Lecture Notes 1

What is Computational Science?

Introduction to Computational Science, Fall 2010

Marcus Pendergrass
Hampden-Sydney College
Outline

1 Basics

2 The Modeling Process

3 Types of Models
Computational science is the theory and practice of using *modeling* and *simulation* to solve problems.
Problem Domains

Definition

The **problem domain** is the field of study that the problem comes from.

Some important problem domains:

- biology
  - epidemiology, genomics, ecology, ...
- meteorology
  - weather prediction, climate modeling
- engineering
  - aircraft design, integrated circuit design, ...
- physics
  - galaxy formation, stellar dynamics, ...
- many more...
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Models

Definition

A **model** is a description of a system that reflects important properties of the system. A **mathematical model** is a model framed in the language of mathematics.

Example

- System: a population whose rate of growth is proportional to the size of the population.
- Mathematical model: \( \frac{dP}{dt} = kP \).
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A simulation is physical system that mimics important properties of some other system. A computer simulation a simulation that is implemented as a computer program.

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note:

MATLAB is a computational environment for carrying out simulations.
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MATLAB is a computational environment for carrying out simulations.
A computational environment is a computer program that facilitates calculations. Computational environments may be fairly simple (e.g. graphing calculators), or very sophisticated. Examples of computational environments include

- Calculators
  - calculator app on iPhone, TI-8x graphing calculators, etc.
- Spreadsheets
  - Microsoft Excel, Apple Numbers, Open Office Calc
- Numerical environments
  - MATLAB, Octave
- Computer algebra systems
  - Maple, Mathematica, Sage
The Practice Of Computational Science

Interdisciplinary

Collaboration across disciplines is typical of computational science.

Teamwork

Teams usually include mathematicians, computer scientists, and experts in the problem domain area (e.g. scientists, engineers).

Reporting

Results of computational science research and practice must be communicated to a wider community in order to have an impact.
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3 Types of Models
The basic modeling process
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Maintaining the model may also require you to revisit earlier steps.
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1. Basics
2. The Modeling Process
3. Types of Models
Deterministic and Stochastic Models

A probabilistic or stochastic model exhibits random effects. A deterministic model does not. Many models are combinations of the two.

Static and Dynamic Models

A static model does not consider time, while a dynamic model changes with time.

Continuous and Discrete Models

A continuous-time model treats time as a continuous variable, able to take on any value. A discrete-time model treats time as a discrete variable, only able to take on certain pre-defined values.
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Practice

Practice 1.1
What is the difference between a model and a simulation? Which comes first in the basic modeling process?

Practice 1.2
Suppose we want to model the angle of the minute hand of a clock (measured from the 12 o’clock position, say). If $\theta$ is the angle in degrees, and $t$ is the time in minutes past the hour, find an equation that models the relationship between $\theta$ and $t$.

Practice 1.3
Suppose I have a spreadsheet that tells me how much I have left to pay on my mortgage at the end of each month. Does this represent a discrete-time model or a continuous-time model?
Practice

Practice 1.4

Give an example of a system for which a probabilistic model would be appropriate. Give another example in which a probabilistic model would not be appropriate.

Practice 1.5

Write an essay describing an example of computational science in action in industry, government, or academia. Carefully delineate the problem that was addressed, and the computational science approach that was used to solve the problem. Reference all sources used in your report.