Computational Modeling

José M. Garrido, Introduction to Elementary Computational Modeling Essential Concepts, Principles, and Problem Solving, CRC Press, Taylor & Francis Group, © 2012

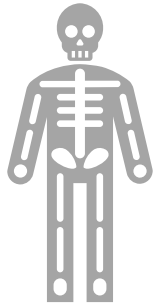
Agenda

- Definition
- Understanding Problem
- Computational Models
- Algorithms and Design Structures

Agenda

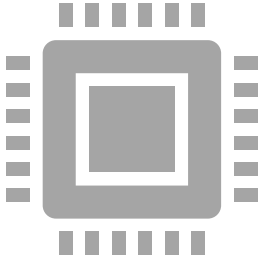
- **Definition**
- Understanding Problem
- Computational Models
- Algorithms and Design Structures

Computational
Science



is an area (or discipline) that includes

concepts,
principles, and
methods
from
applied mathematics and
algorithmic design and computer programming;



these are applied in various areas of science and engineering to solve large-scale scientific problems.

Computational Model

is computer implementation of the solution to a (scientific) problem for which a mathematical representation has been formulated.

is the foundational component of computational science and focuses on reasoning about problems using computational thinking and developing models for problem solving.

Developing a computational model includes formulating the mathematical representation and implementing it by applying computer science concepts, principles and methods.

Computational Thinking

- is an approach for developing computational models and is used for problem solving in the following application areas:
  - Sciences (biology, chemistry, computing, physics, geology, etc.)
  - Social Sciences (psychology, sociology, geography, etc.)
  - Engineering (electrical engineering, civil engineering, mechanical engineering, etc.)
  - Business (accounting, finance, marketing, economics, risk management, etc.).

Agenda

- Definition
- **Understanding Problem**
- Computational Models
- Algorithms and Design Structures

Word Saying
of The Problem

Although a computational problem may be solved using mathematics, a calculator, or a computer program, developing a solution to these problems begins with a description of the problem in a human language (English or Bahasa Indonesia).

To solve such problems, it is necessary to understand what the (English or Bahasa Indonesia) problem statement is saying.

Word Saying
of The Problem: Physics

Calculate the energy needed to heat water from an initial temperature to a final temperature.

The formula to compute the energy is the amount of water in kilograms times the ***difference*** of the ***final*** and ***initial*** temperatures in ***Celsius*** times ***4184***.

Word Saying
of The Problem: Business

A Company may want to predict sales for a brand under alternative prices, advertising spending levels, and package sizes.

Management wants model builders to develop:

an *explicit decision* model, which is *numerically specified*, which can be used to *predict* sales, at the *brand sales* level.

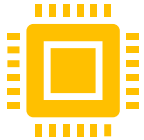
Agenda

- Definition
- Understanding Problem
- **Computational Models**
- Algorithms and Design Structures

Preliminary
Concept

A model is a representation of a real system or part of it.

Modelling is the activity of building models.



A computational model is a mathematical model implemented in a computer system and usually requires high performance computational resources to execute.

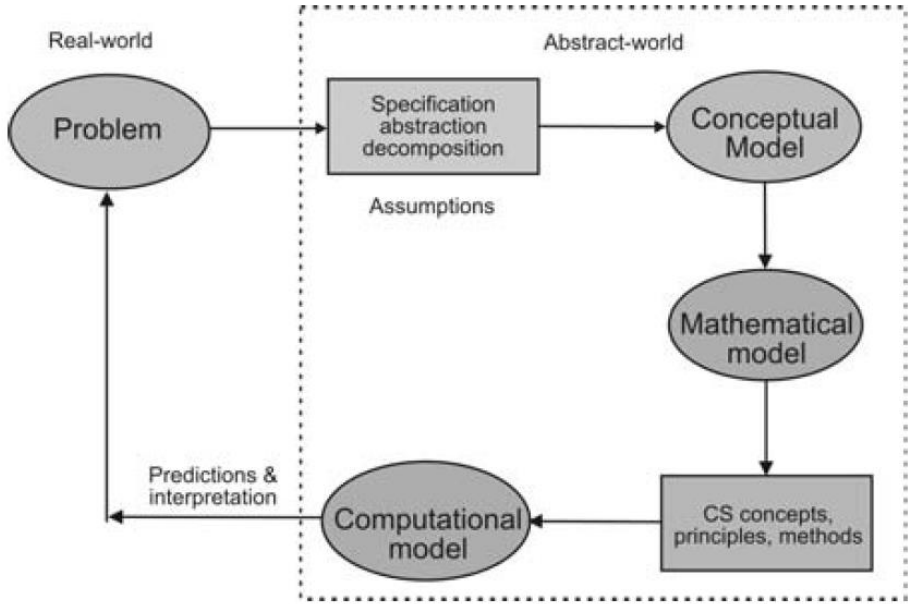
The computer implementations of computational models are essentially programs.

Abstraction is the activity of hiding the details and exposing only the essential features of a particular system.

Proper abstraction will result in a good model that helps solve the problem.

Development of
Computational Models

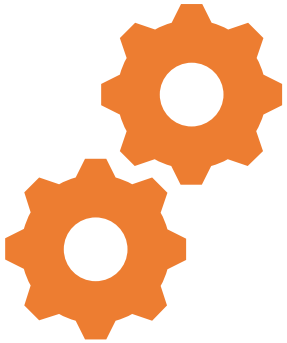
1. problem statement for the computational model: provide the description of the purpose for building the model, the questions it must help to answer, and the type of expected results relevant to these questions.
2. model specification : a description of what is to be accomplished with the computational model to be constructed; and the assumptions (constraints), and domain laws to be followed. It should be clear, precise, complete, concise, and understandable.
3. Conceptual model: formulated from the initial problem statement, informal user requirements, and data and knowledge gathered from analysis of previously developed models.
4. Mathematical model: involves deriving a representation of the problem solution using mathematical entities and expressions and the details of the algorithms for the relationships and dynamic behavior of the model.



Evaluation of
The Models

1. Verification of the model: this stage compares the output results with those that would have been produced by a correct implementation of the conceptual and mathematical models.
2. Validation of the model. This stage compares the outputs of the verified model with the outputs of a real system (or a similar already developed model).

Simulation:
Basic Concepts



Simulation is a set of ***techniques, methods, and tools*** for developing a simulation model of a system and using and manipulating the simulation model to gain more knowledge about the dynamic behavior of a system.

The purpose of simulation is to gain understanding about the behavior of the ***real*** system that the model represents.

Simulation
Model

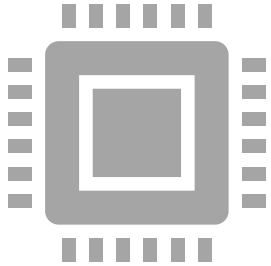
- A simulation model is a computational model that has two main purposes:
  - To study some relevant aspects of the dynamic behavior of a system by observing the operation of the system, using the sequence of events or trace from the simulation runs
  - To estimate various performance measures

Agenda

- Definition
- Understanding Problem
- Computational Models
- **Algorithms and Design Structures**

Algorithms and
Design Structures

Algorithm: The precise, detailed, and complete description of a solution to a known problem



Design structures: sequence, selection, repetition, and input-output.