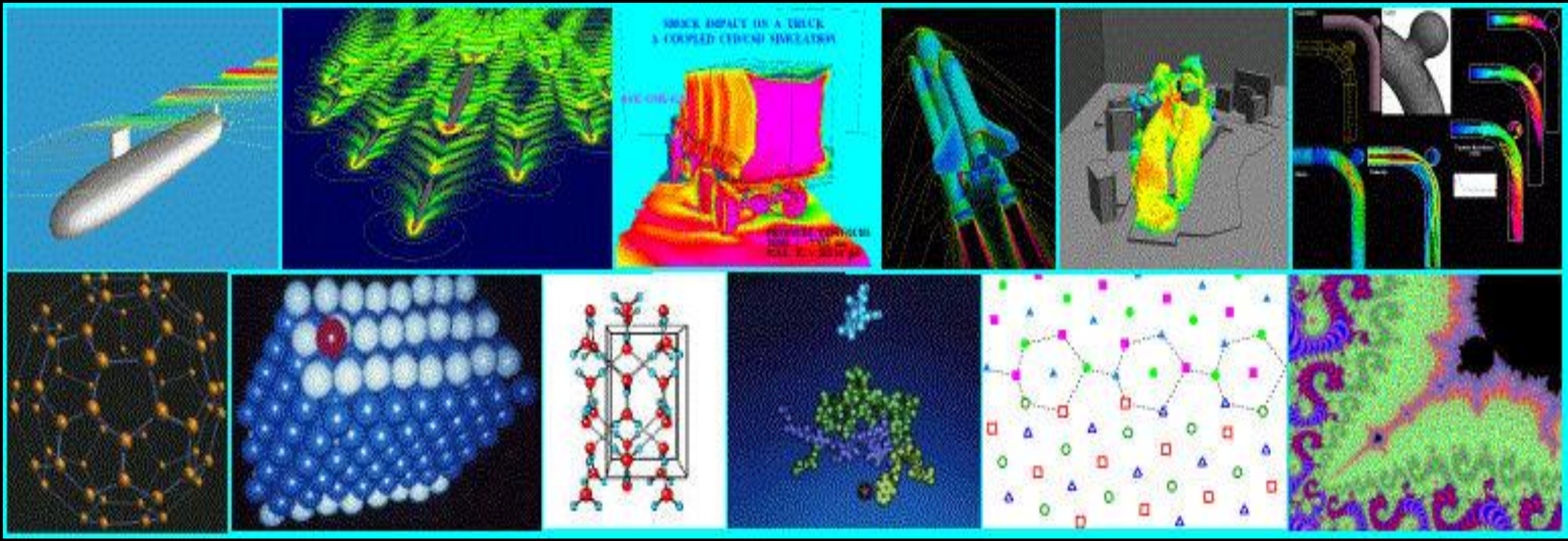
Computing for Scientists
Section 2
Scientific Simulation (SS)

(October 08, 2013 – Nov. 12, 2013)



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CDS 130 - 001
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Scientific Simulation (SS)

CH1. Introduction

CH2. Computational Models

- Predator – Prey Model

CH3. Simulation Basics

- Algorithm, Iteration, Interval, Subinterval

CH4. Differentiation Equation (Not Covered)

CH4. Integration Equation

CH5. Scientific Method

Section 2
Chapter 1

Introduction

(Oct. 08, 2013)

Motivation

- Scientific simulation allows one to

  (1) produce the **quantitative details**, and

  (2) thus **predict the behavior** of a complex scientific system, e.g., biological systems, environmental systems, physical systems, engineering systems etc.

- It is a new way of scientific research, in additional to traditional experimental (including observations) and mathematical approaches.

Example

http://www.ncac.gwu.edu/research/anim/Taurus_to_Taurus_Airbags_Dummies_Seatbelts.mpeg

Full-scale crash testing of several potential crash scenarios is cost-prohibitive and does not achieve comprehensive solutions. Instead, NCAC relies on simulating these scenarios on high-performance computers, which saves time and maximizes research dollars

Example

Cellular Blood Flow:
http://www.youtube.com/watch?v=o11NDvrZMNs&feature=related

The RBCs are modeled as a membrane with hemoglobin inside with a viscosity of 6cP. Each RBC membrane is constructed of linear finite element triangular shells. These shell elements deform due to the fluid-structure interactions with the blood plasma and the hemoglobin.

Example

Merger of the Milky Way:
http://www.youtube.com/watch?v=Cd9cBlvfjow

The Milky Way and the Andromeda galaxy will likely fall together and merge within a few billion years. In this speculative simulation, the two galaxies flyby one another, exciting tidal tails and bridges and collide on a second pass finally merging after several convulsions. The last remnants of the smashed spirals show up as shells and ripples surrounding a newborn elliptical galaxy.

Example: Equations

Many scientific simulations are based on so-called Navier-Stokes Equations (Note: do not worry about the math complexity) http://www.cfd-online.com/Wiki/Navier-Stokes_equations

The instantaneous continuity equation (1), momentum equation (2) and energy equation (3) for a compressible fluid can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j\right] = 0 \qquad (1)$$

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_j}\left[\rho u_i u_j + p\delta_{ij} - \tau_{ji}\right] = 0, \quad i = 1, 2, 3 \qquad (2)$$

$$\frac{\partial}{\partial t}\left(\rho e_0\right) + \frac{\partial}{\partial x_j}\left[\rho u_j e_0 + u_j p + q_j - u_i \tau_{ij}\right] = 0 \qquad (3)$$

Navier-Stokes Equations: three differential equations

A Pipeline of Models

A common way that science gets done

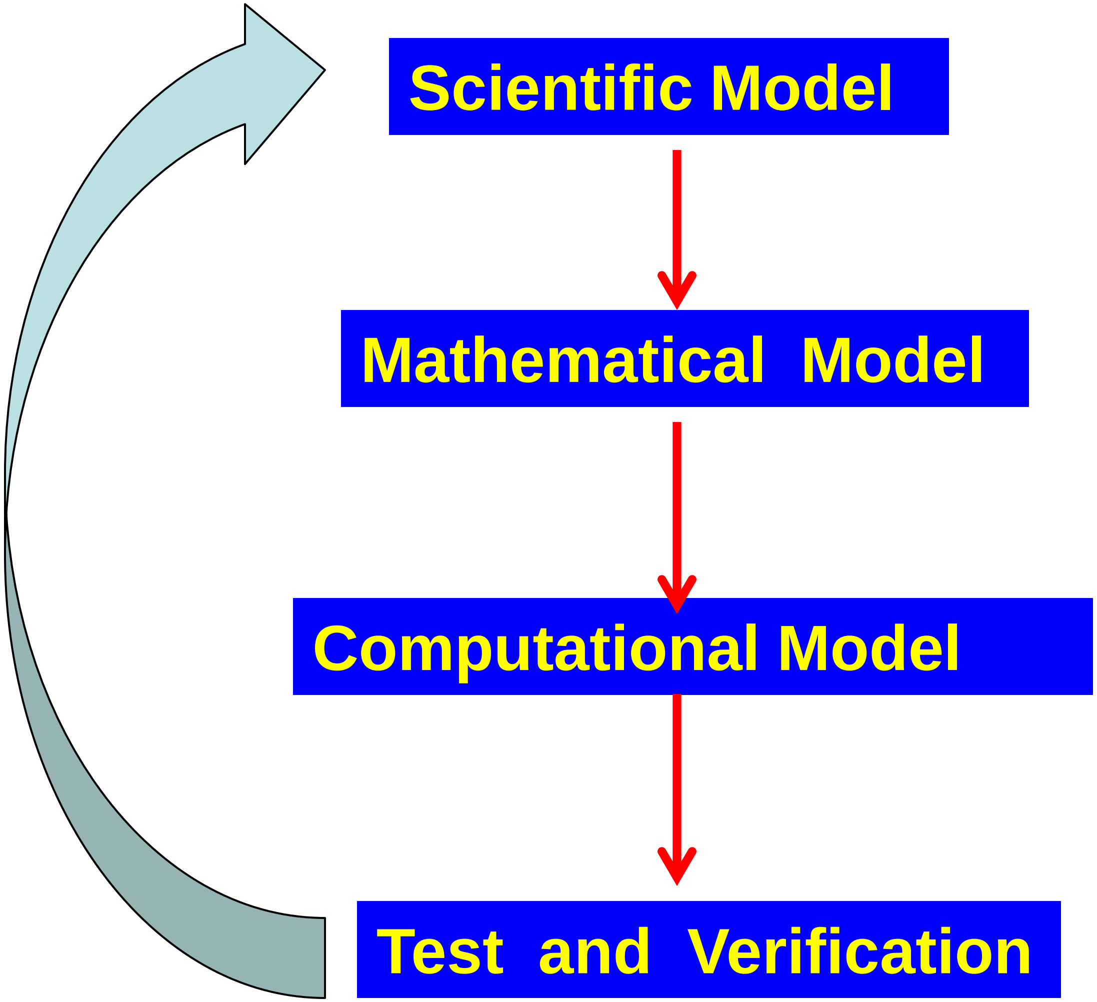
1. Domain specialists (e.g., biologists) develop a conceptual representation of the system, so called **scientific model**

2. The domain specialists collaborate with mathematicians to develop a mathematical representation, or **mathematical model** that corresponds to the scientific model

3. The domain specialists and mathematicians work with computational scientists to implement the equations and explore the results using a computer, that is to develop a **computational model** of the mathematical model.

4. The computational methods need to be **tested**
5. Repeat steps 1 -> 2 -> 3 ->4 -> 1, gain better results.

A Pipeline of Models



The End of Chapter 1

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A Short Review

A pipeline of models in science

Scientific Model

↓

Mathematical Model

↓

Computational Model

↓

Test and Verification

Section 2
Chapter 2

Computational Models

(October 10, 2013)

Questions?

- How to solve a scientific question using computation?
- How to find your bank balance for the next ten years?
- How to predict the populations of foxes and rabbits for the next 50 years in an isolated island?

Objectives

Learn how to create a computational model based on the scientific question that you are asked to solve

Step 1: Create a **mathematic model** that represents a given scientific question

- **Scientific Model → Mathematical Model**

Step 2: convert the mathematical model to a computational model for subsequent calculation

- **Mathematical Model -> Computational Model**

Example 1

Scientific model:

Every year your bank account balance increases by 20%

Mathematical model:

B(next-year) = B(this-year) + 0.2 * B(this-year)   %okay

OR

B(i+1) = B(i) + 0.2 * B(i)   % better mathematically

Example 1 (continued)

Computational Model

```
>> B(i+1)=B(i)+0.2*B(i)  % this is a good algorithm, but
     not good implementation
```

What is wrong with this?

B(1) needs to be defined; B(1): the initial value

```
>> B(1) = 1000   % assuming the balance of the first year
     is1000, or any input number specified by the
     question; the initial value needs to be specified

>> B(2)=B(1)+0.2*B(1)
```

Example 1 (continued)

Better Computational Model

Use FOR loop, but more constrains needed.
(1) The first year is $1000
(2) The balance increases 20% every year
(3) Calculate the balance in the next 10 years.

```
>> B(1) = 1000

>> for i=[1:10]
        B(i+1)=B(i)+0.2*B(i)
   end
```

What is B(11)?

Example 2

scientific model:

Every year your bank account balance increases by 20%.
Every year you pay a fee of $100 to the bank

Mathematical model:

B(next-year) = B(this-year) + 0.2 * B(this-year) – 100

$$B(i+1) = B(i) + 0.2*B(i) - 100$$

Example 2 (continued)

Computational Model

Initial value is needed:
Assuming that the balance of the first year is $1000

```
>> B(1) = 1000
>> B(2)=B(1)+0.2*B(1)-100
```

Example 2 (continued)

Better Computational Model

Use FOR loop.

```
>> B(1) = 1000

>> for i=[1:10]
        B(i+1)=B(i)+0.2*B(i)-100
   end
```

What is B(11)?

Example 3

Scientific Model

Every year your bank account balance doubles.

Question: What is the mathematical model?

Example 3 (continued)

Mathematic Model

Answer:

B(next-year) = 2 * B(this-year)

Or

B(i+1) = 2 * B(i)

Example 3 (continued)

Computational Model

Question:

Every year your bank account balance doubles.
Assuming in the first year, the balance is $1000.

Develop a computational model in Matlab to calculate the balance in the next 10 years?

What is the balance in the 11th year?

Example 3 (continued)

Answer:

```
>> clear    %clear the existing variables

>>B(1)=1000

>>for i=[1:10]
      B(i+1)=B(i)*2
  end

>>B(11)

Ans =
     1024000
```

Example 4

scientific model:

The death rate of the population in a country suffering from war is 3% per year and no babies are born

Question: What is the mathematical model?

Question: Develop a computational model to calculate the population in the next 10 years? What is population in the 11^{th} year?
Assuming the initial population is 20 million.

Example 4 (continued)

Answer: (mathematic model)

P(next-year)=P(this-year) – 0.03*P(this-year)

Answer: (computational model)

```
>> clear    %clear the existing variables
>>P(1)=20000000 %20 million, also expressed by “2e7”
>>for i=[1:10]
   P(i+1)=P(i)-0.03*P(i)
   end

>>P(11)
Ans =
     1.47e+07
```

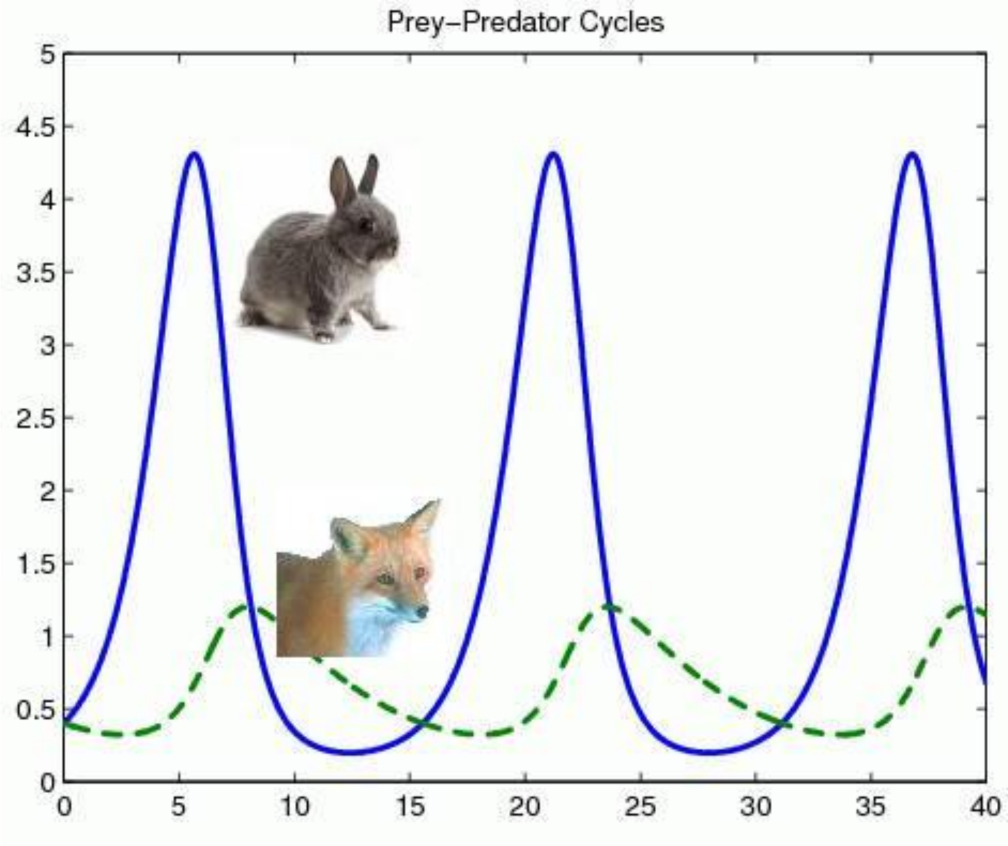
Now consider a scientific model with two inter-dependent variables

Predator – Prey Model

Consider a closed ecosystem, an island with only two species: foxes, the predator, and rabbits, the prey.

Imaging how the two populations change with time?

Predator – Prey Model



Periodical change of populations can happen
http://www.scholarpedia.org/article/Predator-prey_model

Predator – Prey Model

What if the predators are so greedy?

What if the preys are so easy to grow?

Predator – Prey Model

“Predator-prey models are arguably the building blocks of the bio- and ecosystems as biomasses are grown out of their resource masses. Species compete, evolve and disperse simply for the purpose of seeking resources to sustain their struggle for their very existence. Depending on their specific settings of applications, they can take the forms of resource-consumer, plant-herbivore, parasite-host, tumor cells (virus)-immune system, susceptible-infectious interactions, etc.” (http://www.scholarpedia.org/article/Predator-prey_model)

An online simulator:

http://home.messiah.edu/~deroos/CSC171/PredPrey/PRED.htm

Predator – Prey Model

scientific model for rabbits:

The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of foxes. Here, the value of 0.02 is called the interaction constant. The death rate depends on the population of the predator

Mathematical model:

%R(i): number of rabbits in year i
%F(i): number of foxes   in year i

R(i+1)=R(i) + 0.50*R(i) – (0.02*F(i))*R(i)

Predator – Prey Model

Scientific model for foxes:

The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of rabbits. Here, the value of 0.001 is called the interaction constant. The birth rate of the predator depends on the resource, or the food.

Mathematical model:

$$F(i+1) = F(i) - 0.1*F(i) + (0.001*R(i))*F(i)$$

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(Oct. 17, 2013 Starts Here)

A Short Review

Scientific model and question:

Every year your bank account balance increases by 20%. The balance in the first year is $1000. Find the balance in the next 10 years?

Mathematical Model:

B(i+1) = B(i) + 0.20*B(i)

Computational Model:

```
>> B(1) = 1000;
>> for i=[1:10]
        B(i+1)=B(i)+0.20*B(i);
   end
>>B
```

Predator – Prey Model

The observations of this closed ecosystem

- Change in number of rabbits (prey) per year
  - increases in proportion to the number of rabbits (breeding like rabbits!) – **the birth rate of prey**
  - decreases in proportion to (the number of foxes) x (number of rabbits). **The interaction constant** specifies how aggressive is the predator.
  - Does not depend on rabbits dying of natural death (negligible compared with the loss due to predator)
- Change in number of foxes (predator) per year
  - decreases in proportion to the number of foxes due to natural death – **the death rate of predator**
  - increases in proportion to (the number of rabbits) x (the number of foxes) **. The interaction constant specifies how weak is the prey.**
  - Does not depend on the natural birth

Predator – Prey Model

The full scientific model:

- The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of foxes.
- The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of rabbits
- The initial number of rabbits is 100
- The initial number of foxes is 20
- Find out the number of rabbits and foxes in the next 40 years

Predator – Prey Model

Mathematic Model

Answer:

$$R(i+1)=R(i) + 0.50*R(i) - (0.02*F(i))*R(i)$$

$$F(i+1) = F(i) - 0.1*F(i) + (0.001*R(i))*F(i)$$

Predator – Prey Model

Answer: (computational model)

```
>>clear
>>R(1)=100.0   %initial population of rabbits
>>F(1)=20.0    %initial population of foxes
>>BR_rabbit=0.5     %birth rate of rabbits
>>DR_rabbit_INT=0.02   %death date of rabbit (prey) due to interaction
>>DR_fox=0.1     %death rate of fox
>>BR_fox_INT= 0.001 % birth rate of fox (predator) due to interaction

>>for i=1:40
   R(i+1)=R(i)+BR_rabbit*R(i)-DR_rabbit_INT*F(i)*R(i)
   F(i+1)=F(i)-DR_fox*F(i)+BR_fox_INT*R(i)*F(i)
 end

>>R   %print the number of rabbits in 40 years
>>F   %print the number of foxes in 40 years
```

Predator – Prey Model

Answer: (computational model) (continued)

```
>>figure(1);
>>plot(R,'*')   %make a plot showing rabbit evolution

>>figure(2);
>>plot(F,'-')   %make a plot showing fox evolution
```

Predator – Prey Model

Sharpen your MATLAB skill

(1) How to write a program file?

(2) How to make a simple plot

1. It is not convenient to type multiple line programming codes in the command line. Any mistake means re-typing

2. To find the evolution, one needs to use a graphic plot to illustrate the evolution. The plot needs to be well annotated.

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(Oct. 29, 2013 Starts Here)

Predator – Prey Model

The full implementation of the predator-prey model

1. Fully implement the predator-prey mode described in the next page

2. Type-in the MATLAB program and save it as “predator.m”

3. Make a high-quality plot with proper annotations to show the evolution of the population of rabbits and foxes

4. Save the plot as “predator.png”

Predator – Prey Model

The full scientific model:

- The birth rate of rabbits is 50%. The death rate of rabbits is 0.02 times the number of foxes.
- The death rate of foxes is 10%. The birth rate of foxes is 0.001 times the number of rabbits
- The initial number of rabbits is 100
- The initial number of foxes is 20
- Find out the number of rabbits and foxes in the next 50 years

Predator – Prey Model

Answer: “predator.m”

```
clear
R(1)=100.0   %initial population of rabbits
F(1)=20.0    %initial population of foxs
BR_rabbit=0.5     %birth rate of rabbit
DR_rabbit_INT=0.02   %death date of rabbit (prey) due to interaction
DR_fox=0.10     %death rate of fox
BR_fox_INT= 0.001 % birth rate of fox (predator) due to interaction

for i=1:50
 R(i+1)=R(i)+BR_rabbit*R(i)-DR_rabbit_INT*R(i)*F(i)
 F(i+1)=F(i)-DR_fox*F(i)+BR_fox_INT*F(i)*R(i)
end

hold off %clear the previous plot setting
figure(1)  %make plot 1 for rabbit population evolution
plot(R,'-*r')    %line specification: solid line, marker *, red color
hold all  %hold on all previous settings: plotting window, axis, styles
plot(F,':ob')    %line specification: dotted line, marker circle, blue
legend('Rabbit','Fox')


xlabel('Year')    % X axis label
ylabel('Population Numbers')   % Y axis label
title('Predator-prey Model Result',...
    'FontSize',18)
```

(Oct. 29, 2013 ends Here)

(Oct. 31, 2013 Starts Here)

A Short Review

Predator-Prey Model

1. **Download and save the "predator.m" from the class website at http://helio.gmu.edu/public/jzhang/teaching/2013_CDS130_Fall/ClassNotes.html**

2. **Inspect the program for proper styles**
   - **Sufficient comments in the beginning and throughout the program**
   - **Separating the parameters from the calculation**
   - **Proper annotation of the plots**

Gain Insight from Models

Inspecting different models

1. What happens if initial fox population is 50?

2. What happens if the rabbit birth rate is 100%?

3. What happens if the fox interaction constant is 0.005?

4. Play with different parameters as you wish. The goal is to understand the different model results when the input parameters change.

Gain Insight from Models

Studying different models will give you the scientific insight of the underlying scientific system

The End of Chapter 2

Section 2
Chapter 3

Simulation Basics

(October 31, 2013)

Questions?

- How to write a complex program?

- How to make your model accurate?

Objectives

Introduce several basic concepts essential to many computation models

1. **Algorithm**
2. **Iteration**
3. **Initial Condition**
4. **Interval and Sub-interval**

Algorithm

In mathematics and computer science, an algorithm is an effective method expressed as a finite set of well-defined instructions for implementing a function.

Computational Model =

(1) Algorithm (general, universal)

+

(2) Programming (depending on languages you use)

Algorithm

- Algorithm is a generic program instruction.
- It is also called pseudo-code, not specific implementation
- It heavily uses logic and reasoning for solving a problem
- It is essential for a complex program. You need the architect or the designing map before the construction.
- It can then be implemented in any program language, e.g., Matlab, Python, C, C++, Java, Fortune, IDL et al

Algorithm

Question:
Construct an algorithm of finding the largest number in an array?

Algorithm

```
Array A(N)  %input an array of N elements
val_max = 0     % initialize parameter max

Begin Iteration N Times
        IF  val_max < A(i)
             THEN val_max = A(i)
        ELSE do-nothing
End Iteration
```

Algorithm

Question:
Construct an algorithm of finding the largest number in an array? You need to program it using MATLAB

Program (mymax.m)

```
clear
A=[1,4,8,3,2,5]     %provide a sample array

val_max=0;
for i=[1:6]
    if val_max < A(i)
        val_max = A(i);
        display('New max value is found')
    else
        display('DO NOTHING')
    end
end

val_max
```

Algorithm

How to use the self-defined function: simply call the name

```
>>A = [1,2,3,4,3,2,1]     %input array

>>mymax2(A)       %find the maximum value of array A

>>M=mymax2(A)    % return the maximum value to M


>>B=[1, 2, 3, 4, 5, 6, 1]

>>mymax2(B)
```

Iteration

X(i+1) = X(i) + “Function of X(i)”

- Iteration is the act of repeating a process with the aim of approaching a desired result.

- The output of current iteration is used as the input of the next iteration

- Iteration is the **most fundamental method** in computation that represents a dynamic scientific system.
    - For example, the time evolution of populations
    - For example, the change of the bank balances

Iteration

```
>>for i=[1:N]
      X(i+1) = X(i) + “FUNCTION of X(i)”;
end
```

i: the sequence number of the iteration, representing the **independent variable, usually the “time**”, e.g., year in population growth

N: total number of iterations

X: the **dependent variable**, an unknown function, but the model seeks to find

FUNCTION(X(i)): the known function representing the knowledge or model of the system

Initial Condition

- Initial condition defines the initial value of an iteration
- Different initial condition will define a different model

Initial Condition

The result of a real model depends on the initial condition

A specific scientific model:

Every year your bank account balance increases by 10%.

Assuming in the first year, the balance is $1000.

What is the balance in the 10^{th} year?

Question: what is the initial condition?

Initial Condition

Answer: In the first year, the balance is $1000.

Interval and Sub-interval

- In numerical simulation, one has to specify the calculation **interval** and **sub-interval**

- **Interval** is the domain, or the overall range of the calculation

- **Sub-interval** is the step-size in each iteration of the numerical calculation
    - We have assumed that the sub-interval is every one year in many examples. But this is for convenience only, it can be every one month, or even every day

Interval and Sub-Interval

The result of a computational model depends on the interval and sub-interval.

A specific scientific model:

Every year your bank account balance increases by 12%.

Assuming in the first year, the balance is $1000.

What is the balance in the 10th year?

Question: what is the interval of the model?

What is the sub-interval of the model?

Interval and Sub-Interval

Answer: The interval is from year 1 to year 10.
The sub-interval is every one year.

Question: what happens if the sub-interval changes? Will this change the result?

Interval and Sub-Interval

Specific scientific models:

Model 1:
Every year your bank account balance increases by 12%.
Assuming in the first year, the balance is $1000.
What is the balance in the 10th year?

Model 2:
Every month your bank account increases by 1%
Assuming in the first month of the first year, the balance is $1000.
What is the balance at the end month of the10th year?

What are the commons and differences of the two models?

Interval and Sub-Interval

Answer:

The two models share the same scientific knowledge or algorithm: increasing by 12% on a yearly base, or "equivalently" by 1% on a monthly base

The two models have the "same" interval: 10 years or 120 months

The difference is that the two models have different sub-intervals: every year versus every month

Interval and Sub-Interval

Question: implement the following models in a single program

Model 1:
Every year your bank account balance increases by 12%.
Assuming in the first year, the balance is $1000.
What is the balance in the 10th year?

Model 2:
Every month your bank account increases by 1%
Assuming in the first month of the first year, the balance is $1000.
What is the balance at the end month of 10th year?

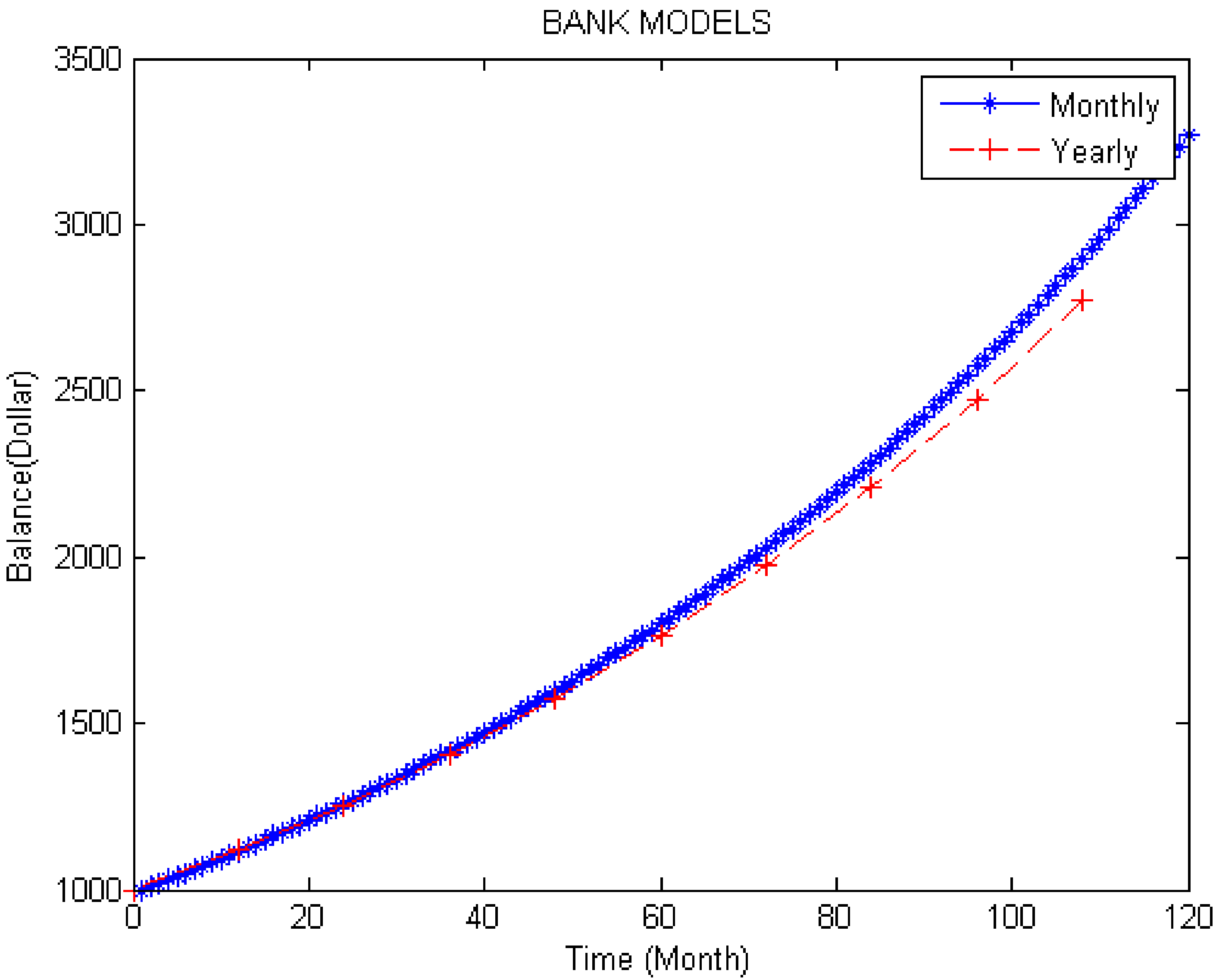
Write a program code to implement the two models, and make a plot to show the results?

Interval and Sub-Interval

“bank_interval.m”

```
clear;clc
BM1(1)=1000;  %model 1 initial condition
BM2(1)=1000;  %model 2 initial condition

for i=[1:9]
    BM1(i+1)=BM1(i)+0.12*BM1(i);
end

for i=[1:119]
    BM2(i+1)=BM2(i)+0.01*BM2(i);
end

%figure(1)
hold off
x2=[1:120];
plot(x2,BM2,'-*b')

xlabel('Time (Month)')
ylabel('Balance(Dollar)')
title('BANK MODELS')

hold all
x1=[1:10]*12-12;
plot(x1,BM1,'--+r')

legend('Monthly','Yearly')
```

Interval and Sub-Interval



Interval and Sub-Interval

Yearly	Model	Monthly	Model
i=1 (Beginning of year 1)	$1000	i=1 (Beginning of Month 1)	$1000
i=2 (Beginning of year 2) (Beginning of month 13)	$1120	i=13 i=1+12*(2-1) (Beginning of month 13)	$1127
i=5 (Beginning of year 5) (Beginning of month = 1 + 12*4 = 49	$1574	i=49 i=1+12*(5-1) (beginning of month 49)	$1612
i=10 (Beginning of year 10) (Beginning of month = 1+12*9=109)	$2773	i=109 i=1+12*(10-1) (beginning of month 109)	$2929

The Effects of Sub-interval

- A smaller sub-interval requires more steps of calculation

- But, a smaller sub-interval provides more detailed evolution

- Furthermore, a smaller sub-interval provides a more accurate result
    - This conclusion will be further illustrated in the context of integration (the next chapter)

(Oct. 31, 2013 ends Here)

(Nov. 05, 2013 Starts Here)

A Short Review

1. **Algorithm**

2. **Iteration**

3. **Initial Condition**

4. **Interval and Sub-interval**

Interval and Sub-Interval

Specific scientific models:

Model 1:
Every year your bank account balance increases by 12%.
Assuming in the first year, the balance is $1000.
What is the balance in the 10th year?

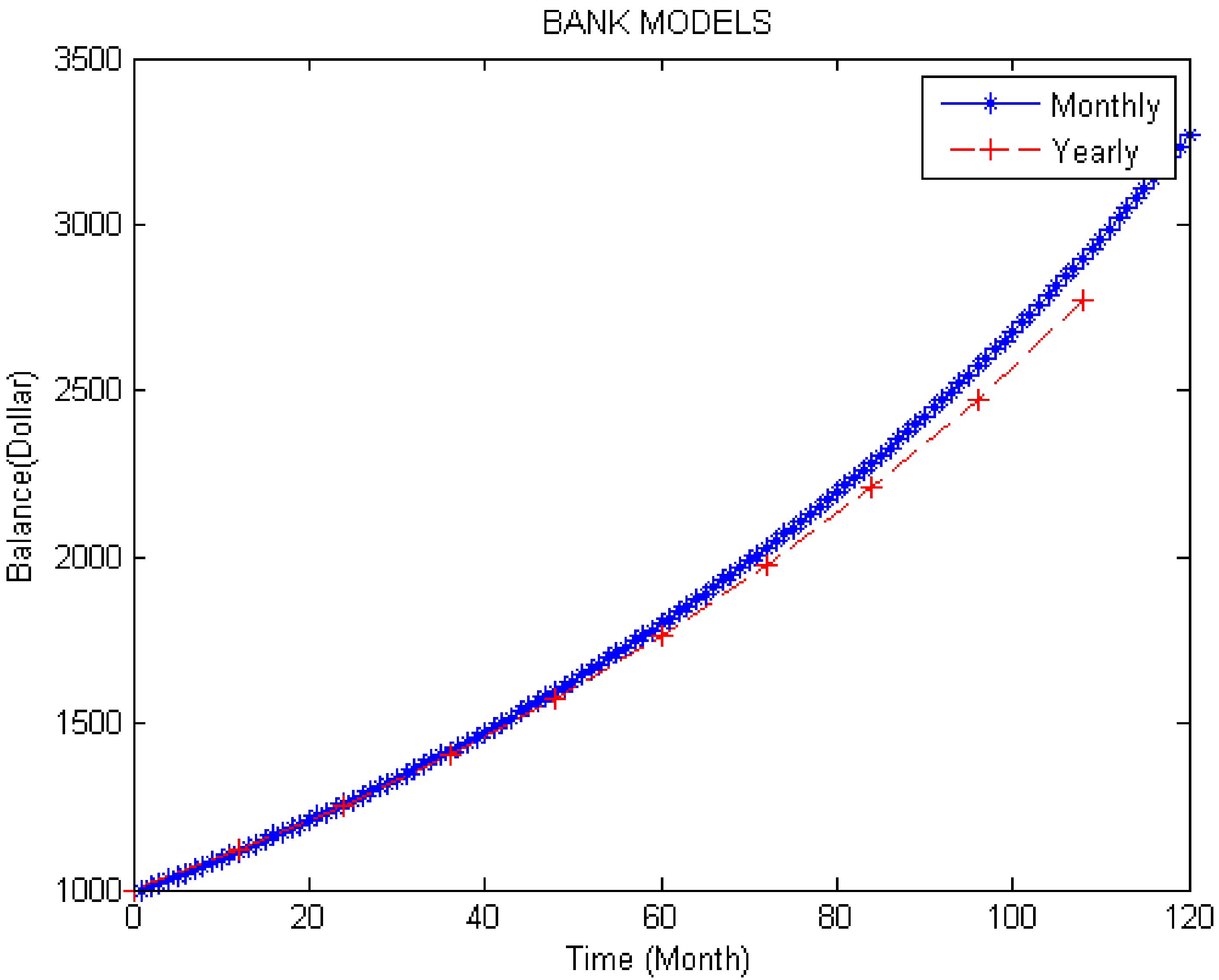
Model 2:
Every month your bank account increases by 1%
Assuming in the first month of the first year, the balance is $1000.
What is the balance at the end month of the10th year?

Interval and Sub-Interval

"bank_interval.m"

```
clear;clc
BM1(1)=1000;  %model 1 initial condition
BM2(1)=1000;  %model 2 initial condition

for i=[1:9]
   BM1(i+1)=BM1(i)+0.12*BM1(i);
end

for i=[1:119]
   BM2(i+1)=BM2(i)+0.01*BM2(i);
end

%figure(1)
hold off
x2=[1:120];
plot(x2,BM2,'-*b')

xlabel('Time (Month)')
ylabel('Balance(Dollar)')
title('BANK MODELS')

hold all
x1=[1:10]*12-12;
plot(x1,BM1,'--+r')

legend('Monthly','Yearly')
```

Interval and Sub-Interval



The End of Chapter 3

Section 2
Chapter 4

Integration Equation

(November 05, 2013)

Questions?

- Known the radius, how to find the area of a circle?

- For an arbitrary curve in the X-Y plane, how to find the area covered by the curve?

- How to find the value of pi?

Objectives

1. Understand the meaning of integration

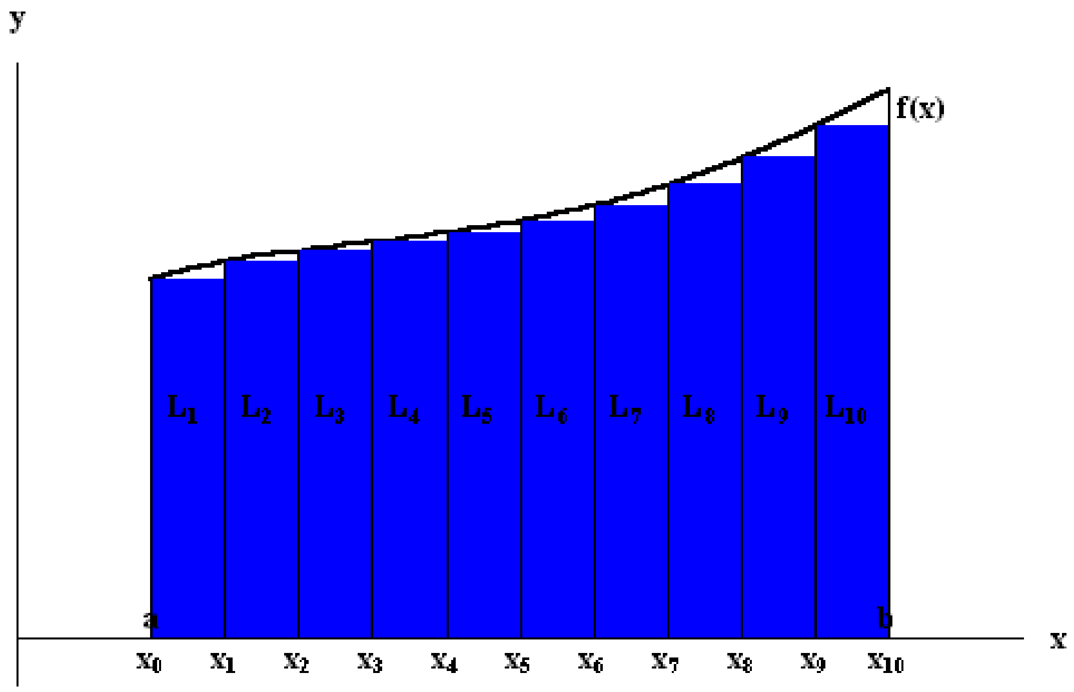
2. Learn the mathematical expression of an integration equation

3. Know how to obtain the result of an arbitrary integration equation using numerical calculation

Integration

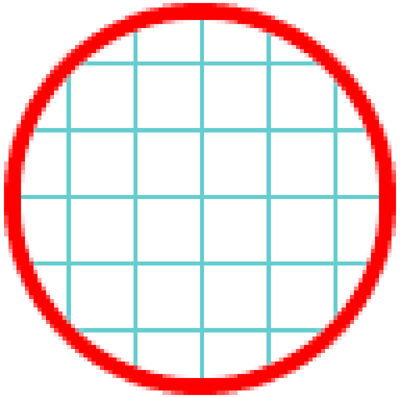
Integration can be defined as the sum of pieces

For example: Integration can be defined as the total area enclosed by the function f(x) and the X-axis. The pieces are those small rectangles.



Primitive Integration

- Primitive integration method has long been used by ancient mathematicians
- A good example is to find the area size of a circle, that leads to the discovery of π
  - The **piece-wise approach**
  - Count the small tiles with known size
  - The smaller the tile, the more accurate the circular area, thus the π
  - **In other words, the smaller the sub-interval, the more the accuracy**
  - For example. One circle has a radius of 1 meter. If filling the circle with 10 cm tiles, how many tiles will fit in?
  - The answer is ~ 314, thus the π

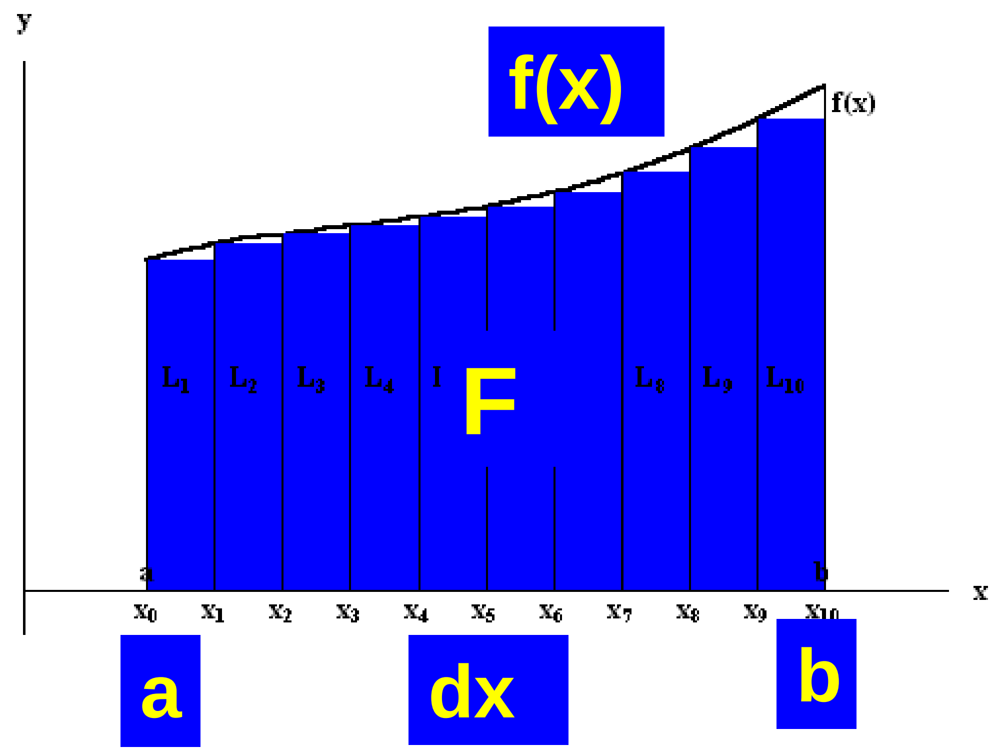


$S = \pi r^2$

Integration in Calculus

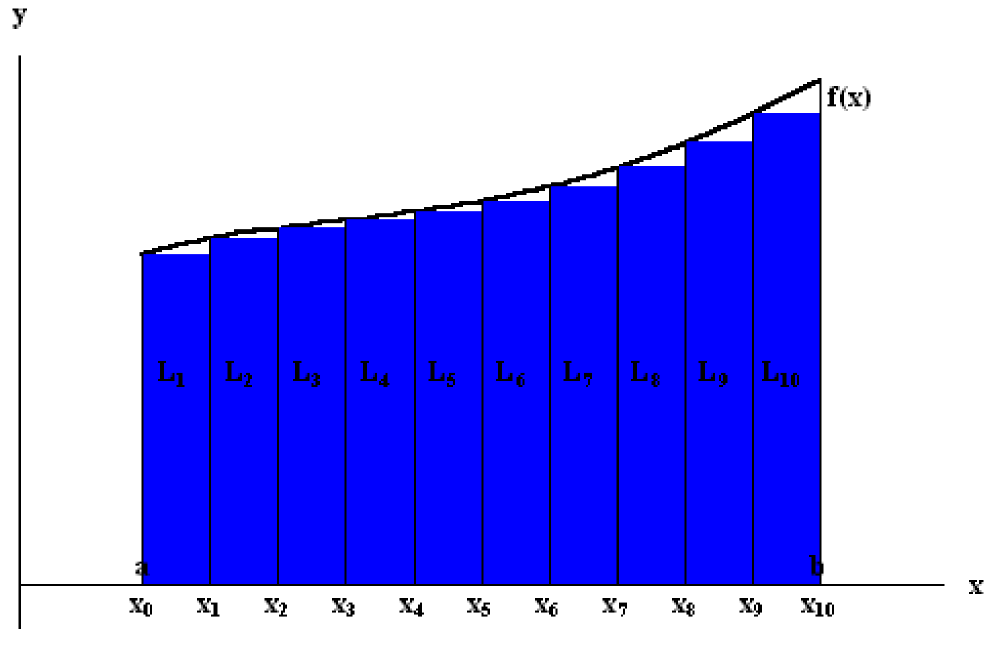
$$F = \int_a^b f(x)dx$$

•f(x): the given function
•F: the integration value
•[a, b]: the **interval** of the integration
    • a: the lower limit
    • b: upper limit
•dx: the **sub-interval** of the integration, which is infinitely small in calculus



Integration in Computation Piece-wise Approach

The total area is approximated by the sum of the sizes of the rectangles (L1+L2+L3….). The size of each rectangle can be easily calculated over each sub-interval: $L_i = f(x_i) * \Delta x$, where Δx is a finite interval



Integration To Summation

$$F = \int_a^b f(x)dx$$

$$dx \to \Delta x; \qquad f(x) \to f(x_i)$$

$$F = \sum_{i=1}^{N} f(x_i) \cdot \Delta x$$

$$F = f(x_1) \cdot \Delta x + f(x_2) \cdot \Delta x + \ldots. f(x_N) \cdot \Delta x$$

N : number of rectangles, or number of iterations

Δx : sub-interval = (b - a)/N

Integration To Summation To Iteration

$$\Delta x : \text{sub - interval} = (\text{b - a})/\text{N}$$

$$\text{x}(1) = \text{a}$$

$$\text{x}(2) = \text{x}(1) + \Delta x$$

$$\text{x}_{\text{i+1}} = \text{x}_{\text{i}} + \Delta x$$

$$\Longrightarrow$$

$$F(1) = f(x(1)) \cdot \Delta x$$

$$F(2) = F(1) + f(x(2)) \cdot \Delta x$$

$$F(i+1) = F(i) + f(x_{i+1}) \cdot \Delta x$$

$$\Longrightarrow F(N)\ \text{is the result}$$

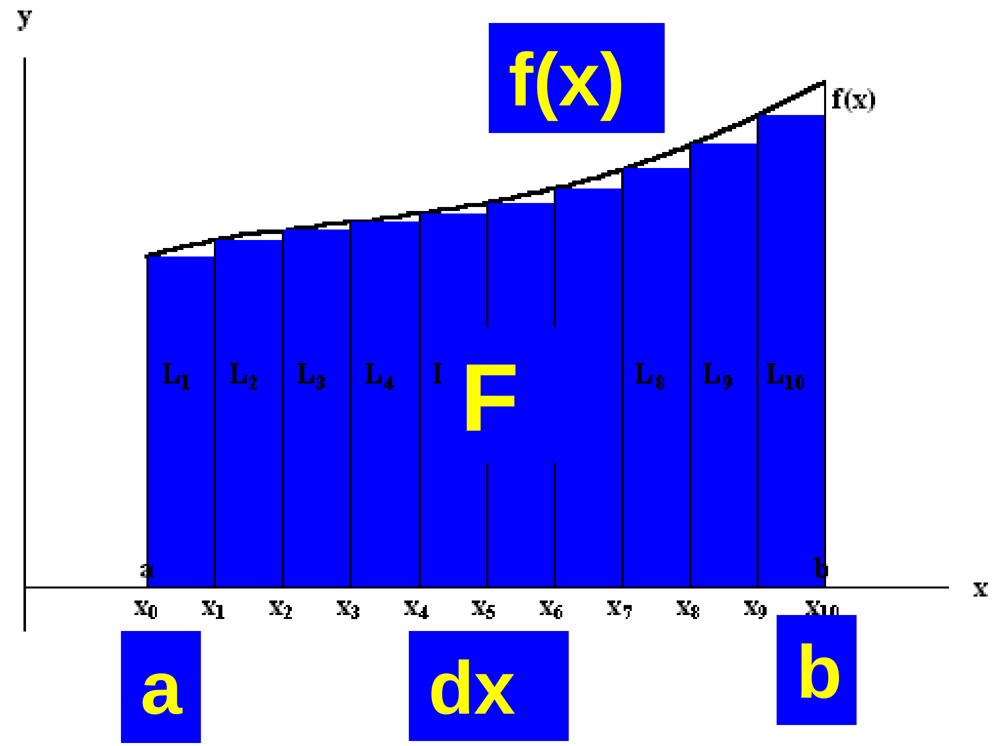
(Nov. 05, 2013 ends Here)

(Nov. 07, 2013 Starts Here)

A Short Review

1. **What is integration?**
   - **The sum of pieces**
2. **Integration in the notion of calculus**

$$F = \int_a^b f(x)dx$$



A Short Review

3. Integration in the form of summation

$$F = \underbrace{\underbrace{\underbrace{f(x_1)\cdot\Delta x}_{F(1)} + f(x_2)\cdot\Delta x}_{F(2)} + \dots f(x_N)\cdot\Delta x}_{F(N)}$$

4. Integration to Iteration

$$F(1) = f(x(1))\cdot\Delta x$$

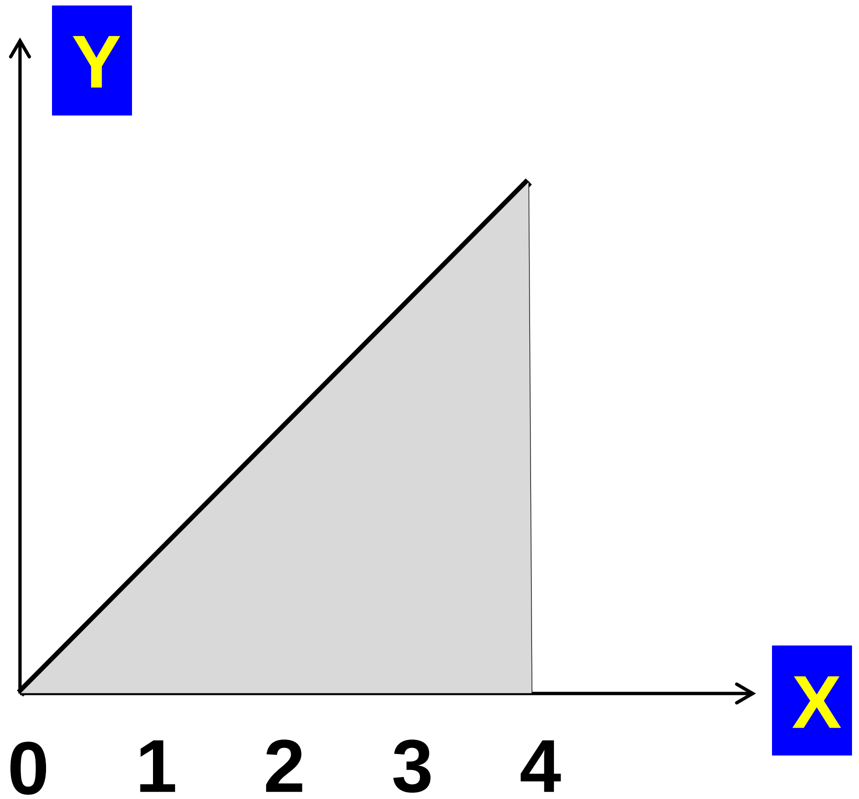
$$F(i+1) = F(i) + f(x_{i+1})\cdot\Delta x$$

$$\Rightarrow F(N)\ \text{is the result}$$

Example 1: f(x)=x

$$f(x) = x$$

$$F = \int_0^4 x\,dx$$



It is equivalent to find the area of a right triangle with the base size of 4 and the height of 4.
The area value is expected to be 4 X 4 / 2 = 8

Example 1: f(x)=x

Question: integrate the function f(x)=x from the interval x=0 to x=4.

$$f(x) = x$$

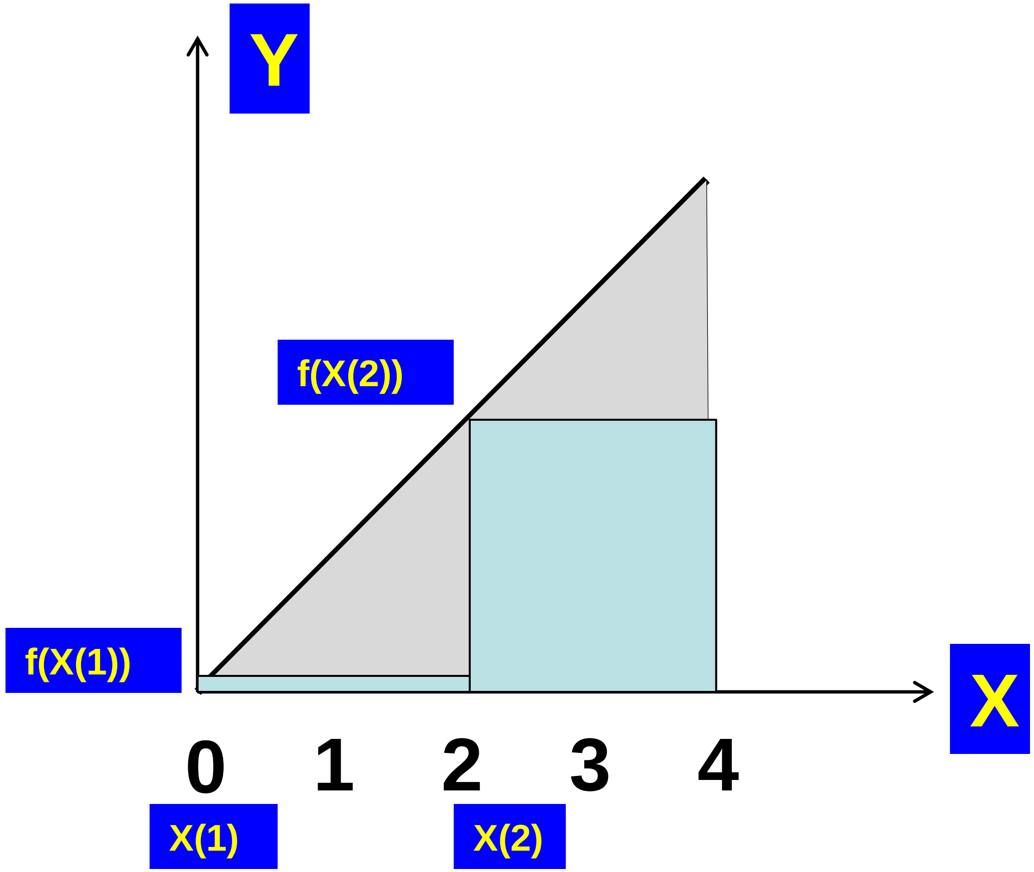
$$F = \int_0^4 x dx$$

(1) Take the number of sub-intervals as 2, use your pencil to calculate the integration using the summation method?
(2) Take the number of sub-intervals as 4, use your pencil to calculate the integration using the summation method?
(3) Convert the integration to iteration. Implement a computational model. Write a MATLAB program to do the calculation. Find the values when the numbers of sub-interval are 10, 100, 1000, 10000 ,respectively

Example 1: f(x)=x

Answer

(1) Take the number of sub-intervals as 2. The area is approximated by two rectangles



Example 1: f(x)=x

Answer

(1) Take the number of sub-interval as 2

$$F = f(1)\cdot\Delta x + f(2)\cdot\Delta x$$

$$\Delta x = (b-a)/N = (4-0)/2 = 2\cdot$$

$$x(1) = a = 0;$$

$$f(1) = x(1) = 0$$

$$x(2) = x(1) + \Delta x = 2$$

$$f(2) = x(2) = 2$$

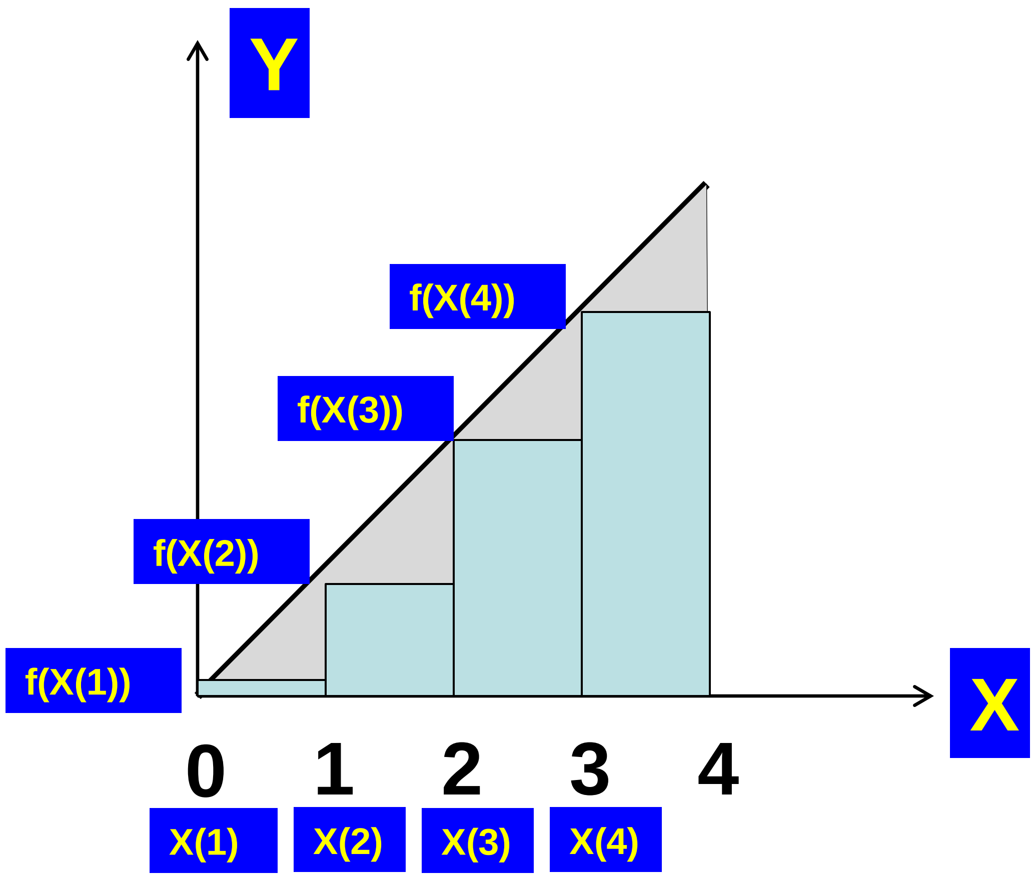
$$F = 0\cdot 2 + 2\cdot 2 = 4$$

The approximation value of 4 is smaller than the true value 8. Why?

Example 1: f(x)=x

Answer

(2) Take the number of sub-intervals as 4. The area is approximated by four rectangles



Example 1: f(x)=x

Answer

(2) Take the number of sub-interval as 4

$$F = f(1)\cdot\Delta x + f(2)\cdot\Delta x + f(3)\cdot\Delta x + f(4)\cdot\Delta x$$

$$\Delta x = (b-a)/N = (4-0)/4 = 1\cdot$$

$$x(1) = a = 0$$

$$f(1) = x(1) = 0$$

$$x(2) = x(1) + \Delta x = 1$$

$$f(2) = x(2) = 1$$

$$x(3) = x(2) + \Delta x = 2$$

$$f(3) = x(3) = 2$$

$$x(4) = x(3) + \Delta x = 3$$

$$f(4) = x(4) = 3$$

$$F = 0\cdot 1 + 1\cdot 1 + 2\cdot 1 + 3\cdot 1 = 6$$

Example 1: f(x)=x

Answer:

(3) Convert the integration to iteration

$$F = \int_a^b f(x)dx$$

$$dx \rightarrow \Delta x$$

$$f(x) \rightarrow f(x_i)$$

$$F = f(x_1)\cdot \Delta x + f(x_2)\cdot \Delta x + ... f(x_N)\cdot \Delta x$$

N : number of rectangles, or number of iterations

Δx : sub-interval = (b - a)/N

Algorithm for the computational model : the usage of iteration

$\mathrm{x}(1) = \mathrm{a}$

$\mathrm{F}(1) = f(x_1)\cdot \Delta x$

$\mathrm{x}(\mathrm{i}+1) = \mathrm{x}(\mathrm{i}) + \Delta x$

$F(i+1) = F(i) + f(x(i+1))\cdot \Delta x$ until find F(N)

Example 1: f(x)=x

Answer (3). The Implementation “area1.m”

```
a=0;    % lower limit
b=4;  % upper limit
N=10;  %Number of iterations
 dx=(b-a)/N;  %the sub-interval

%specify the initial value
x(1)=a;   % a=0
F(1)=x(1)*dx;

%iteration to find the integration value
for i=[1:N-1]
  x(i+1)=x(i)+dx;
  f(i+1) = x(i+1)
  F(i+1)=F(i)+f(i+1)*dx;
end

sprintf('The integration value = %f',F(N))
```

Example 1: f(x)=x

Using 10 rectangles: N=10, sub-interval Δx=0.4

F=7.20000

Using 100 rectangles: N=100, sub-interval Δx=0.04

F=7.92000

Using 1000 rectangles: N=5000, sub-interval Δx=0.004

F=7.99200

Using 10000 rectangles: N=10000, sub-interval Δx=0.0004

F=7.99920

Therefore, the smaller the sub-interval, the better the accuracy

Example 2: $f(x)=x^2$

Question: integrate the function $f(x)=x^2$ from the interval x=0 to x=3.

$$f(x) = x^2$$

$$F = \int_0^3 x^2 dx$$

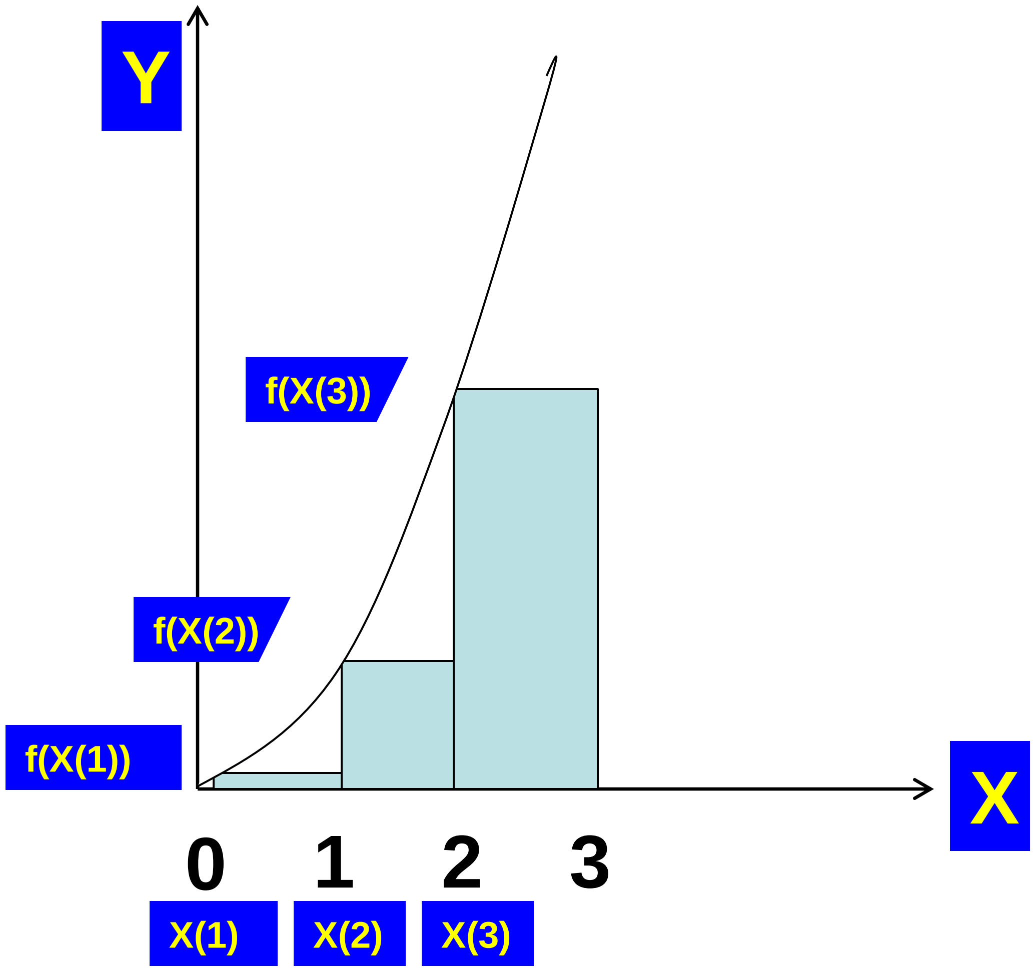
(1) Take the number of sub-interval as 3, use your pencil to calculate the integration?

(2) Convert the integration to iteration. Implement the computational model. Write a MATLAB program to do the calculation. Find the values when the numbers of sub-interval are 10, 100, 1000, 10000 ,respectively

Example 2: $f(x)=x^2$

Answer

(1) Take the number of sub-intervals as 3. The area is approximated by four rectangles



Example 2: $f(x)=x^2$

Answer

(1) Take the number of sub-interval as 3

$$F = f(1)\cdot\Delta x + f(2)\cdot\Delta x + f(3)\cdot\Delta x$$

$$\Delta x = (b-a)/N = (3-0)/3 = 1\cdot$$

$$x(1) = a = 0$$

$$f(1) = x(1)^2 = 0$$

$$x(2) = x(1) + \Delta x = 1$$

$$f(2) = x(2)^2 = 1$$

$$x(3) = x(2) + \Delta x = 2$$

$$f(3) = x(3)^2 = 4$$

$$F = 0\cdot 1 + 1\cdot 1 + 4\cdot 1 = 5$$

Example 2: $f(x)=x^2$

Answer:

(2) Convert the integration to iteration

$$F=\int_a^b f(x)dx$$

$$dx \rightarrow \Delta x$$

$$f(x) \rightarrow f(x_i)$$

$$F=f(x_1)\cdot\Delta x+f(x_2)\cdot\Delta x+....f(x_N)\cdot\Delta x$$

N : number of rectangles, or number of iterations

Δx : sub-interval = (b - a)/N

Algorithm for the computational model : the usage of iteration

$$\mathrm{x}(1)=\mathrm{a}$$

$$\mathrm{F}(1)=f(x_1)\cdot\Delta x$$

$$\mathrm{x}(\mathrm{i}+1)=\mathrm{x}(\mathrm{i})+\Delta x$$

$$F(i+1)=F(i)+f(x(i+1))\cdot\Delta x \quad \text{until find F(N)}$$

Example 2: $f(x)=x^2$

Answer (2). The Implementation “area2.m”

```
a=0;    % lower limit
b=3;  % upper limit
N=10;  %Number of iterations
 dx=(b-a)/N;  %the sub-interval

%specify the initial value
x(1)=a;   % a=0
F(1)=x(1)^2*dx;

%iteration to find the integration value
for i=[1:N-1]
  x(i+1)=x(i)+dx;
  f(i+1)=x(i+1)^2
  F(i+1)=F(i)+f(i+1)*dx;
end

sprintf('The integration value = %f',F(N))
```

Example 2: $f(x)=X^2$

Using 10 rectangles: N=10, sub-interval $\Delta x=0.3$

F=7.695000

Using 100 rectangles: N=100, sub-interval $\Delta x=0.03$

F=8.865450

Using 1000 rectangles: N=1000, sub-interval $\Delta x=0.003$

F=8.986504

Using 10000 rectangles: N=10000, sub-interval $\Delta x=0.0003$

F=8.998650

The true value is 9. Therefore, the smaller the sub-interval, the better the accuracy

(Nov. 07, 2013 ends Here)

(Nov. 12, 2013 Starts Here)

A Short Review

Integration To Summation

$$F = \int_a^b f(x)dx$$

$$dx \to \Delta x; \qquad f(x) \to f(x_i)$$

$$F = \sum_{i=1}^{N} f(x_i) \cdot \Delta x$$

$$F = f(x_1) \cdot \Delta x + f(x_2) \cdot \Delta x + \ldots . f(x_N) \cdot \Delta x$$

N : number of rectangles, or number of iterations

Δx : sub-interval = (b - a)/N

A Short Review

Integration To Iteration

$$\Delta x : \text{sub - interval} = (\text{b - a})/\text{N}$$

$$\text{x}(1) = \text{a}$$

$$\text{x}(2) = \text{x}(1) + \Delta x$$

$$\text{x}_{\text{i+1}} = \text{x}_{\text{i}} + \Delta x$$

$$\Longrightarrow$$

$$F(1) = f(x(1)) \cdot \Delta x$$

$$F(2) = F(1) + f(x(2)) \cdot \Delta x$$

$$F(i+1) = F(i) + f(x_{i+1}) \cdot \Delta x$$

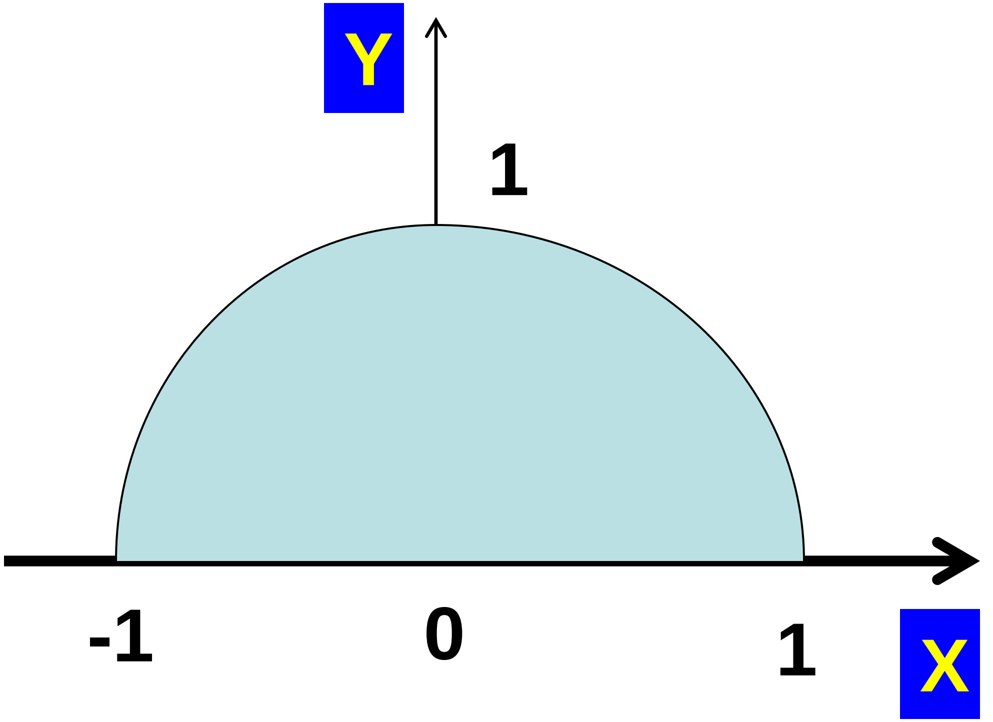
$$\Longrightarrow F(N) \text{ is the result}$$

Example 3: Find π

$$f(x) = \sqrt{1 - x^2}$$

$$F = \int_{-1}^{+1} f(x)dx$$

$$F = \int_{-1}^{+1} \sqrt{1 - x^2}\,dx$$



It is equivalent to find the area of a half circle, which is F = ½ (πr^2) = π/2, in other words π = 2 F.

We know, π = 3.141592653

Example 3: Find π

Question: integrate the following function to find F, then convert F to π

$$F = \int_{-1}^{+1} \sqrt{1 - x^2}\, dx$$

$$\pi = 2F$$

(1) Write a MATLAB program to do the calculation. Find F and π when the numbers of sub-interval are 10, 100, 1000, 10000 ,respectively.

Example 3: Find π

Answer: “find_pi.m”

```
format long   % use long digital format to increase the accuracy
a=-1;    % lower limit
b=+1;  % upper limit
N=10000;  % Number of iterations

dx=(b-a)/N;  %the sub-interval

%specify the initial value
x(1)=a;
f(1)=sqrt(1-(x(1))^2);
F(1)=f(1)*dx;

%iteration to find the integration value
for i=[1:N-1]
  x(i+1)=x(i)+dx;
  f(i+1)=sqrt(1-(x(i+1))^2);
  F(i+1)=F(i)+f(i+1)*dx;
end
my_pi=2*F(N);

sprintf('My Pi value = %12.9f,  when N=%i', my_pi,N)
```

Example 3: Find π

Using 10 rectangles: N=10, sub-interval $\Delta x=0.2$

π = 3.037048829

Using 100 rectangles: N=100, sub-interval $\Delta x=0.02$

π = 3.138268511

Using 1000 rectangles: N=1000, sub-interval $\Delta x=0.002$

π = 3.141487477

Using 10000 rectangles: N=10000, sub-interval $\Delta x=0.0002$

π = 3.141589327

The End of Chapter 4

Section 2
Chapter 5

Scientific Method

(November 12, 2013)

Scientific Method

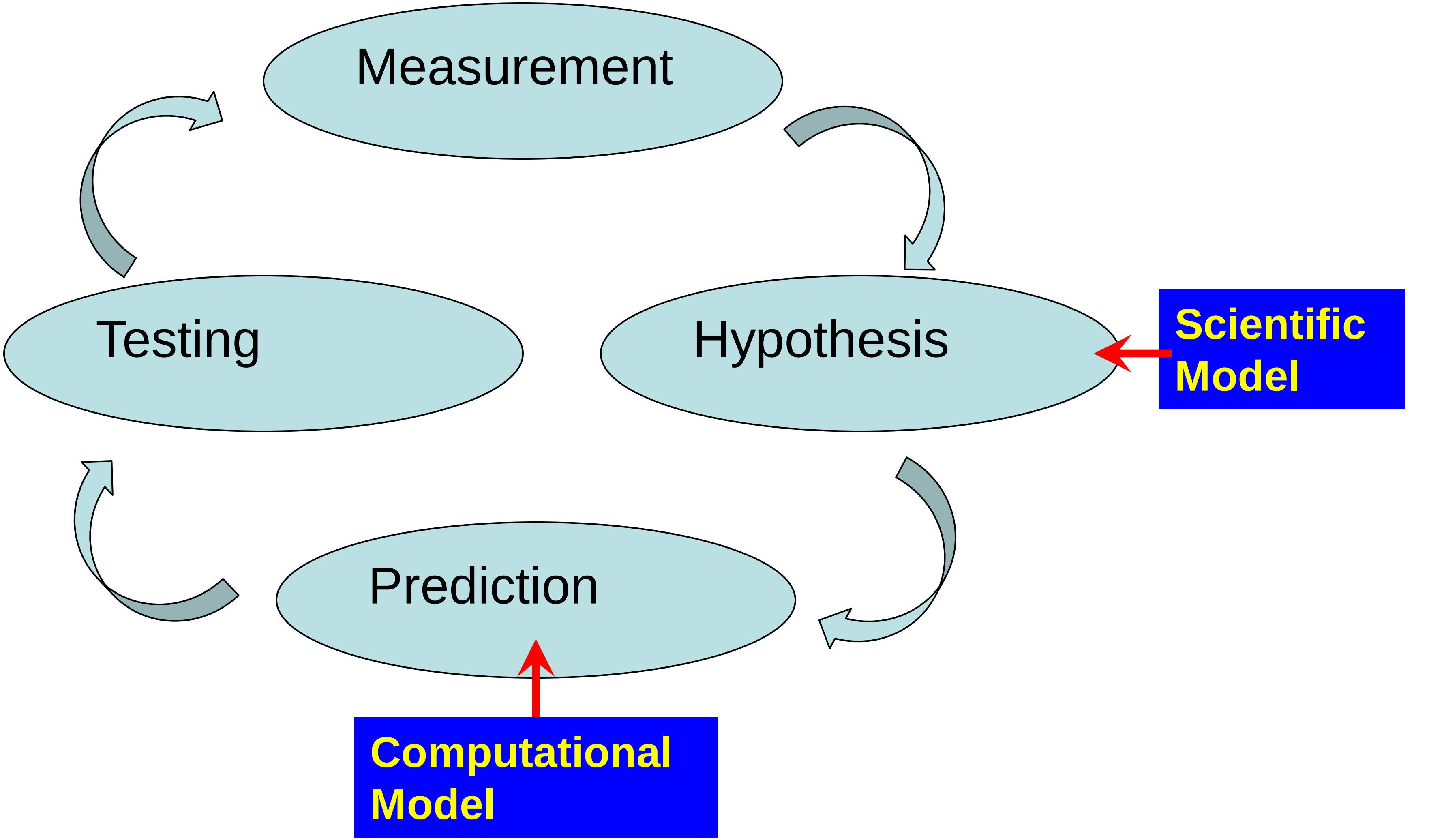
- The scientific method defines how scientific research is conducted. It consists of four essential elements:

1. Measurement (or observation)
2. Hypothesis
3. Prediction
4. Testing

- It is a cyclic process until the testing fully verifies the results

- Then, the hypothesis becomes a theory.

Scientific Method



The End of Chapter 4

The End of Section 2:

Scientific Simulation

(Nov. 12, 2013 ends Here)