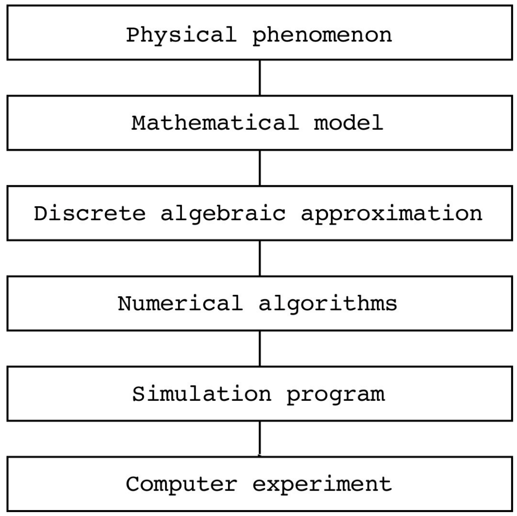
Introduction

COMPUTER EXPERIMENT

- **Computational physics**: An area of physics, in which computers play a central role.
- **Computational physics approach**



1. **Mathematical model** is developed for the **physical phenomenon** of interest.

   Example: Newton's second law of motion for interacting particles. (Three laws of motion were published by Isaac Newton in *Mathematical Principles of Natural Philosophy*, 1686.)

$$m\frac{d^2\vec{r}_i(t)}{dt^2} = \vec{F}_i(t) \quad (i = 1,\ldots,N) \tag{1}$$

2. The equations of the mathematical model are cast into a **discrete algebraic form**, which is amenable to numerical solution.

   Example: Time discretization of the Newton's second law of motion.

$$m\frac{\vec{r}_i(t+\Delta t) - 2\vec{r}_i(t) + \vec{r}_i(t-\Delta t)}{\Delta t^2} = \vec{F}_i(t) \quad (i = 1,\ldots,N; t = 0, \Delta t, 2\Delta t, \ldots)$$

3. **Numerical algorithms** are used to convert the algebraic equation system into a **simulation program**.

   Example 1: Verlet algorithm.

```
compute F_i(t) as a function of x_i(t)
x_i(t+Dt) = 2x_i(t) - x_i(t-Dt) + F_i(t)Dt^2/m
v_i(t) = [x_i(t+Dt) - x_i(t-Dt)]/2Dt
```

   Example 2: velocity-Verlet algorithm.

```
compute F_i(t) as a function of x_i(t)
v_i(t+Dt/2) = v_i(t) + F_i(t)Dt/2m
x_i(t+Dt) = x_i(t) + v_i(t+Dt/2)Dt
compute F_i(t+Dt) as a function of x_i(t+Dt)
v_i(t+Dt) = v_i(t+Dt/2) + F_i(t+Dt)Dt/2m
```

4. **Computer experiments** are performed to follow the time evolution of the model physical system.

- **Type of mathematical models**

	Discrete/particle model (ordinary differential equations)	Continuum model (partial differential equations)
Deterministic	Molecular dynamics	Computational fluid dynamics, continuum mechanics
Stochastic	Monte Carlo particle simulation	Quantum Monte Carlo

- **Discrete (particle) vs. continuum models**: Mathematical models are either the particle type or the continuum type. Particle models trace the motion of many interacting particles, an example being Newton's second law of motion. Particle-type laws are typically formulated as coupled ordinary differential equations.

  Continuum models deal with functions extending over the space. For example, the dynamics of a quantum particle is described by a parabolic partial differential equation called the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=\left(-\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+v(\vec{r})\right)\psi(\vec{r},t)\,, \tag{2}$$

  where $i = \sqrt{-1}$, $\hbar = 1.05\times10^{-34}$ Js is the Planck constant, and $\psi(\vec{r},t)$ is a complex-valued wave function. The square, $|\psi(\vec{r},t)|^2$, of the wave function is the probability to find the particle at position $\vec{r}$ at time t.

- **Molecular dynamics**: Follows Newton's second law of motion for interacting particles.
- **Deterministic vs. stochastic simulations**: Computer simulations are either deterministic or stochastic. Deterministic simulations usually deal with mathematical initial value problems, i.e., differential equations such as Eqs. (1) and (2) are integrated forward in time starting with some initial configuration.

  Stochastic simulations use random numbers to: i) provide approximate solutions to large-scale problems where deterministic solutions are intractable (e.g., statistical mechanics in physics); or ii) simulate stochastic natural phenomena (e.g., stock price).

- **Monte Carlo (MC) method**: A computational method that utilizes random numbers.

WHAT YOU WILL LEARN IN THIS COURSE

The ability to implement the solution of mathematically formulated problems on a computer. We will learn basic elements of computational methods in the context of several computer simulations. Our lecture notes will be organized according to the simulations that we will cover, whereas, in each simulation, we will learn several computational methods covered in the textbook, *An Introduction to Computational Physics*, *2nd Ed*. by Tao Pang. The following diagram summarizes the relationships between the simulations to be covered in the lectures and the computational methods in Tao Pang's textbook.

- **Computational physicists' survival kit**: The following two references will provide sufficient tools to most computational research. After this course, I hope that the students will be able to read and use relevant parts of these books as necessary for their own research projects.

1. **Mathematical methods in physics**: Any book you are familiar with, e.g., G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists, 7th Ed*. (Academic Press, 2012).
2. **Numerical algorithms**: W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes, 3rd Ed*. (Cambridge U Press, 2007)—available online (C: www.nrbook.com/a/bookcpdf.php, Fortran: www.nrbook.com/a/bookfpdf.php, and Fortran90: www.nrbook.com/a/bookf90pdf.php).

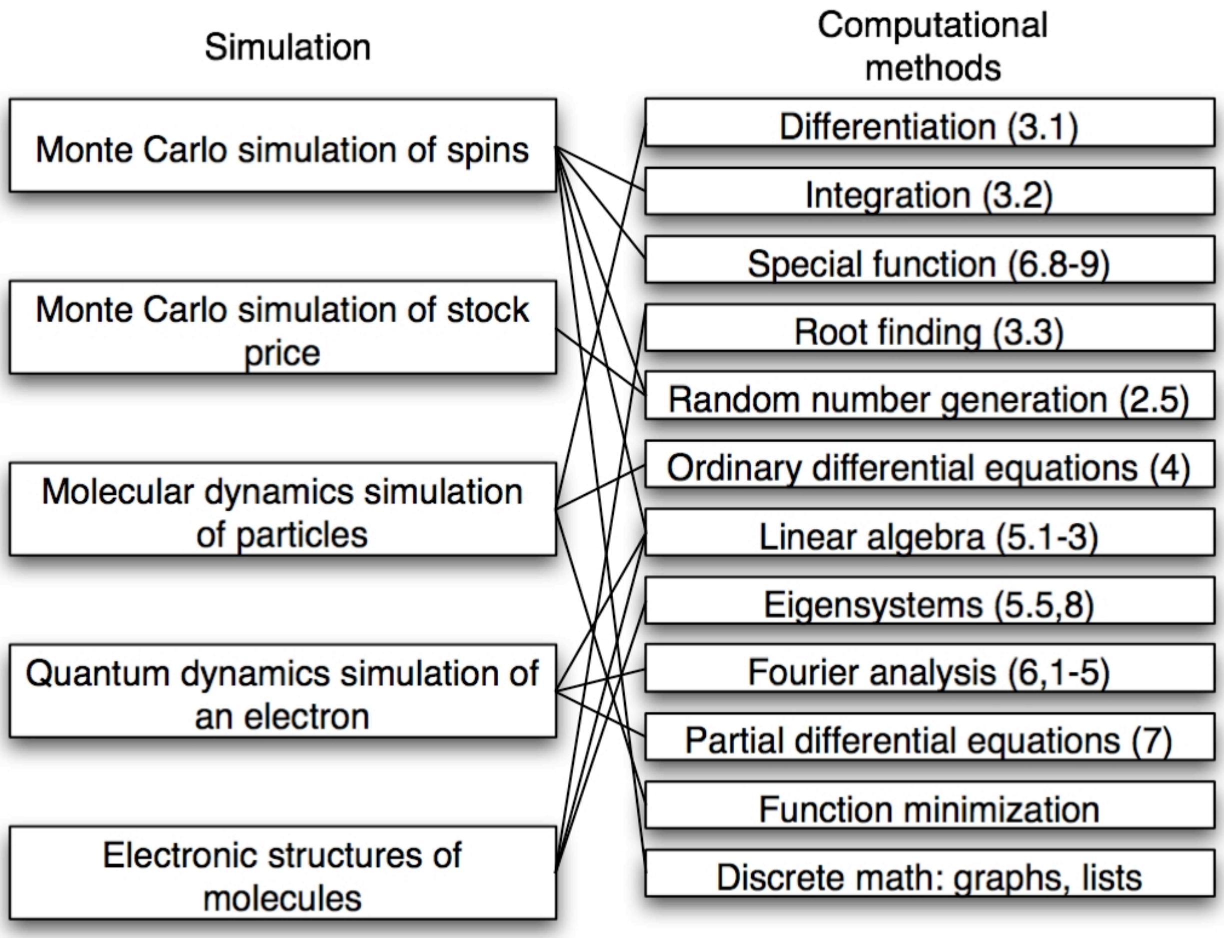


Figure: Computer simulations to be covered in this course (left column) and the associated computational methods (right column) to be learned, in which the numbers represent the chapter/section numbers in Tao Pang's textbook.

ENABLING TECHNOLOGIES

For real-life research, you will need more advanced computational methods, which will not be covered within this course. These topics will be taught in CSCI596—Scientific Computing and Visualization and CSCI653—High Performance Computing and Simulations:

- Parallel and distributed computing;
- Visualization;
- Data management and mining (knowledge discovery);
- Advanced numerical methods (mostly multi-resolution techniques).