Introduction Computational Science:

Introduction to the 3rd Paradigm

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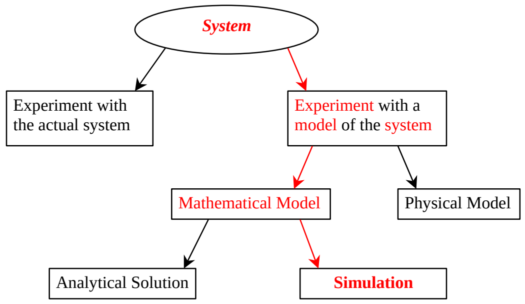
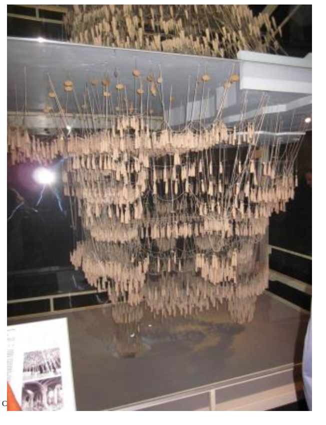
Two questions to start

- What is a system?
- What is a model?
- What is the difference between a model and a simulation?

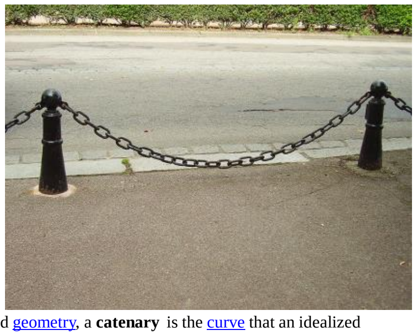
Ways to Study a System


System
Experiment with the actual system
Experiment with a model of the system
Mathematical Model
Physical Model
Analytical Solution
Simulation

Model Sagrada familia

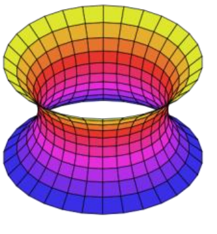


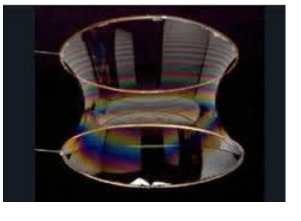
Model Sagrada familia



In physics and geometry, a **catenary** is the curve that an idealized hanging chain or cable assumes under its own weight when supported only at its ends. The curve has a U-like shape, superficially similar in appearance to a parabola, but it is not a parabola: it is a (scaled, rotated) graph of the hyperbolic cosine

Model Sagrada familia

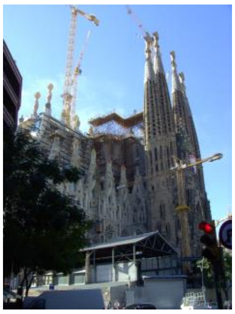




The catenary curve is the graph of the hyperbolic cosine function. The surface of revolution of the catenary curve, the catenoid, is a minimal surface, specifically a minimal surface of revolution

Model Sagrada familia

Sagrada familia Barcelona



Definitions - 1

What is a **SYSTEM** ?

"A distinguishable piece of the universe", *or*

"A system is a potential source of data"

Bernard Ziegler, *Theory of Modeling and Simulation*, 1976.

What is an **EXPERIMENT** ?

"An experiment is the process of extracting data from a system by exerting it through its inputs."

François Cellier, *Continuous System Modelling*, 1990. (read 1st chapter)

Definitions - 2

What is a **MODEL?**

" A model (*M*) for a system (*S*) and an experiment (*E*) is anything to which E can be applied in order to answer questions about S."

Marvin Minski, *Models, Minds, Machines*, 1965.

Note that ...

- A model is not necessarily a computer program !
- Here we concentrate on models that can be expressed as computer programs.
- By definition, a model can be qualified as a system, which allows to cut out smaller pieces to generate a new model (*hierarchy of models*)
  - Jack Kleijnen, "Concept of Meta-Models," in *Progress in Modelling and Simualation,* 1982.
- A model is always related to the tuple *System* and *Experiment*.
- Model validation relates to an experiment to be performed on a system.

Definitions - 3

What is a **SIMULATION?**

"A simulation is an experiment performed on a model."

Granino Korn and John Wait, *digital continuous system simulation*, 1978.

Definitions -4

What is an **EXPERIMENTAL FRAME?**

"An experimental frame is a specification of the conditions under which the system observed is experimented with."

Bernard Ziegler, *Theory of Modeling and Simulation*, 1976.

Note that ...

- A mathematical simulation is a coded description of an experiment with a reference to the model to which this experiment is applied.
- Note the (important) separation between model description and experiment description.
- Also note the potential danger of this separation; it is very easy to apply an experiment to a model for which the model is not *valid*.

The Dangers of Simulation

- Both its strength and weakness: generality and ease of its application…

"All too often, simulation is a love story with an unhappy ending. We create a model of a system, and then fall in love with it. Since love is usually blind, we immediately forget all about the experimental frame, we forget that this is *not* the real world, but that it represents the world only under a very limited set of experimental conditions (we become 'model addicts')."

F. Cellier, *Continuous System Modeling*, 1990

in other words...

"Don't fall in love with your model !"

Francois Cellier

quants de alchemisten van wall street

http://tegenlicht.vpro.nl/afleveringen/2009-2010/Crisis-als-kans/quants-de-alchemisten-van-wall-street.html

Why is Modeling Important ?

"Modeling means the process of organizing knowledge about a given system"

Bernard Ziegler, *Multifaceted Modeling and Discrete Event Simulation*, 1984

"... it can thus be said that modeling is the single most central activity that unites *all* scientific and engineering endeavors. While the scientist is happy to simply *observe* and *understand* the world, i.e., create a model of the world, the engineer wants to *modify* it to his advantage. While science is all *analysis*, the essence of engineering is *design*.."

"... *simulation* can be used not only for analysis (direct problems) but also for design (inverse problems)."

François Cellier, *Continuous System Modelling*, 1990

Prediction? – 16 other reasons

"But, more to the point, I can quickly think of 16 reasons other than prediction (at least in this bald sense) to build a model … off the top of my head, and in no particular order, such modeling goals include:

1.Explain (very distinct from predict)
2.Guide data collection
3.Illuminate core dynamics
4.Suggest dynamical analogies
5.Discover new questions
6.Promote a scientific habit of mind
7.Bound (bracket) outcomes to plausible ranges
8.Illuminate core uncertainties.
9.Offer crisis options in near-real time
10.Demonstrate tradeoffs / suggest efficiencies
11.Challenge the robustness of prevailing theory through perturbations
12.Expose prevailing wisdom as incompatible with available data
13.Train practitioners
14.Discipline the policy dialogue
15.Educate the general public
16.Reveal the apparently simple (complex) to be complex (simple) "

Epstein, Joshua M. (2008). 'Why Model?'. Journal of Artificial Societies and Social Simulation 11(4)12 <http://jasss.soc.surrey.ac.uk/11/4/12.html>.

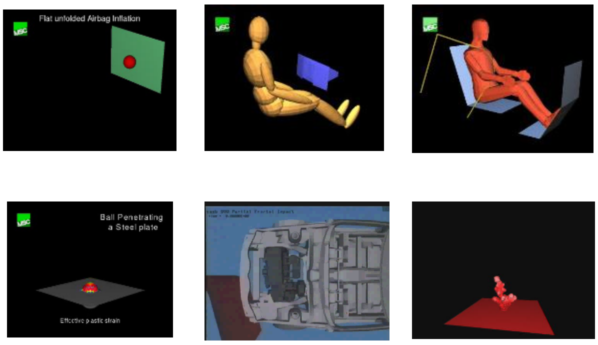
Reasons to use Simulation

- The physical system in not available
- The experiment may be dangerous
- The cost of the experiment is too high
- The time constants of the system are not compatible with those of the experimenter
- Control variables may be inaccessible
- Suppression of disturbances

Examples

- Car crashworthiness
- Airplane
- Galaxy evolution
- Molecular docking
- Stock-exchange
- Computer/Network

Examples


Flat unfolded Airbag Inflation
Ball Penetrating a Steel plate
Effective plastic strain

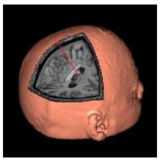
More Examples...

Car crashes

and even more examples...

air flows in and around cars

Examples from healthcare



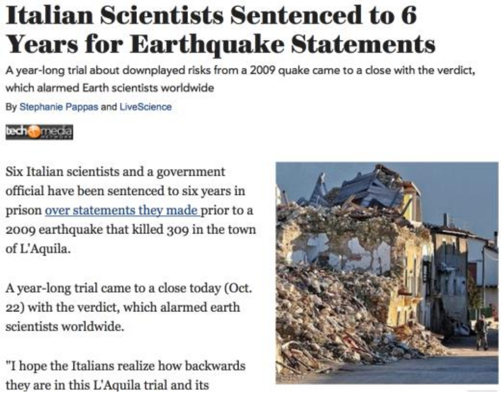
Interactive MRI

The virtual hand

Things can go wrong...

- Crash NW255 1987
  - Flap signal worked in simulation but not in real
  - 155 people killed
- Hartford Civic Center Coliseum (1978)
  - 2.4 acre roof collapse.
  - Computer results mis-interpreted
- Love Parade disaster (2010)
  - Crowd simulation used to verify safety

The expectation of models



Italian Scientists Sentenced to 6 Years for Earthquake Statements

A year-long trial about downplayed risks from a 2009 quake came to a close with the verdict, which alarmed Earth scientists worldwide

By Stephanie Pappas and LiveScience

Six Italian scientists and a government official have been sentenced to six years in prison over statements they made prior to a 2009 earthquake that killed 309 in the town of L'Aquila.

A year-long trial came to a close today (Oct. 22) with the verdict, which alarmed earth scientists worldwide.

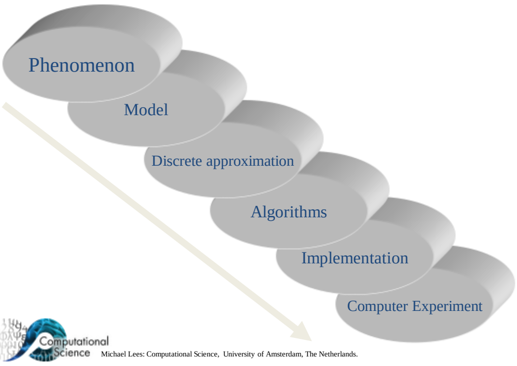
"I hope the Italians realize how backwards they are in this L'Aquila trial and its

Things could have gone right...

Things could have gone right...

- Tacoma narrow collapse
- Erasmus bridge singing
- Automatic debiting in car-portals
- Traffic…(contention, road-changes)
- …
- … any other examples ??

The Computer Experiment I



Phenomenon

Model

Discrete approximation

Algorithms

Implementation

Computer Experiment

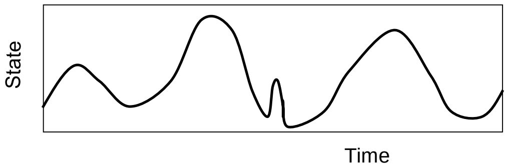
The Computer Experiment II

- Data interpretation
  - – Visualization & Virtual Reality
- Sensitivity Analyses
- Performance optimization
- Model refinement
- Interactive Simulation
  - – man-in-the-loop
  - – VR-HPC

Types of models

Mathematical Models

- Continuous-Time Models
  - **State** changes *continuously* over time:



Growth of a population N(t), logistic model

$$\frac{dN}{dt} = rN(1 - \frac{N}{K})$$

- *r* is intrinsic rate of increase, K carrying capacity
- Assumption 1: every living organism must have at least one parent of like kind
- Assumption 2:In finite space, due to limiting effect of the environment, there is an upper limit to the number of organisms that can occupy that space

Lotka-Volterra model

$$\frac{dH}{dt} = bH - sHP$$

$$\frac{dP}{dt} = -dP + esHP$$

- H herbivores, P predators, and four parameters: b birth rate prey, s searching efficiency predator, e efficiency food->predators

Mathematical Models continued

- Within a finite time span, the state variables change their values infinitely often
- Represented by: Set of differential Equations
  - Lumped parameter models: ODE

$$\frac{dx}{dt} = f(x, u, t)$$

  - Distributed parameter models: PDE

$$\frac{\partial u}{\partial t} = \sigma . \frac{\partial^2 u}{\partial x^2}$$

Simple pendulum

$$\frac{d^2\theta}{dt^2} + \frac{g}{l}\sin(\theta) = 0$$

- *Where θ is the displacement angle, g accelaration of gravity, l length of pendulum*

Simple pendulum

- *Any system of differential equations of higher order than one , can be written as a system of first order equations, assume*

$$x_1 = \theta$$

$$x_2 = \dot{\theta}$$

Simple pendulum

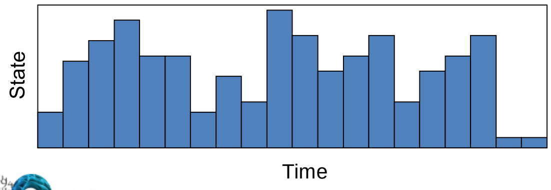
- *Any system of differential equations of higher order than one , can be written as a system of first order equations:*

$$\frac{dx_1}{dt} = x_2$$

$$\frac{dx_2}{dt} = -\frac{g}{l}\sin(x_1)$$

Mathematical Models continued

- Discrete-Time Models
  - Time-Axis is discretized
  - Represented by difference equations
  - $X(t_{k+1}) = f(x_k, u_k, t_k)$



Example discrete time population growth model (Verhulst model)

- *Xn is population size in year n, R is relative increase population*

$$R = (x_{n+1} - x_n)/x_n$$

- *If R is constant*

$$x_{n+1} = (1+r)x_n$$

- *After n years exponential growth*

$$x_n = (1+r)^n x_0$$

Example discrete time population growth model (Verhulst model)

- *If R is proportional to 1-Xn*

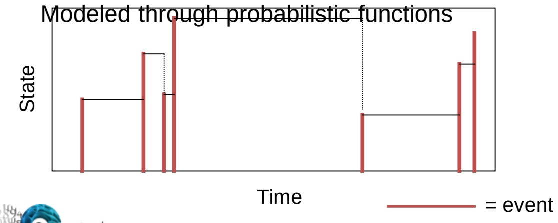
$$R = r(1 - X_n)$$

$$\frac{x_{n+1} - x_n}{x_n} = r(1 - x_n)$$

$$x_{n+1} = (1+r)x_n - rx_n^2$$

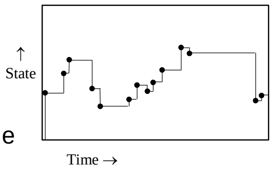
Mathematical Models continued

- Discrete-Event Models
  - State change changes at certain points in time and ‘jumps’ in time. Events can happen at any time
- *No* analogue mathematical representation. Modeled through probabilistic functions

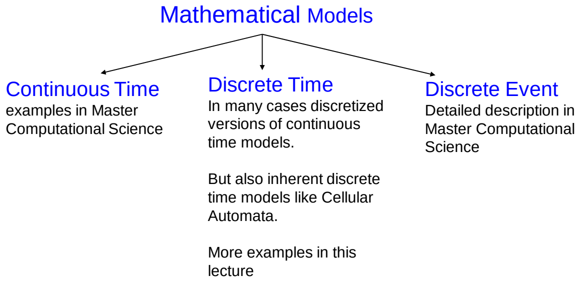


Types of Mathematical Models III

- Discrete Event model
  - State variables change at discrete events.
  - Paradoxically, both the time axis and the state axis in Discrete Event Models are continuous.
  - In a finite time span only a finite number of changes may occur.



Overview Mathematical Models


Mathematical Models

Continuous Time
examples in Master Computational Science

Discrete Time
In many cases discretized versions of continuous time models.

But also inherent discrete time models like Cellular Automata.

More examples in this lecture

Discrete Event
Detailed description in Master Computational Science

Execution Models

- Time-driven simulation

- Event driven simulation

Time Driven

- the simulation clock is advanced in increments of exactly Δt time units

- the time step Δt is small enough to capture every event in the system

Event Driven

- Step 1: The simulation clock is initialized to zero and the times of occurrence of future events are determined.

- Step 2: The simulation clock is advanced to the time of the occurrence of the most imminent (i.e. first) of the future events.

- Step 3: The state of the system is updated to account for the fact that an event has occurred.

- Step 4: Knowledge of the times of occurrence of future events is updated and the first step is repeated.

Billiard-ball example

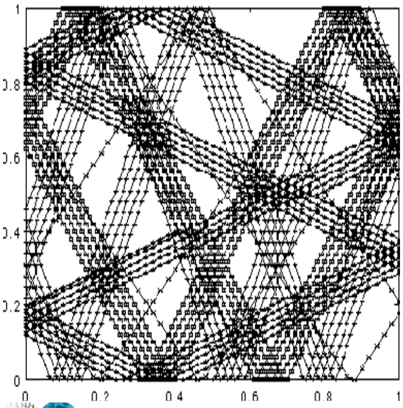
- Gas dynamics of 4 gas molecules, v=const.

- 2D kinetic energy conservation

- Consider Time and Event driven:

Billiard-ball Time Driven Simulation

```
input stop, simulation time, Δt;
initialize balls with x,y position and velocity
vx,vy in x,y direction;
time = 0.0;
while (time < stop simulation)
{
for each ball do {
          x += Δt * vx;
          y += Δt * vy;
          if (x == 0) vx = -vx;
          if (y == 0) vy = -vy;
     }
time += Δt;
}
```



Result Time Driven

Δt = 0.001
1000 state evaluations

Billiard Balls event driven I

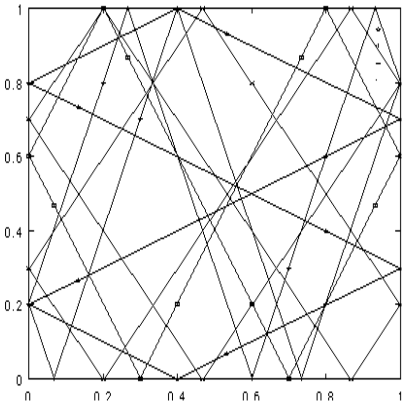
```
input stop_simulation_time;
initialize balls with x,y position and velocity vx,vy
in x,y direction;
for each ball do {
     impact_time = collision_time(ball);
     schedule(MOVE, impact_time, ball);
}
prev_time = 0.0;
while (time() < stop_simulation_time) {
     next_event(&event, &ball);
     switch(event) {
     case MOVE:
          update_positions(time() - prev_time);
          impact_time = collision_time(ball);
          schedule(MOVE, impact_time, ball);
          prev_time = time();
          break;
     }
```

Billiard Balls event driven II

```
collision_time(ball)
{
     if (vx >= 0) {
          t0 = (1 - x) / xv;
     }
          else {
          t0 = -x / xv;
          }
     if (vy >= 0) {
          t1 = (1 - y) / yv;
     }
          else {
          t1 = -y / yv;
          }
     return min(t0, t1);}
```

Billiard Balls event driven III

```
update_positions(Δt)
{
     for each ball do {
          x += Δt * vx;
          y += Δt * vy;
          if (x == 0 || x == 1)
               vx = -vx;
          if (y == 0 || x == 1)
               vy = -vy;
     }
```



Result Event Driven

60 state evaluations

Some Observations

- If the time between the succeeding events becomes small, time driven is preferred. This is the *frequency* parameter.

- The overhead per event (i.e., the state update) is larger with event-driven simulation. This is referred to as the *event overhead*.

- The amount of work between any two events plays an important role. This we call the *granularity* of the system.

Validation and Verification

- Validation
  - Check the validity of the model.
  - *Does the model reproduce the real data?*

- Verification
  - Check the correctness of the simulation.
  - *Does the simulation program do what it is supposed to? Bugs, hidden errors?*