Introduction

"A model is a representation of the structure of a real-life system". [1]

Types of models [1]:

- Iconic – exact replica in smaller scale e.g. wind tunnel, doll house, model train
- Analogue – the properties of one physical system are used to represent another one
  spring to represent an molecular bond
- Symbolic – mathematical expressions and computer code for an abstract representation harmonic oscillator: spring force $F_x = -kx$

Models describe the natural world using idealizations that

- simplify ..the physical system
- capture ..key aspects of the system
- match ...existing expt data
- enable predictions ... that can be tested against expt. data

[1] From Harry Perros, Computer Science Department, NC State University Raleigh, NC, *Computer Simulation Techniques: The definitive introduction!*, http://www.csc.ncsu.edu/faculty/perros//simulation.pdf

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Which idealized models do you remember from your physics classes?

- Simple pendulum
- inclined planes
- perfectly conducting wires
- ohmic resistance
- projectile motion
- infinitely long wires in Gauss's law application

In which ways were they idealized?

- Massless string
- ignore friction, gravity independent of height of elevation
- ignore resistance
- temperature dependence of R, frequency dep
- drag force
- edge effects

How did you work with these models? How did you find solutions?

- force diagrams → Newton's 2nd → acceleration → integrate with appr. initial conditions
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- for electric fields in systems with a lot of symmetry use Gauss's law

What are simulations?

Example for an analogue simulation:

Simulation of traveling waves with the aid of a crowd in a stadium.

- How would you instruct the spectators in a stadium to simulate a pulse traveling along a string?
- How would you tell them to simulate a traveling wave?
- How would you tell them to simulate, a standing wave?
- How would you simulate a two-dimensional plane wave or a spherical wave

Simulations require:

- a model, i.e. a representation of the physical system
- a set of instructions

Simulations provide an alternative to exact or approximate analytical solutions.

They are often used

- for complex systems, where exact solutions are not available and approximations difficult to find
- to test approximations used in analytical solutions
- to explore a system and find out where "interesting things" happen
- as an alternative to costly experimentation

Examples for simulation techniques:

- Monte Carlo — stochastic (non-deterministic)
- Molecular dynamics
- Finite element methods
- Variational methods
- Finite difference methods
- Spectral methods

(Molecular dynamics through Spectral methods: deterministic)