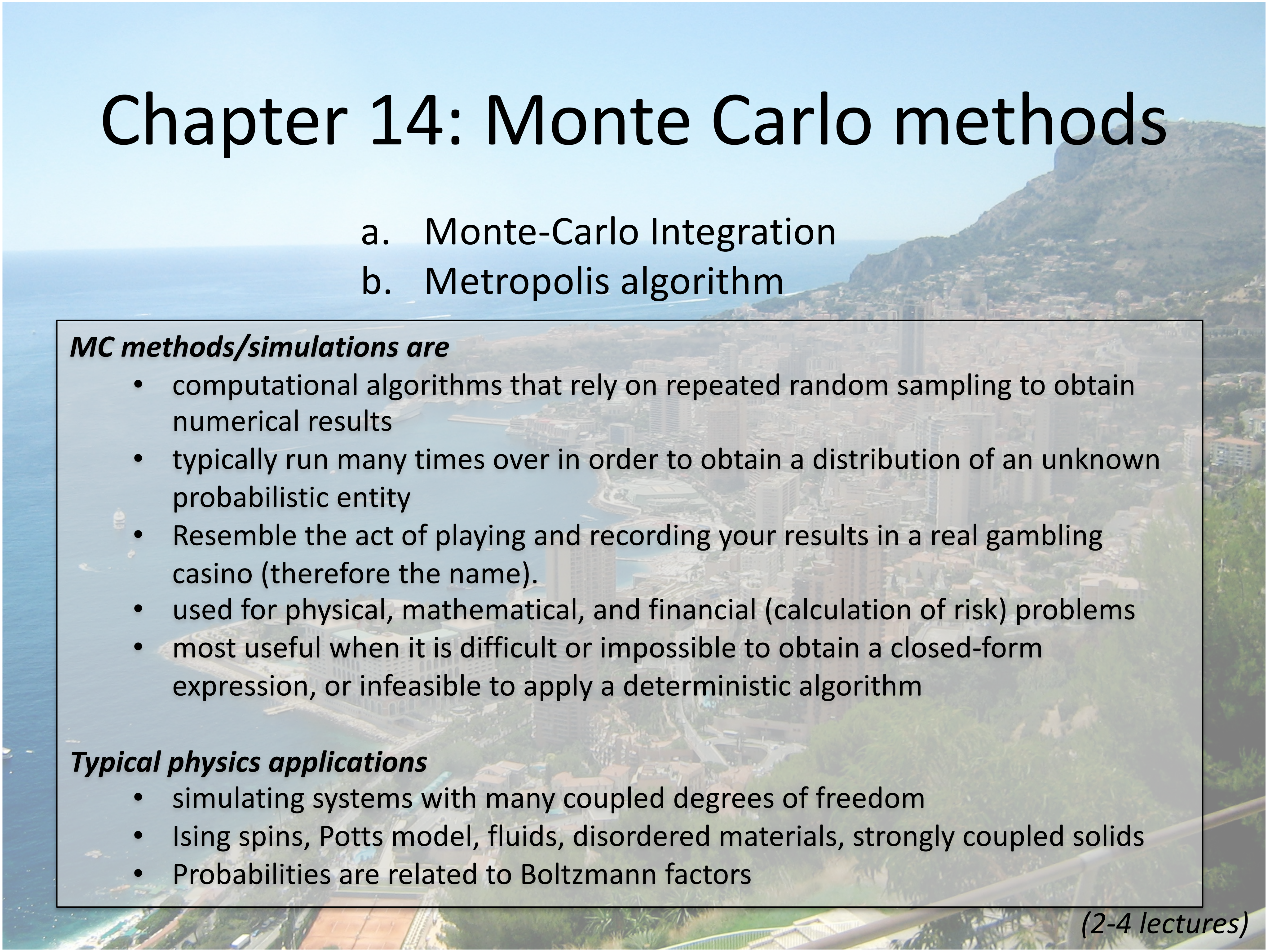
Stochastic Methods

Based on random numbers!

Chapter 12: Pseudo-Random numbers

a. Different methods
b. Quality tests





Chapter 14: Monte Carlo methods

a. Monte-Carlo Integration
b. Metropolis algorithm

MC methods/simulations are

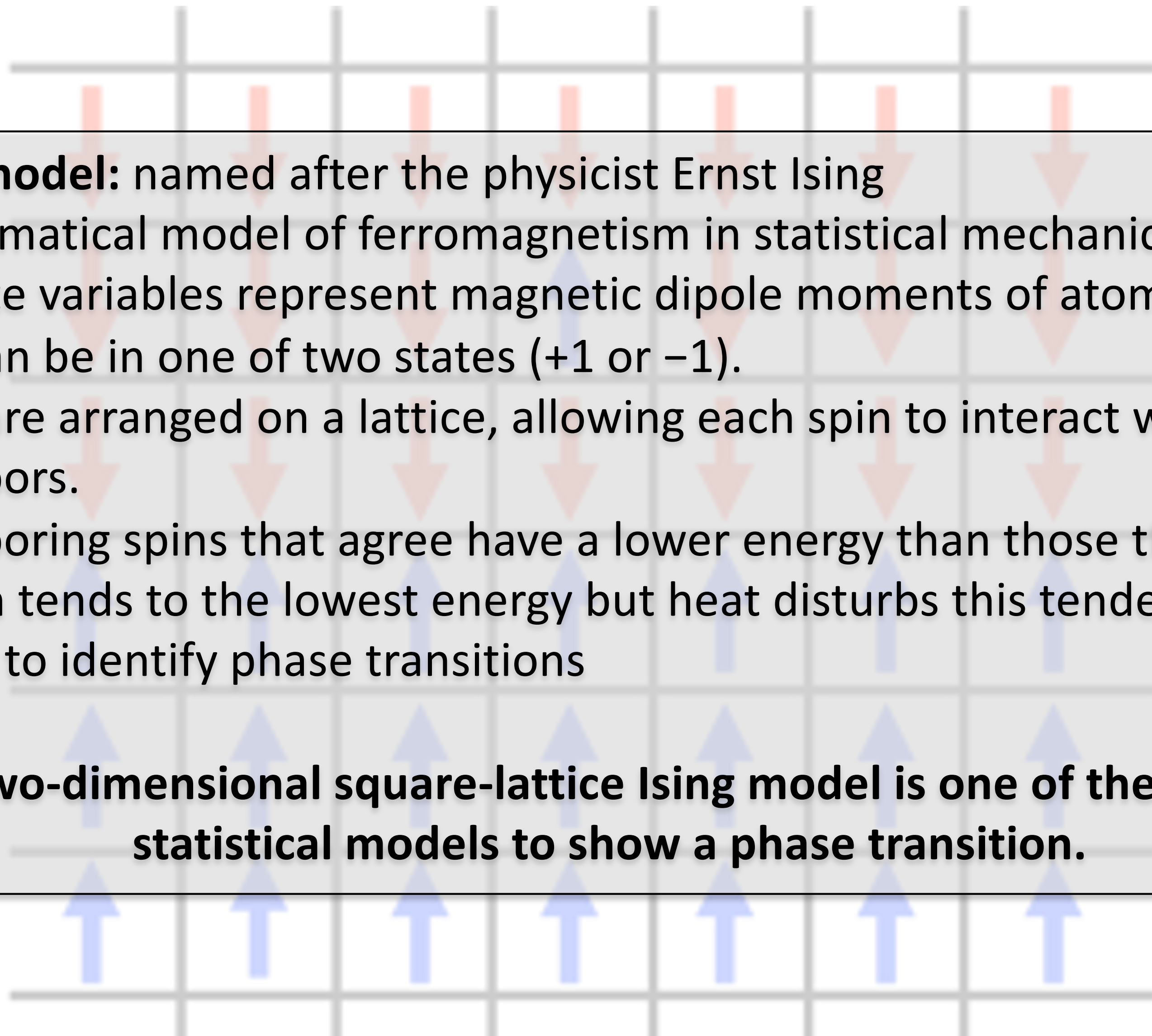
- computational algorithms that rely on repeated random sampling to obtain numerical results
- typically run many times over in order to obtain a distribution of an unknown probabilistic entity
- Resemble the act of playing and recording your results in a real gambling casino (therefore the name).
- used for physical, mathematical, and financial (calculation of risk) problems
- most useful when it is difficult or impossible to obtain a closed-form expression, or infeasible to apply a deterministic algorithm

Typical physics applications

- simulating systems with many coupled degrees of freedom
- Ising spins, Potts model, fluids, disordered materials, strongly coupled solids
- Probabilities are related to Boltzmann factors

(2-4 lectures)

Chapter 15: Ising Model



- **Ising model:** named after the physicist Ernst Ising
- mathematical model of ferromagnetism in statistical mechanics.
- discrete variables represent magnetic dipole moments of atomic "spins" that can be in one of two states (+1 or −1).
- spins are arranged on a lattice, allowing each spin to interact with its neighbors.
- neighboring spins that agree have a lower energy than those that disagree
- system tends to the lowest energy but heat disturbs this tendency
- allows to identify phase transitions

The two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition.

Literature

Additional Textbook suggestions for more details

J. Franklin, *Computational Methods for Physics***,** Cambridge University Press (July 15, 2013)

Nicholas J. Giordano, Hisao Nakanishi, *Computational Physics,* Addison-Wesley; 2 edition (July 31, 2005)

Alfio Quarteroni, Riccardo Sacco and Fausto Saleri, *Numerical Mathematics*, Springer; 2nd edition (October 19, 2006)

Curtis F. Gerald and Patrick O. Wheatley, *Applied Numerical Analysis, Pearson*; 7 edition (August 10, 2003)

Germund Dahlquist and Åke Björck, *Numerical Methods in Scientific Computing: Volume 1*, Society for Industrial and Applied Mathematics (September 4, 2008)

See also course website

Demos

Jupyter-lab (python)

- Plotting with matplotlib
- Magic commands

Command-line

- C program
- Compilation
- Output
- Plotting with gnuplot

Alternative to Jupyter Lab/Notebook:

- Google Colaboratory: colab.research.google.com (requires gmail account)

Other (free) plotting software:

- Labplot (GUI) for 2D plots: labplot.kde.org
- paraview (3D visualization, python scriptable): www.paraview.org

Please do not use Excel for plotting!