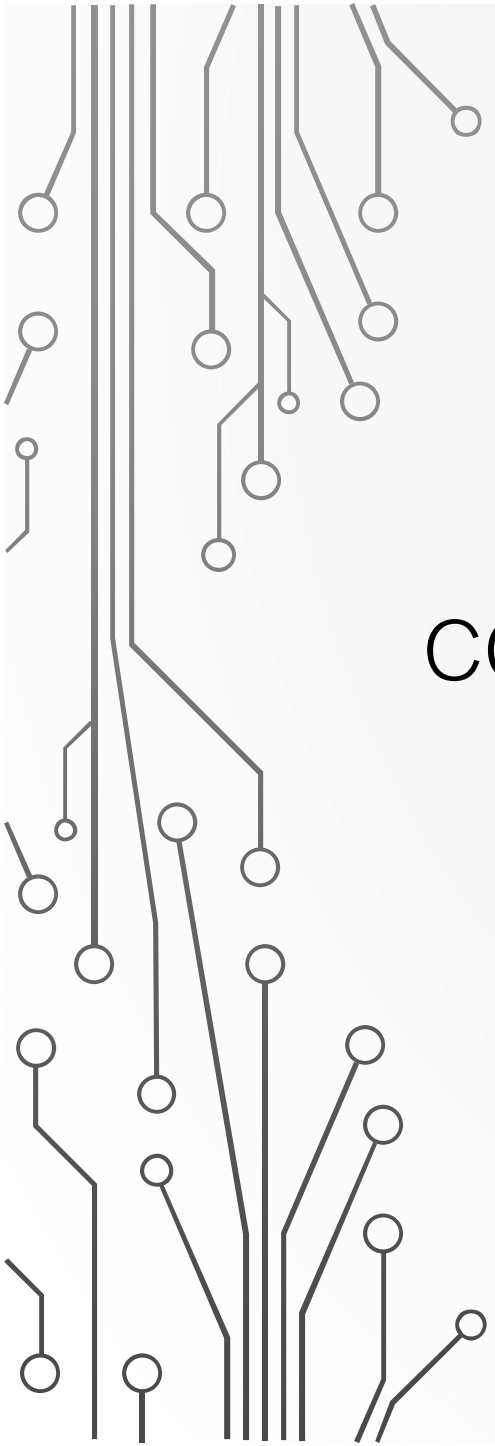


COMPUTER SIMULATION

OUTLINE

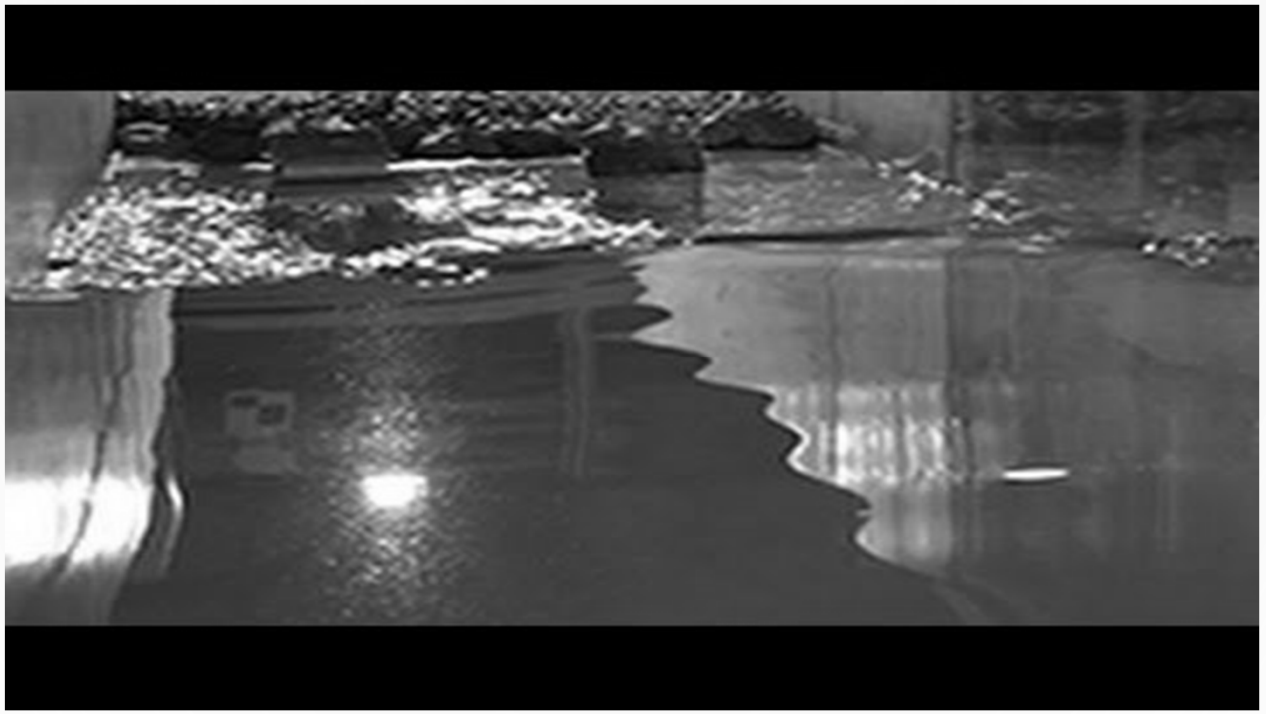
In this module, we will focus on the act simulation, taking mathematical models and implement them on computer systems.

- Simulation & Computer Simulations
- Mathematical (Simulation) Model
- Computer Simulation Tools
- Computer Simulation Examples
  - Deterministic and Stochastic
  - With spreadsheet program

WHAT IS SIMULATION?

- **Simulation** is the imitation of the operation of a real-world process or system over time. Can be physical, or mathematical.
  - Physical simulation: physical objects (physical model) are substituted for the real thing based on laws of physics. Can be interactive (with human components)
  - Mathematical simulation: simulation with mathematical models.

PHYSICAL SIMULATION EXAMPLE: A TSUNAMI SIMULATOR

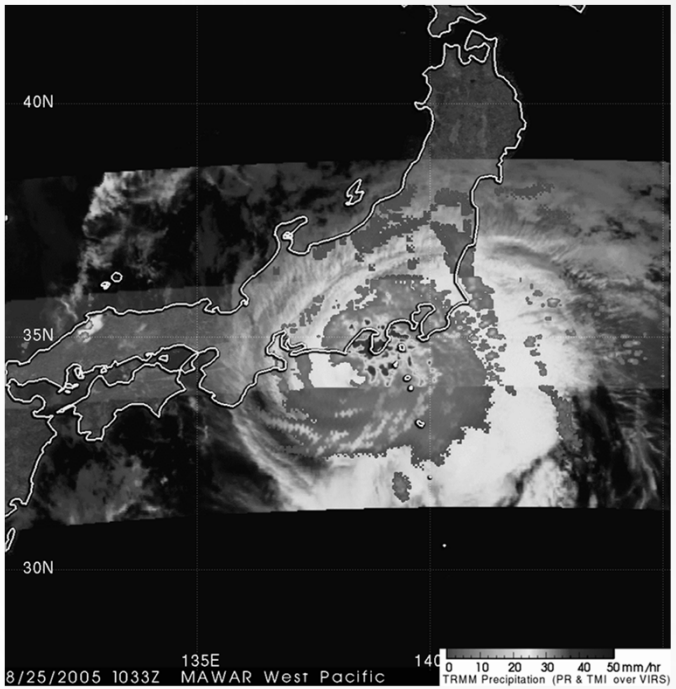


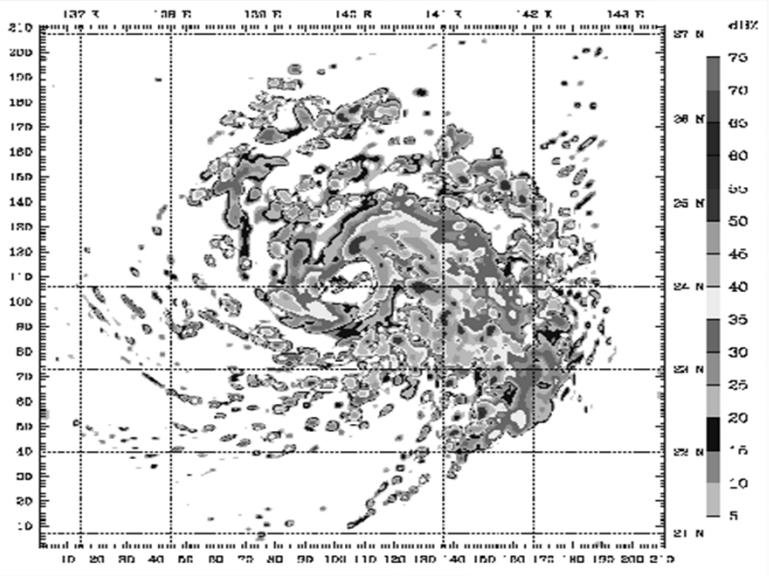
https://www.youtube.com/watch?v=Ez_TOJe-oaA

COMPUTER SIMULATION

- A **computer simulation** is a simulation, run on computers to reproduce behavior of a system.
- The simulation uses an abstract model (a **computational model** or sometime called **mathematical model**) to simulate the system.
- Computer simulation has become a useful part of mathematical modeling many natural systems in **physics**, **astrophysics**, **climatology**, **chemistry**, **biology**, and human systems such as **economics**, **psychology**, **social science**, and **engineering**.

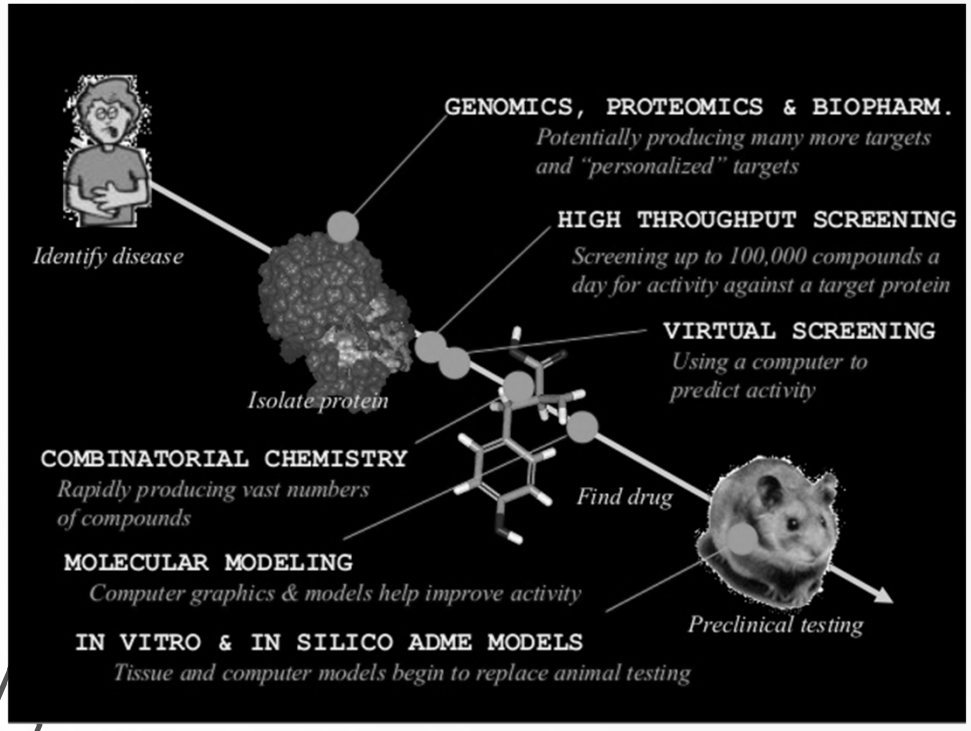
SIMULATION OF TYPHOON

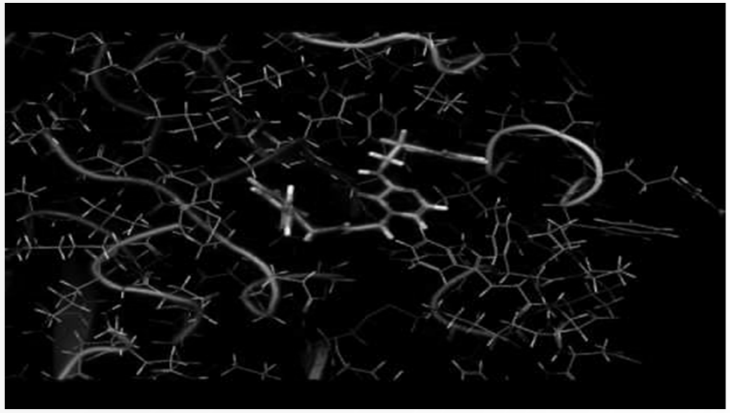




Simulation of Typhoon Mawar, Japan, 2005

COMPUTATIONAL CHEMISTRY FOR DRUG DESIGN





MATHEMATICAL MODELS AND SIMULATION IN MATERIAL SCIENCE

The **lim-inf**

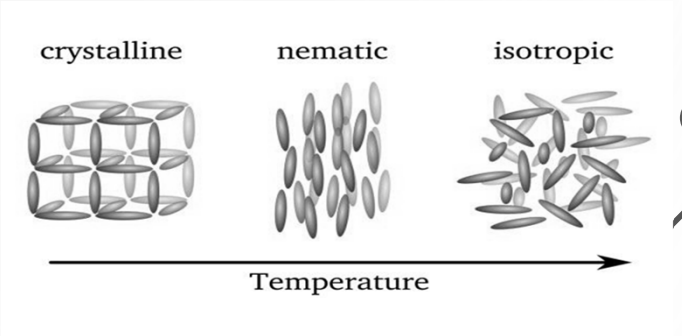
$$\liminf_{h\to 0} E_1^h[s_h, \mathbf{n}_h]$$

$$\geq \int_\Omega (\kappa - 1)|\nabla|\widetilde{\mathbf{u}}||^2 + |\nabla\widetilde{\mathbf{u}}|^2 dx$$

...using $\widetilde{\mathbf{u}} = |s|\mathbf{n}$...

$$= \int_\Omega \kappa|\nabla s|^2 + s^2|\nabla\mathbf{n}|^2 dx$$

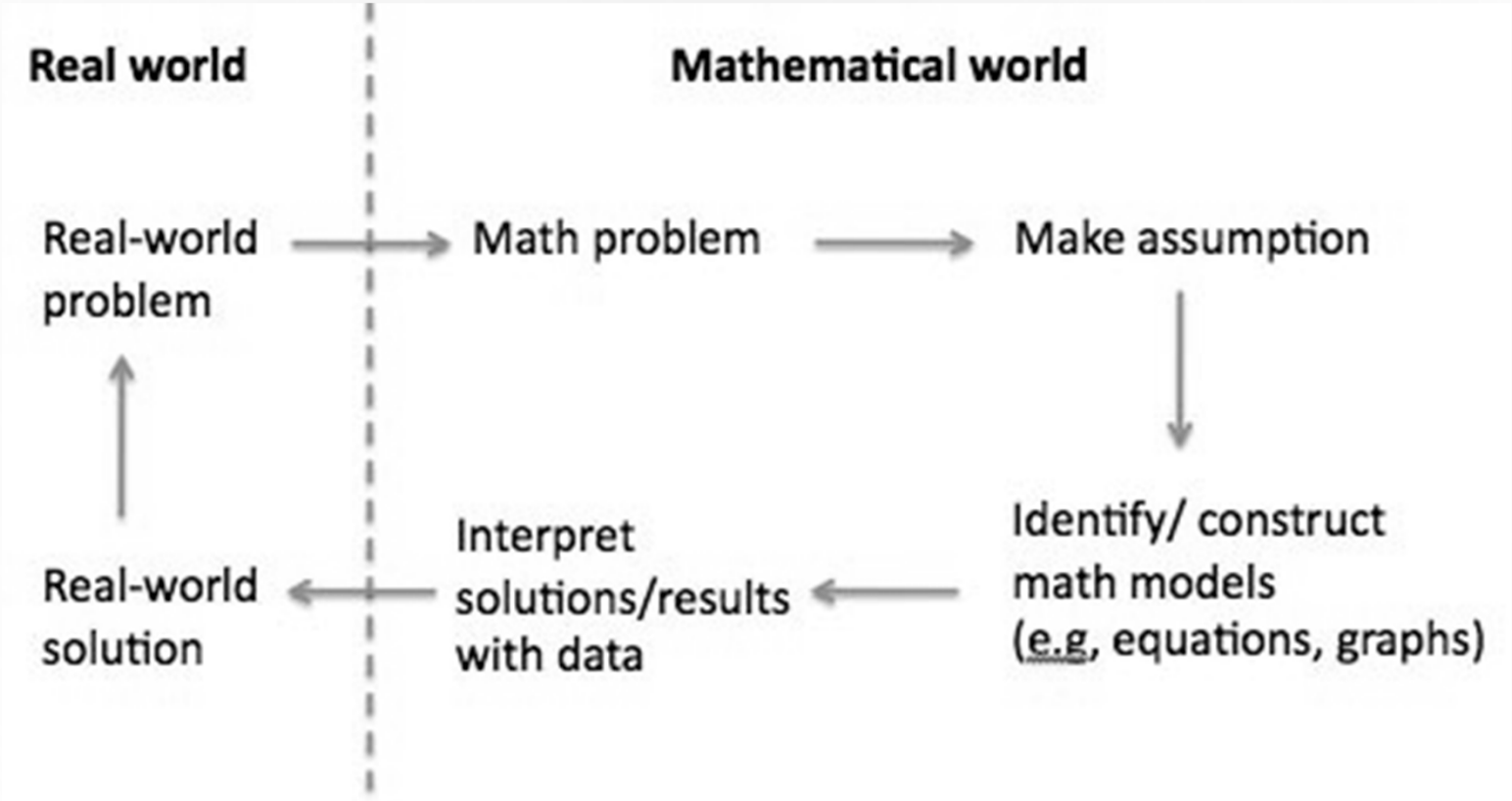
Simulation of Nematic Liquid Crystals



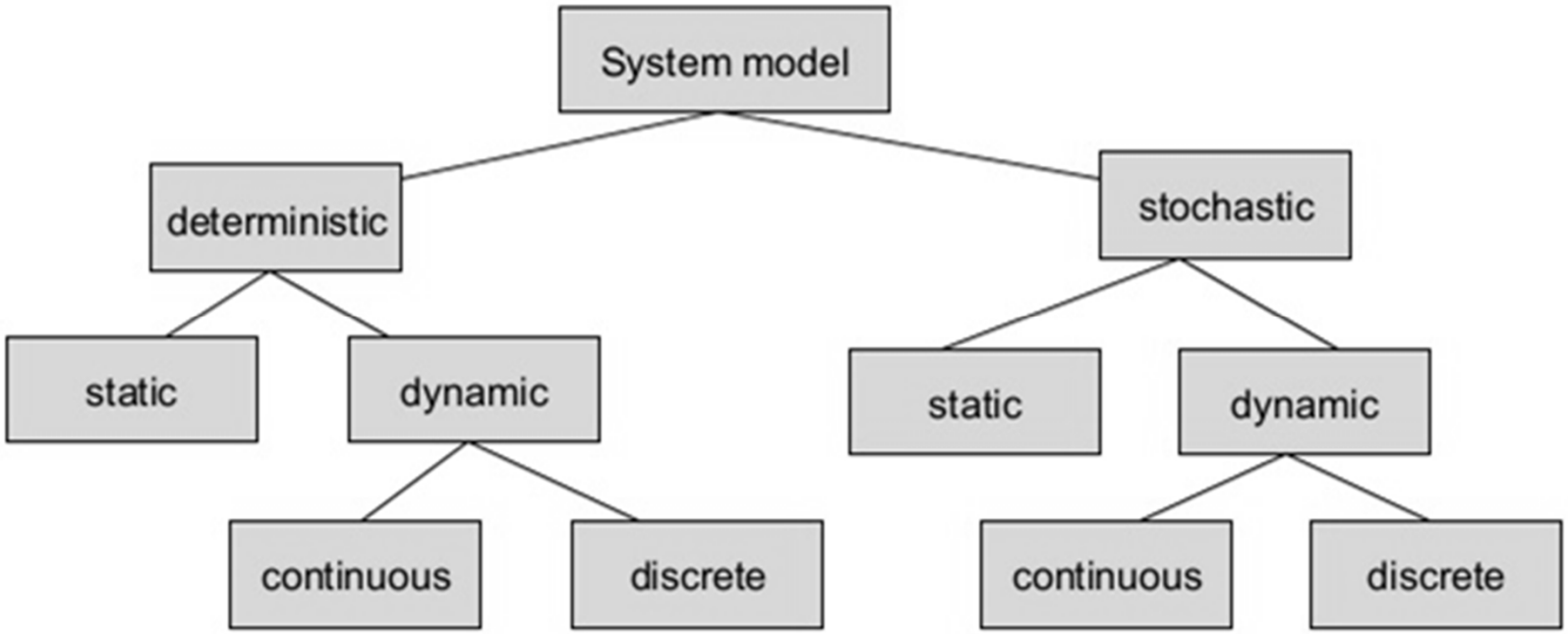
WHAT YOU NEED FOR COMPUTER SIMULATION

- Mathematical Model, Simulation Model, or just Model
  - Represents the key characteristics or behaviors/functions of the selected physical or abstract system or process.
  - What are the variables? How do they change over time?
- Data
  - For input parameters, and validation.
- Tools
  - Where/how are you going to implement the model into computer simulation?
- And you

MATHEMATICAL MODELING



TYPES OF MATHEMATICAL MODELS



CONTINUOUS-TIME AND DISCRETE-TIME MATHEMATICAL MODELS

Continuous-Time Systems

Most continuous time systems represent how continuous signals are transformed via **differential equations**.

E.g. circuit, car velocity

$$\frac{dv_c(t)}{dt} + \frac{1}{RC} v_c(t) = \frac{1}{RC} v_s(t)$$

$$m\frac{dv(t)}{dt} + \rho v(t) = f(t)$$

First order differential equations

Discrete-Time Systems

Most discrete time systems represent how discrete signals are transformed via **difference equations**

E.g. bank account, discrete car velocity system

$$y[n] = 1.01y[n-1] + x[n]$$

$$v[n] - \frac{m}{m+\rho\Delta} v[n-1] = \frac{\Delta}{m+\rho\Delta} f[n]$$

$$\frac{dv(n\Delta)}{dt} = \frac{v(n\Delta) - v((n-1)\Delta)}{\Delta}$$

DIFFERENTIAL EQUATIONS (CONTINUOUS TIME MODELS)

- A **differential equation** is a mathematical equation that

ODE (ORDINARY DIFFERENTIAL EQUATION):

An equation contains only ordinary derivates of one or more dependent variables of a single independent variable.

For Example,

$dy/dx + 5y = e^x$, $(dx/dt) + (dy/dt) = 2x + y$

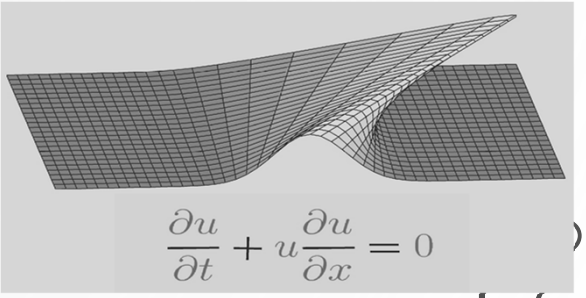
PDE (PARTIAL DIFFERENTIAL EQUATION):

An equation contains partial derivates of one or more dependent variables of two or more independent variables.

For Example,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial t^2} = 2\frac{\partial u}{\partial t} \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

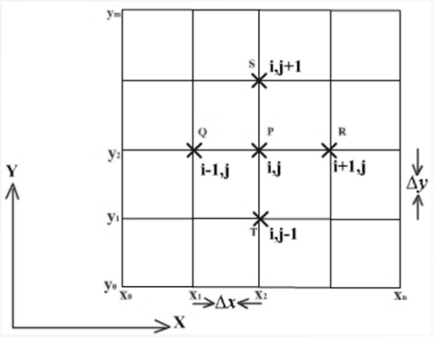
$$S(t) = \frac{t^2}{2}\frac{d^2 s}{dt^2} + t\frac{ds}{dt} + s_0$$



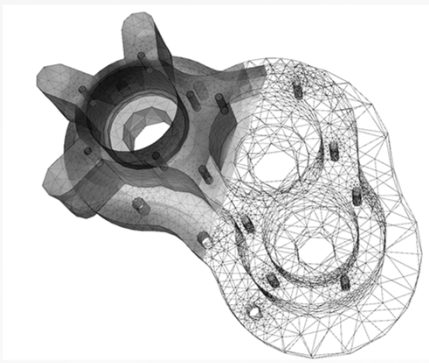
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

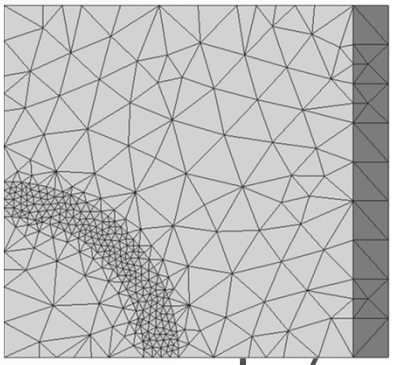
DIFFERENCE EQUATIONS (DISCRETE-TIME MODELS)

- The finite-difference methods are numerical methods for solving differential equations by approximating them with difference equations, in which finite differences approximate the derivatives.



- The finite element methods are numerical techniques for finding approximate solutions to boundary value problems for partial differential equations.

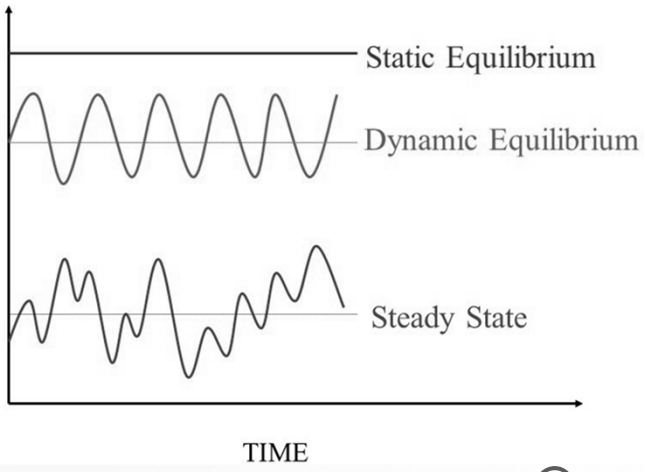




STATIC AND DYNAMIC MODELS

STATIC MODEL A static (or steady-state) model calculates the system in equilibrium, and thus is time-invariant. A static model cannot be changed, and one cannot enter edit mode when static model is open for detail view.

DYNAMIC MODEL A dynamic model accounts for time-dependent changes in the state of the system. Dynamic models are typically represented by differential equations.



STATIC MODELS

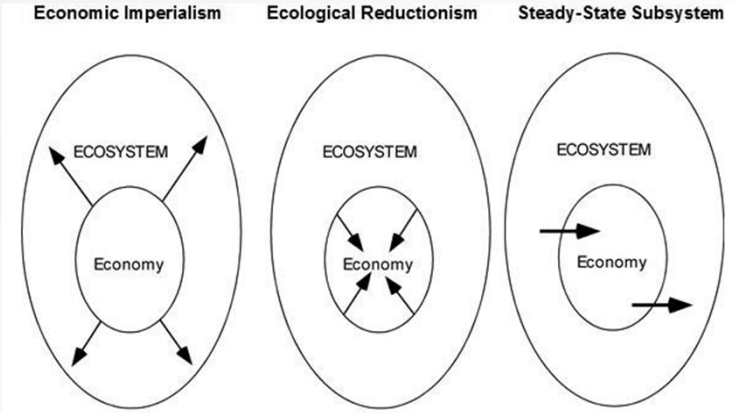
- A system is in a steady state if the variables which define the behavior of the system or the process are unchanging in time.
- In continuous time, this means that for those properties p of the system, the partial derivative with respect to time is zero.

$$\frac{\partial p}{\partial t} = 0 \qquad \text{for all t}$$

- In discrete time, it means that the first difference of each property is zero.

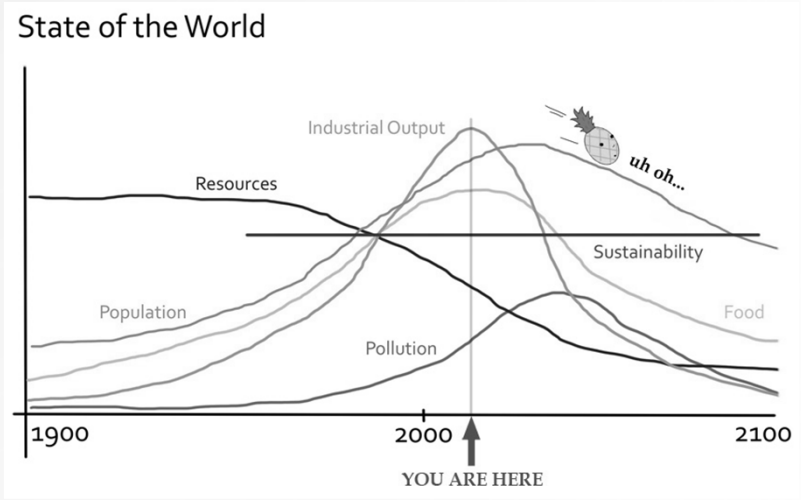
$$p_{t+1} - p_t = 0 \qquad \text{for all t}$$

Economic System



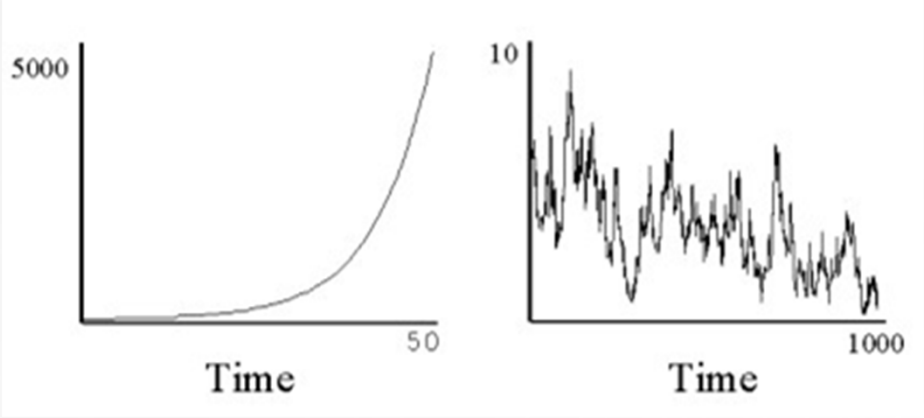
DYNAMIC MODELS

- A **dynamic model** represents the behavior of a system over time.
- It is used where the system's behavior is best described as a set of states that occur in a sequence of time.
- The components of the **dynamic model** are: **States.**



DETERMINISTIC AND STOCHASTIC MODELS

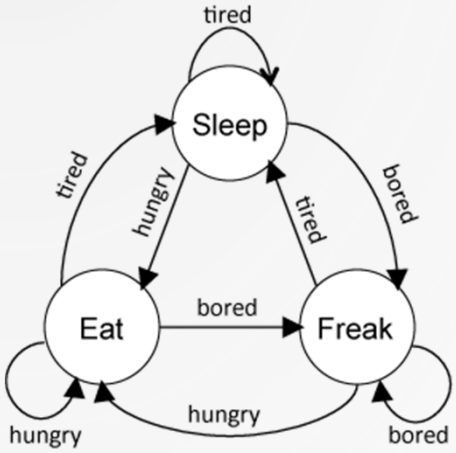
- In **deterministic models**, the output of the model is fully determined by the parameter values and the initial conditions.
- **Stochastic models** possess some inherent randomness. The same set of parameter values and initial conditions will lead to an ensemble of different outputs.



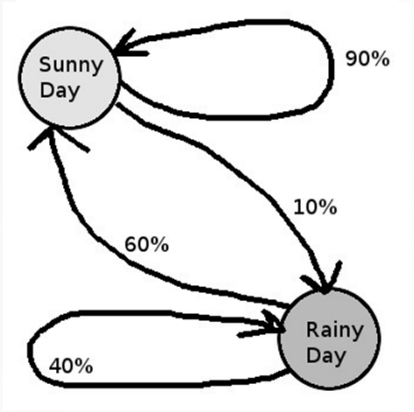
Continuous Deterministic Continuous Stochastic

DETERMINISTIC MODELS

- A **deterministic system** is a system in which no randomness is involved in the development of future states of the system.
- A deterministic model will always produce the same output from a given starting condition or initial state.



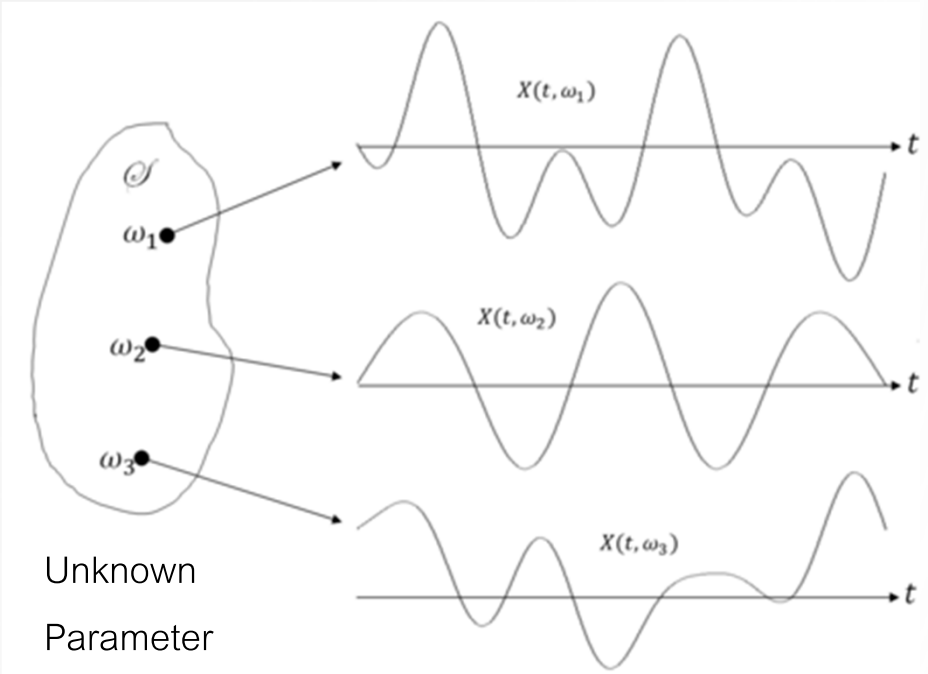
Finite State Machine
(Discrete Deterministic Model)



Markov Chain
(Discrete Stochastic Model)

STOCHASTIC PROCESS

- A stochastic process is a random process evolving with time.
- The evolution of the stochastic system is represented by a set of random variables.



Unknown Parameter

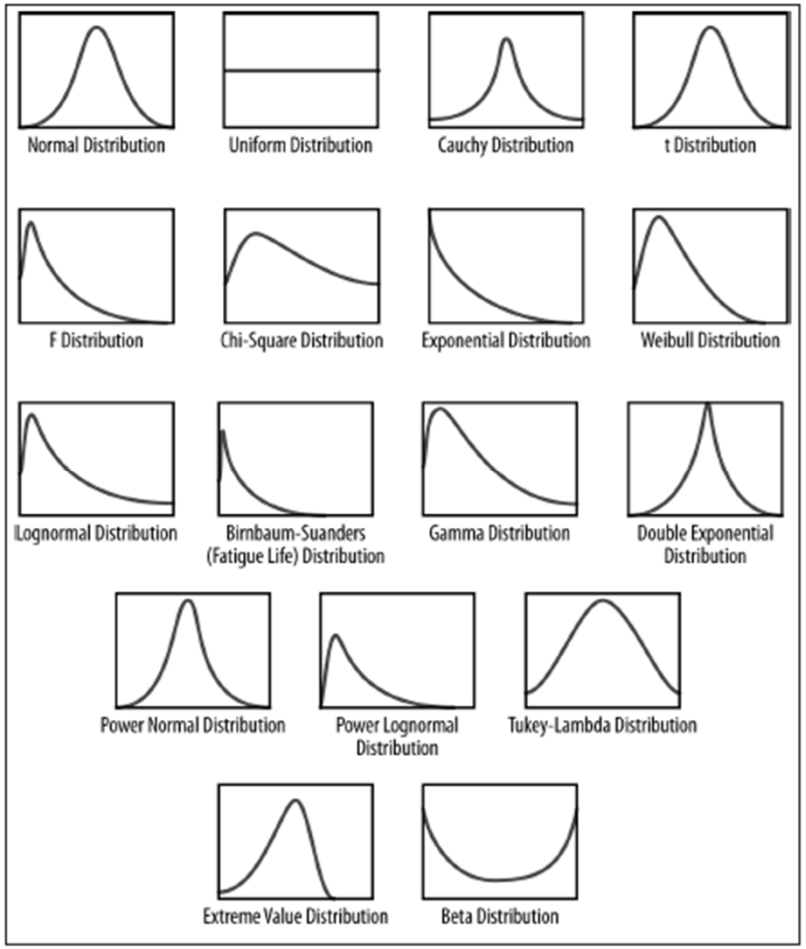
$\omega \sim P(\Theta)$?

Observations

PROBABILITY DISTRIBUTIONS

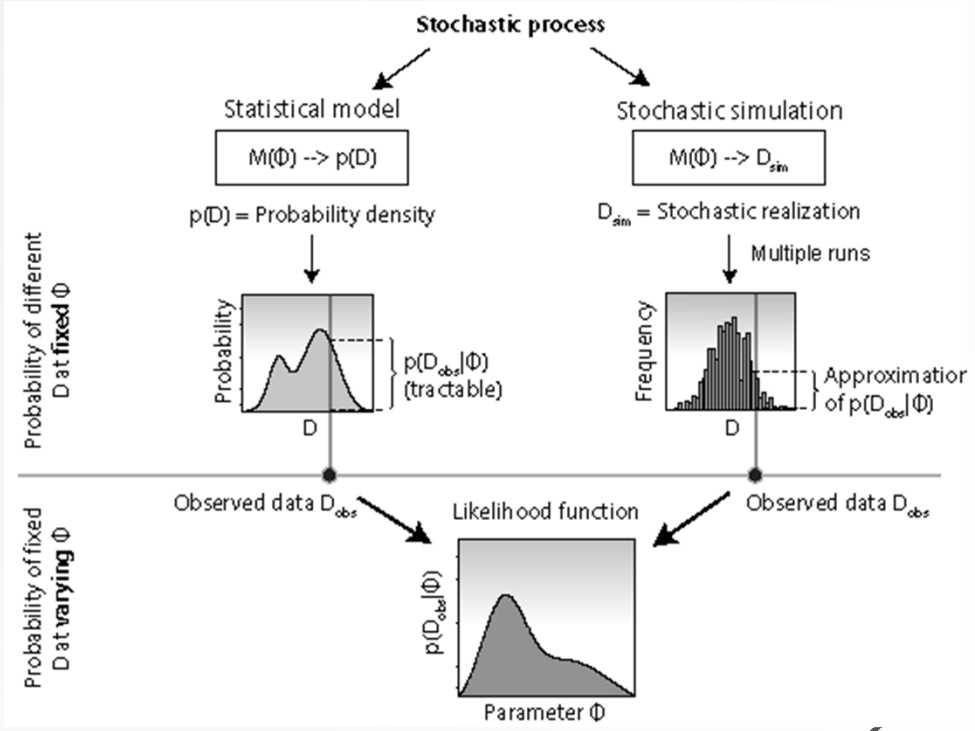
- A **probability distribution** is used to describe the potential outcome of a random variable.

$$\omega \sim P(\Theta)\ ?$$



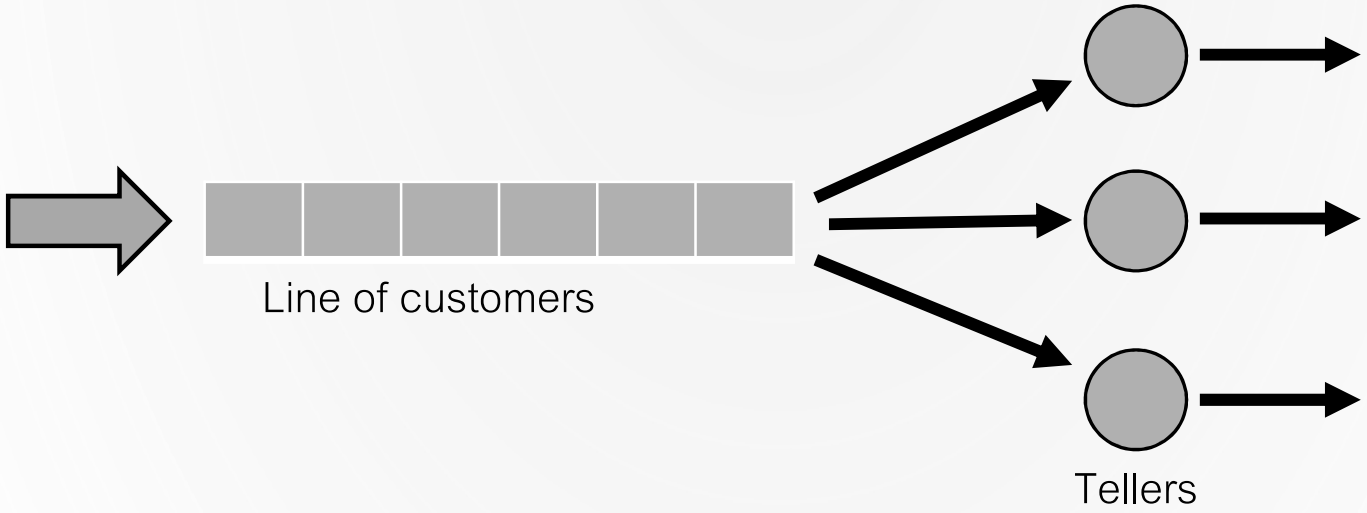
STOCHASTIC SIMULATION

- A **stochastic simulation** is a simulation that traces the evolution of random variables that can change stochastically (randomly) with certain probabilities.



DETERMINISTIC VS. STOCHASTIC

Queueing model for bank (customer & tellers)



Deterministic

- Customer arrives every 10 minutes during 9:00-10:59 and every 5 minutes during 11:00-12:00
- Each customer will take 12 minutes of Teller's time.

Stochastic

- Next customer will arrive 8-11 minutes, using uniform distribution.
- The time a customer will take with the teller is normally distributed, with mean of 9 minutes and s.d. of 2.5 minutes.

COMPUTER SIMULATION TOOLS

- General purpose language
  - C, Java, Python
- Mathematical/Statistical programming languages
  - MATLAB, R, SciLab
- Special Purpose Language/Software
- Spreadsheet
  - Excel, Google Sheet

COMPUTER SIMULATION AND STOCHASTIC MODEL

- To simulate a stochastic system, computer system need a way to introduce randomness into the simulation.
- However, computer system cannot generate true randomness.
- It can, however, generate approximated randomness, using pseudorandom number generator, or just random number generator.

PSEUDORANDOM NUMBER GENERATOR

- Pseudorandom number generator (PRNG) produce a number based on sequence of hard-to-guess numbers.
- User needs to provide PRNG algorithm with seed, basically select which sequence to use. With a PRNG algorithm, one seed will always the same sequence.
- If seed is known, random number can be guessed.
- Other data source, such as computer clock, can help with randomness.

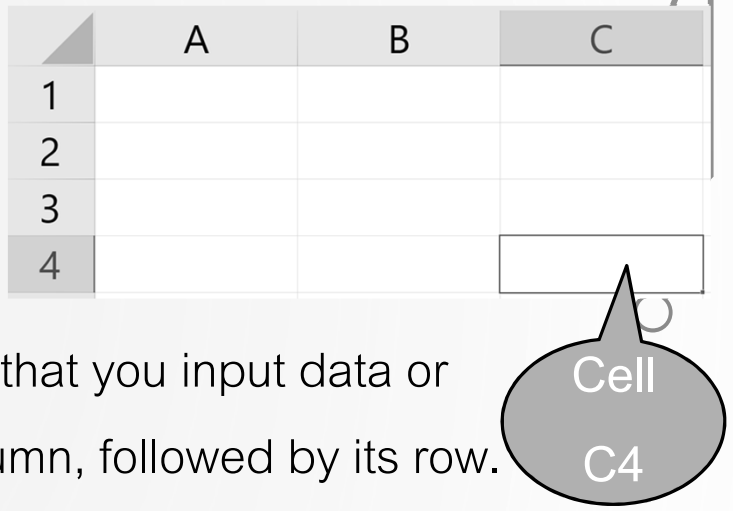
SPREADSHEET SIMULATION

- Today examples will use spreadsheet simulation.
- Spreadsheet = Large table
- Users can enter data and perform calculation on the spreadsheet
- Spreadsheet program provides prewritten calculation routines
- No need of (deep) programming knowledge

SPREADSHEET APPLICATIONS

- Google Sheet
  - Provided by Google, for “free”.
  - Access via Google Drive (https://drive.google.com)
  - Need Google account to use online version. Without Google account, can still download spreadsheet that is shared to you.
- Microsoft Excel
  - Applications from Microsoft, need to buy license to use.
  - For CMU students, can download for free at http://o365.cmu.ac.th/
  - More functionalities than Google Drive, but you may not need them.

SPREADSHEET BASICS



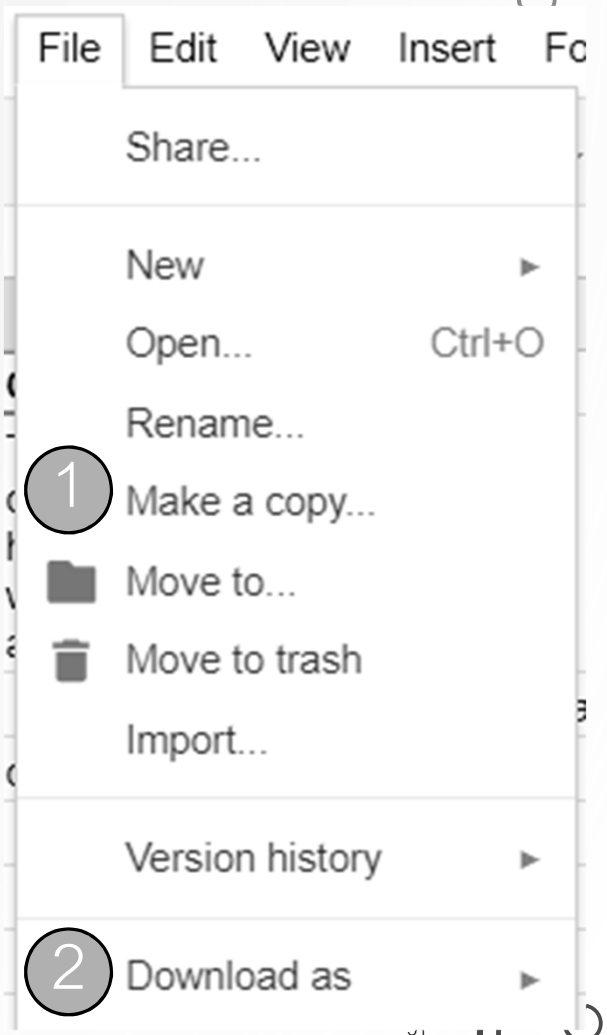
- A spreadsheet has many blocks, or cells that you input data or calculation (formula). Cell name is its column, followed by its row. For example, cell C4 is located at column C and row 4.
- Putting equal sign (=) as a starting symbol in a cell will tell Excel that this cell is a **formula** cell. Excel will perform calculation base on the formula on this cell and display the result. For example, putting "=1+4" at cell C4 will show 5 on cell C4.
- Functions are pre-written calculation you can use in a formula. For example, SUM(1,2,3) will give the result of sum of 1,2, and 3, which is 6.

SPREADSHEET BASICS (CONT.)

- You use values in another cell by using **reference.**
  - For example, C1 will get the value in cell C1.
  - Reference can be relative reference (C1) or absolute reference ($C$1). This will affect what the reference cells will be when you copy the cell with formula and paste it somewhere else.
  - You can also use semi-colon (:) to refer to a group of cells. For example, A1:B3 will refer to cell A1 to cell B3 (A1, A2, A3, B1, B2, and B3)

NOTE ABOUT EXAMPLE SPREADSHEETS

- There are two examples.
  - Projectile Motion: https://goo.gl/ypFrms
  - 10-coins Toss: https://goo.gl/VSsuWm
- When you go to the link, the file is at lecturer's Google Drive account. You can only read, that file.
- If you want to make change, like changing values, you need to either:
  1. Make a copy. A copy of the spreadsheet will be created in your Google Drive account. Or.
  2. Download as → Microsoft Excel (.xlsx), you will get an excel file on your PC.



DETERMINISTIC MODEL EXAMPLE: PROJECTILE MOTION

- Launch an object at an angle.
  - Horizontal (x-axis) velocity is constant
  - Vertical (y-axis) velocity is affected by gravity. Object will go up at first, then come back down.
  - Example question:
    - When will the object come down? How far can it go before it comes back down?

PROJECTILE MOTION MODEL

- Initial coordinates:

$$x_0 = y_0 = 0$$

- Launch angle: θ
- Initial velocity: v_0

$$v_{x,0} = v_0 \cos(\theta)$$

$$v_{y,0} = v_0 \sin(\theta)$$

- Acceleration:

$$a_x = 0$$

$$a_y = -g = -9.8$$

- Velocity at time t

$$v_{x,t} = v_{x,0} = v_0 \cos(\theta)$$

$$v_{y,t} = v_0 \sin(\theta) - gt$$

- Coordinates at time t

$$x_t = v_{x,t} t = v_0 \cos(\theta)\, t$$

$$y_t = v_0 \sin(\theta) - \frac{1}{2} g t^2$$

PROJECTILE MOTION SIMULATION

- Initial Parameters: v_0, θ, g, x_0, y_0
- Time step
  - What is the size of the time step, 10s?, 1s? 0.01s?
  - What is the range of time we want to perform simulation?
- Formula
  - Formula for *x* and *y* are provided. But if they are not provided directly, but only differential function of them is provided (velocity in this case). You may need to solve (or approximately solve) the differential function to get the changes in value first.

$$\Delta y(a,b) = \int_{t=a}^{t=b} v_{y,t}\,dt$$

PROJECTILE MOTION SIMULATION

	A	B	C	D	E	F	G	H	I	J
1	**Parameters**									
2	v{0} (m/s)	7.0000								
3	theta (radian)	0.7854		(degree)	45					
4	g (m/s^2)	9.8000								
5	vx{0} (m/s)	4.9497								
6	vy{0} (m/s)	4.9497								
7										
8	x{0} (m)	0.0000								
9	y{0} (m)	0.0000								
10										
11	**Simulation**									
12	t (s)	0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4
13	vx{t} (m/s)	4.950	4.950	4.950	4.950	4.950	4.950	4.950	4.950	4.950
14	vy{t} (m/s)	4.950	4.460	3.970	3.480	2.990	2.500	2.010	1.520	1.030
15	x{t} (m)	0.000	0.247	0.495	0.742	0.990	1.237	1.485	1.732	1.980
16	y{t} (m)	0.000	0.235	0.446	0.632	0.794	0.931	1.044	1.132	1.196

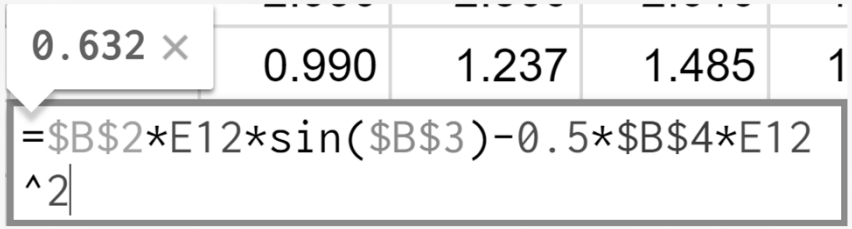
Initial Values

Values at t = 0.15

https://goo.gl/ypFrms

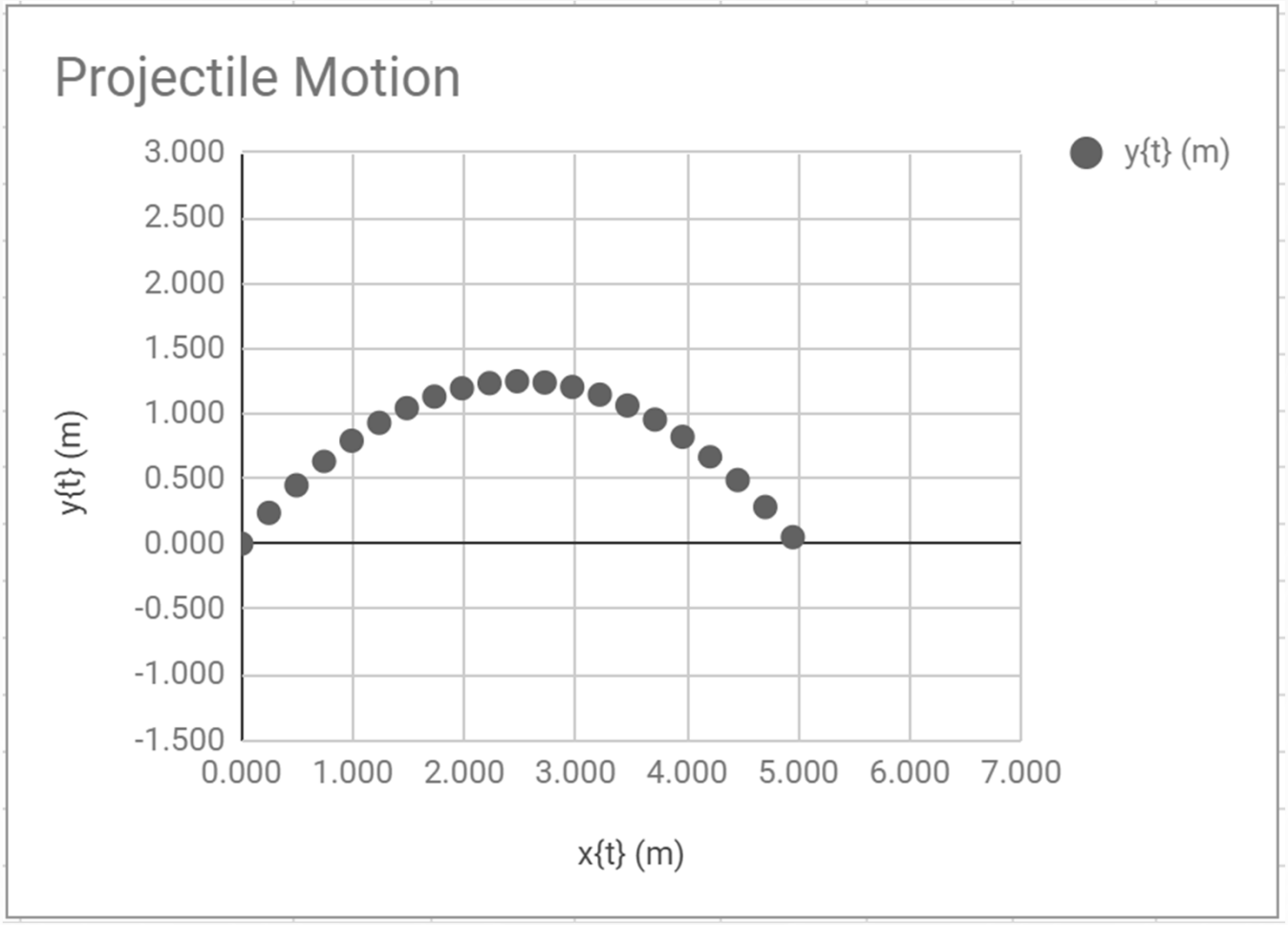
PROJECTILE MOTION SIMULATION

- The Simulation
  - Formulas are used to updated values of cells



    - E12 holds value t = 0.15, cell, $B$2 and $B$4 holds contants v_0 and g respectively, and thus use absolute reference. sin() is a function provided by Google sheet.
    - And when the initial values are changed, the values in the simulation will change according.
  - Charts
    - You can also make charts out of the data in the cells

PROJECTILE MOTION SIMULATION – CHART EXAMPLE



STOCHASTIC MODEL EXAMPLE: 10-COINS TOSS

- Tossing 10 fair coins, count how many come up head.
  - What is the expected value of this?
  - How likely will the experiment yield this result?
- The model for 10-coins toss
  - Each coin toss is independent.
  - Can be said that fair coin tosses are i.i.d.
  - So, the simulation will perform coin toss 10 separate times for one trials.

10-COINS TOSS SIMULATION

Each trial consist of 10 coins toss.

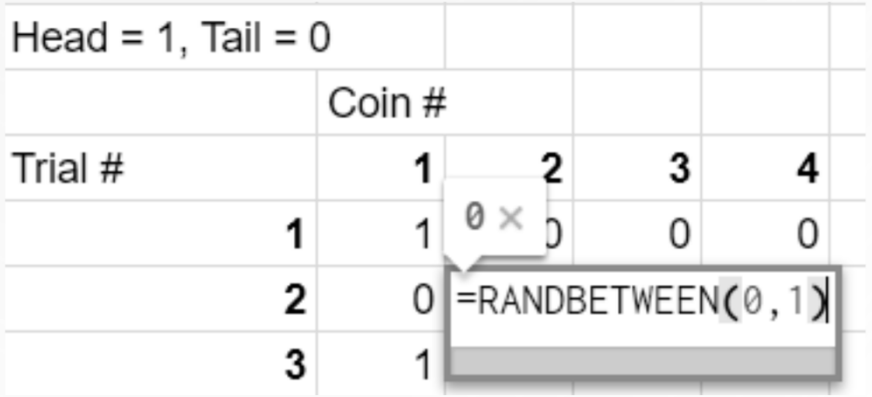
We perform 10 trails. (Why?)

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	**Coin Simulation**												
2	Tossing 10 fair coins for 10 times how many times will we get 5 heads and 5 tails?												
3		Head = 1, Tail = 0											
4	ctrl-R to reroll		Coin #										
		Trial #		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**Number of Heads**
			1	0	1	0	0	0	1	1	1	0	0	**4**
			2	1	1	1	0	0	0	1	1	1	0	**6**
			3	0	1	0	0	0	0	0	1	1	1	**4**
			4	1	0	0	1	0	0	0	1	0	1	**4**
			5	1	1	0	0	0	0	0	0	0	1	**3**
			6	0	1	0	1	1	0	1	0	1	0	**5**
			7	0	1	0	1	1	0	0	1	1	1	**6**
			8	0	1	0	0	0	1	1	0	0	1	**4**
			9	1	0	1	1	1	0	0	1	1	1	**7**
			10	0	1	0	0	1	1	0	0	0	1	**4**
16													
17	**Number of times we actually get 5**	1											
18	**Average number of heads from the simulation**	4.7											

https://goo.gl/VSsuWm

10-COINS TOSS SIMULATION (CONT.)

- How do we get random number?
  - Google Sheet provides a few random functions, which can be use to generate random number.
  - RAND() generate a real number between 0 and 1, inclusive.
  - RANDBETWEEN(A, B) generates an integer between A and B, inclusive.



10-COINS TOSS SIMULATION (CONT.)

- How to count number of head?
  - Since head is 1 and tail is 0, we can just SUM() function to add up the 1's.

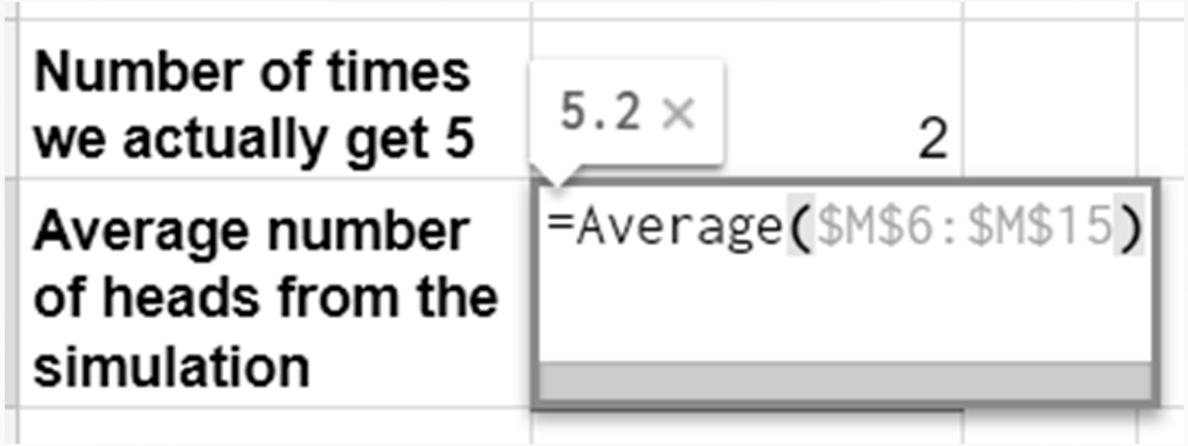
	1	2	3	4	5	6	7	8	9	10	2 × ber of Heads
1	1	0	0	0	0	0	1	0	0	0	=SUM(C6:L6)
2	0	1	0	0	1	1	0	0	1	1	

- How to count number of trial with exactly 5 heads?
  - COUNTIF() function

	2 ×
Number of times we actually get 5	=COUNTIF($M$6:$M$15,5)

10-COINS TOSS SIMULATION (CONT.)

- How to get average number of heads in 10 trials
  - AVERAGE() function



TO LEARN MORE...

- If you want to know more about spreadsheet, Computer Science off 204100: IT& Everyday Life, which cover Microsoft Excel.
- 204100's materials are also available for download.
  - Thai: http://www.cs.science.cmu.ac.th/course/204100/doku.php
  - English:

    http://www.cs.science.cmu.ac.th/course/204100/doku.php?id=english_section
- Many guides and tutorials are also available online, or in book forms.