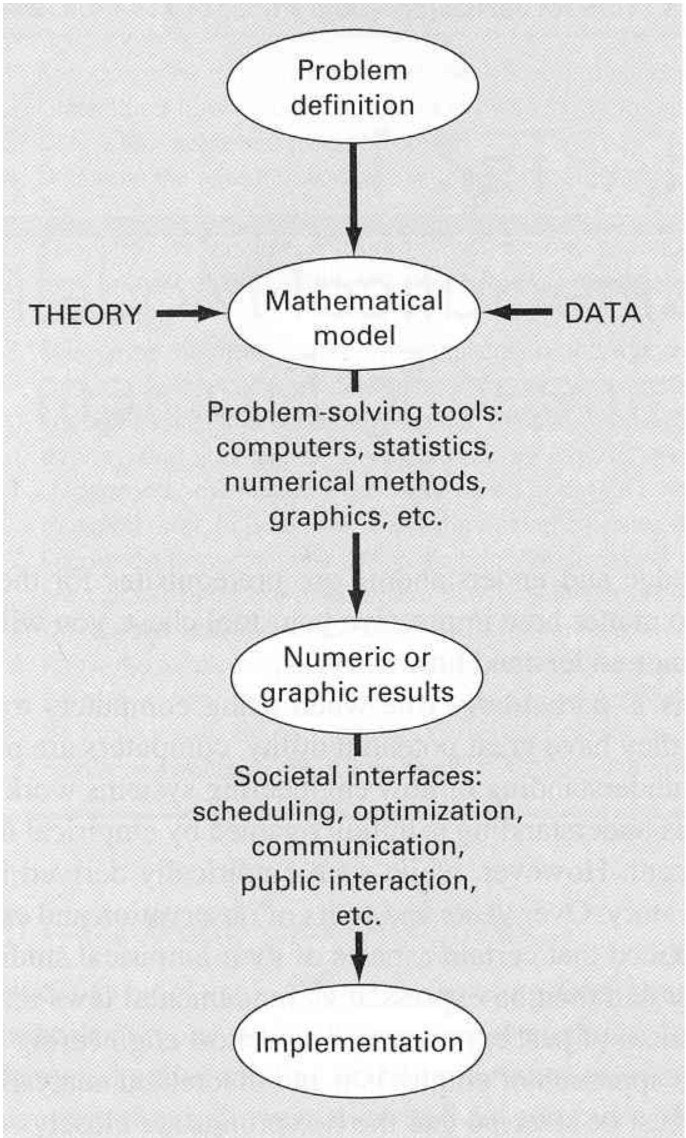
Contents

- Mathematical modeling
  - Differential equations considered as nature laws
  - Constitutive differential equations
  - Conservative differential equations
- Approximations and round-off errors (반올림오차)
  - Significant figures
  - Accuracy and precision
  - Error definitions
- Taylor series and truncation errors (단절오차)
  - Error propagation
  - Total numerical error
- Verification and Validation

Introduction

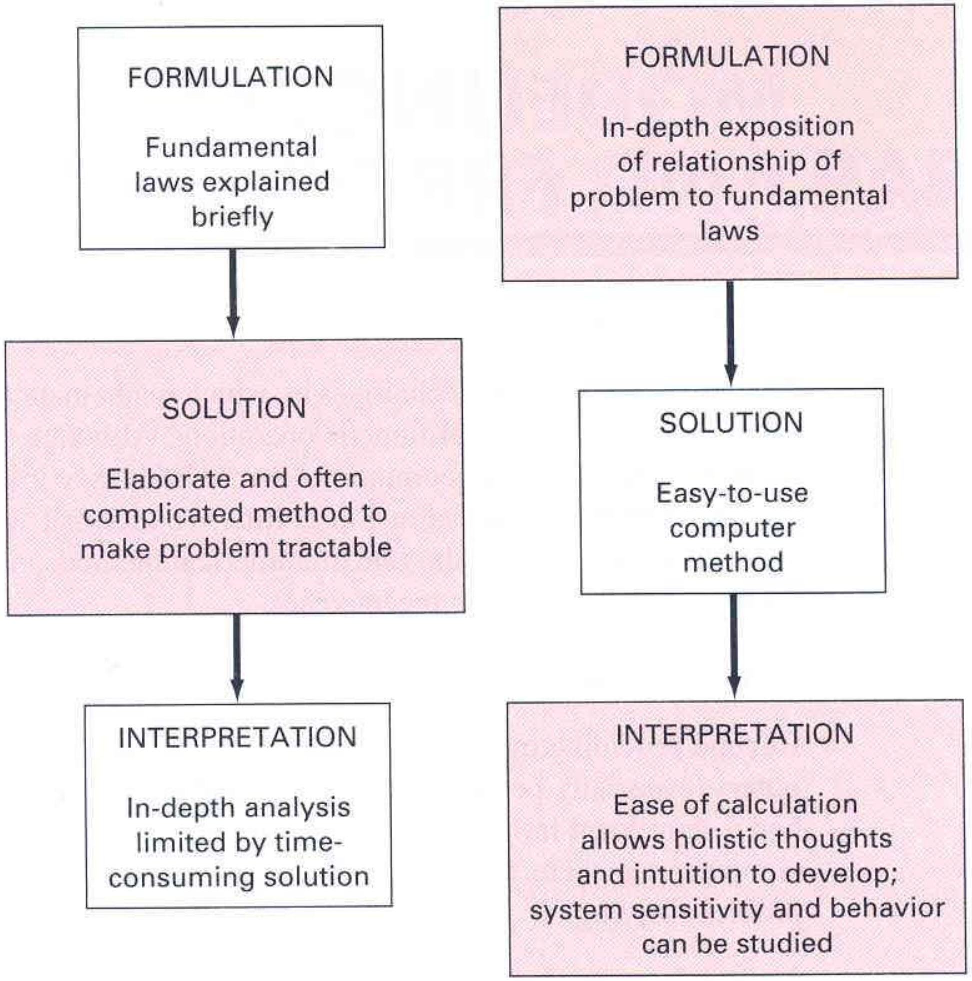
- Mathematical Modeling and Engineering Problem Solving requires understanding of engineering systems
  - Empiricism: observation and experiment
  - Theoretical analysis: generalization
- Computers are great tools, however, without fundamental understanding of engineering problems, they will be useless

Engineering Problem-Solving Process



Three Phases of Engineering Problem Solving

- Precomputer era
- Computer era



Mathematical Model

$$\boxed{\begin{matrix}\text{dependent}\\ \text{variables}\end{matrix}} = f\begin{pmatrix}\text{independent} & & \text{forcing}\\ & \text{parameters,} & \\ \text{variables,} & & \text{functions}\end{pmatrix}$$

- Dependent variable: characteristic that usually reflects the state of the system
- Independent variables: dimensions such as time and space along which the systems behavior is being determined
- Parameters: reflect the system's properties or composition
- Forcing functions: external influences acting upon the system

Mathematical Modeling

- Are there any basic principles to follow when a differential equation is set up?
  - No general answer
- Modeling: art
  - Problem types, simplifying assumptions
  - Chemical engineering: conservation principles
  - Electromagnetic field theory: Maxwell's equations
  - Control theory: block diagram
- Classification
  - Differential equations considered as nature laws
  - Constitutive differential equations
  - Conservative differential equations

Nature Laws

- Mathematical relation that cannot be derived from physical facts
  - Observations
  - No experiment has been designed that contradicts the law
- Examples
  - Newton’s law for the motion of a particle
  - Maxwell’s laws for the electromagnetic field
  - Schrödinger’s equation in quantum mechanics

Newton's 2nd Law of Motion

- States that "the time rate change of momentum of a body is equal to the resulting force acting on it."

$$F = ma$$

F : net force acting on the body [N]

m : mass of the object [kg]

a : its acceleration [m/s^2]

- Characteristics
  - It describes a natural process or system in mathematical terms
  - It represents an idealization and simplification of reality
  - Finally, it yields reproducible results, consequently, can be used for predictive purposes

Parachutist Problem (1)

- Mathematical model

$$F = ma \rightarrow a = \frac{F}{m} \rightarrow \frac{dv}{dt} = \frac{mg - cv}{m} \rightarrow \frac{dv}{dt} = g - \frac{c}{m}v$$

$$\frac{dv}{dt} + \frac{c}{m}v = g : \text{differential equation}$$

$$v_h = c_1 e^{\lambda t} \rightarrow \lambda = -\frac{c}{m}$$

$$v = c_1 e^{\left(-\frac{c}{m}\right)t} + c_2 \rightarrow \frac{c}{m}c_2 = g \rightarrow c_2 = \frac{gm}{c}$$

$$v = c_1 e^{\left(-\frac{c}{m}\right)t} + \frac{gm}{c} \leftarrow (t = 0, v = 0) \Rightarrow c_1 = -\frac{gm}{c}$$

$$v = \frac{gm}{c}\left[1 - e^{\left(-\frac{c}{m}\right)t}\right] : \text{analytical (or exact) solution}$$


```
>> dsolve('Dv=g-c/m*v','v(0)=0')
```

Parachutist Problem (2)

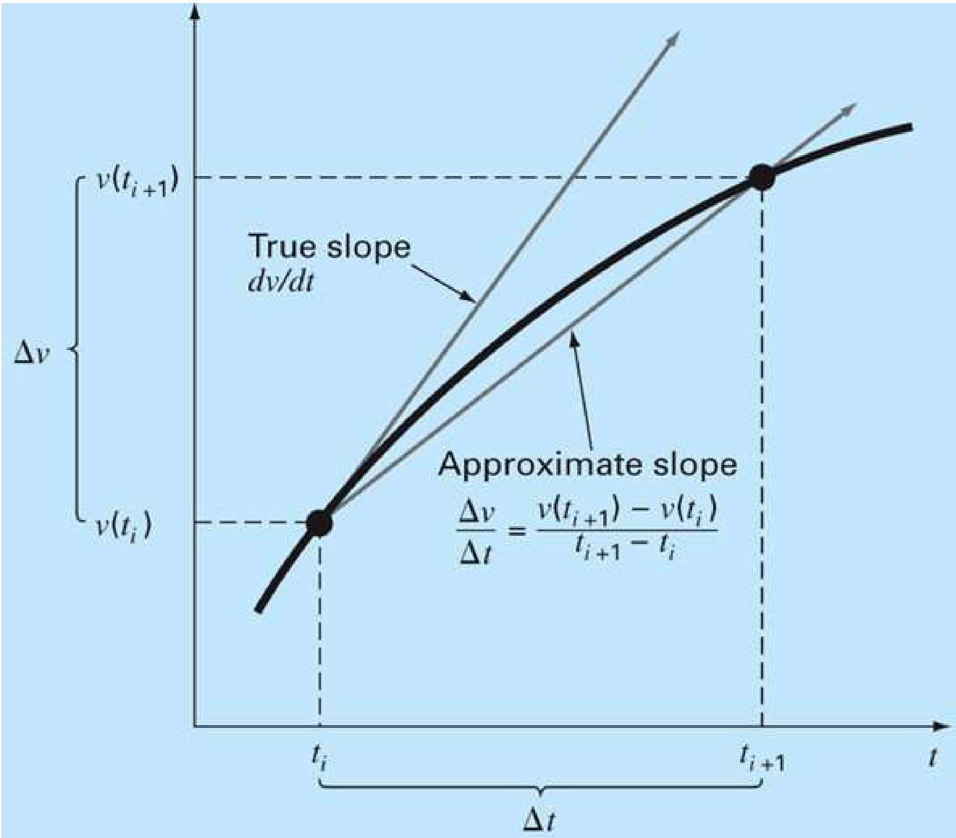
- Numerical methods

$$\frac{dv}{dt} = \lim_{\Delta t \to 0} \frac{\Delta v}{\Delta t} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

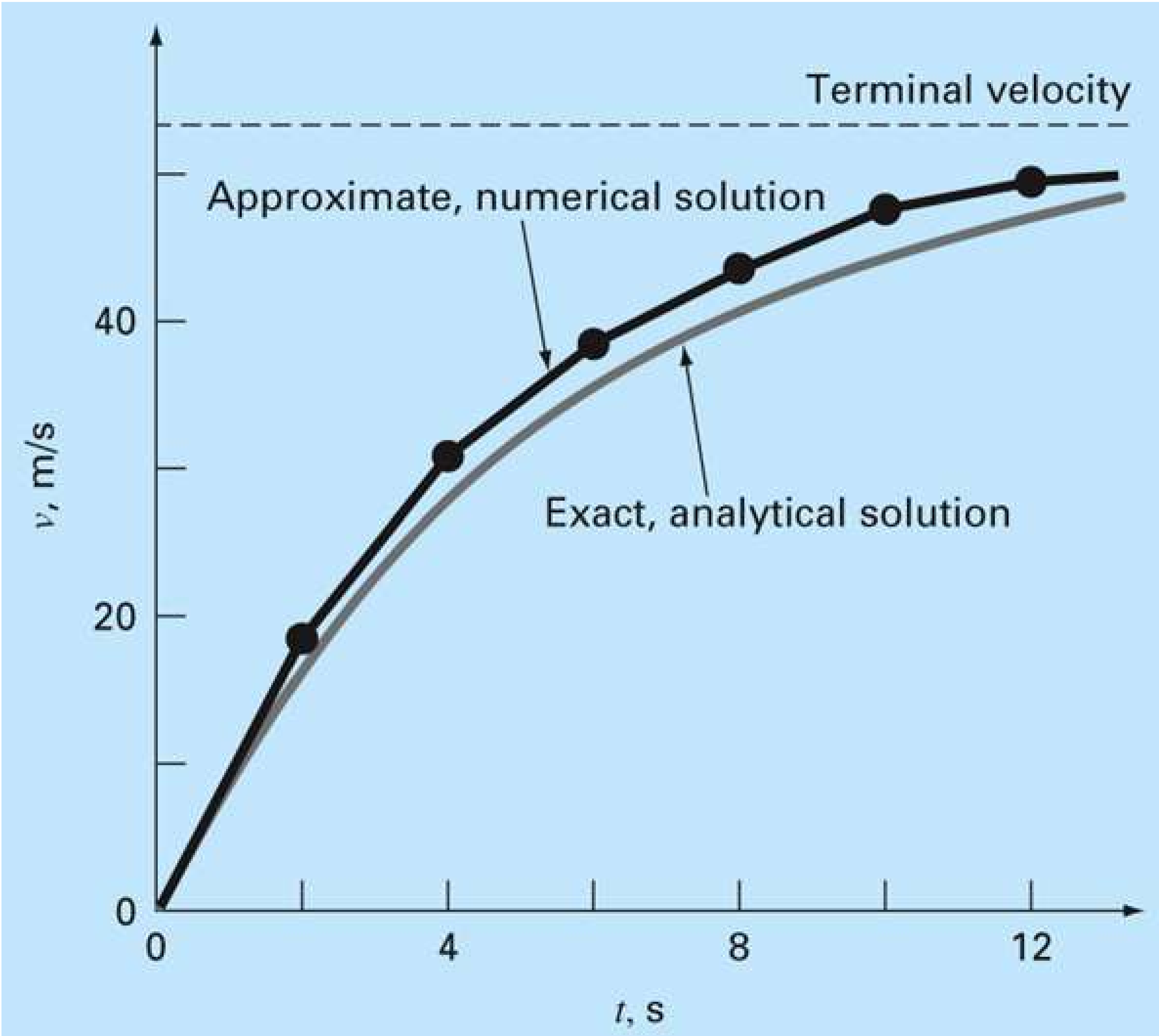
$$\frac{dv}{dt} = g - \frac{c}{m} v \rightarrow \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} = g - \frac{c}{m} v(t_i)$$

$$\underbrace{v(t_{i+1})}_{new} = \underbrace{v(t_i)}_{old} + \underbrace{\left[g - \frac{c}{m} v(t_i) \right]}_{slope} \underbrace{(t_{i+1} - t_i)}_{step\ size}$$

: Euler's method



Parachutist Problem (3)



Constitutive Equations

- Mathematical model of the physical properties of a gas, fluid, or solid: empirical nature
  - Observations of a phenomenon
  - Measurements of an experiment
- Examples
  - Equations in heat transfer problems
  - Equations in mass diffusion problems
  - Equations in mechanical moment diffusion problems
  - Equations in elastic solid mechanics problems
  - Equations in chemical reaction engineering problems
  - Equations in electrical engineering problems

Heat Transfer Problems

- Fourier's law of heat diffusion: conduction (전도)

$$q = -\kappa \frac{dT}{dx} \xrightarrow{E=\rho C_p T} q = -\alpha \frac{dE}{dx}$$

- Newton's law of cooling: convection (대류)

$$Q = -kA\left(T_0 - T\right)$$

- Stefan-Boltzmann's law for temperature radiation loss (복사)

$$Q = -Ae\sigma\left(T_0^{\,4} - T^4\right)$$

Heat Transfer Problems

q : heat flux $\left[J/\left(m^2 \cdot s\right)\right]$

κ : thermal conductivity $\left[J/\left(K \cdot m \cdot s\right)\right]$

ρ : density $\left[kg/m^3\right]$

C_p : heat capacity at constant pressure $\left[J/K \cdot kg\right]$

E : thermal energy $\left[J/m^3\right]$

α : thermal diffusivity $\left[m^2/s\right]$

Q : heat flow $\left[J/s\right]$

A : area $\left[m^2\right]$

k : convection heat transfer coefficient $\left[J/\left(K \cdot m^2 \cdot s\right)\right]$

e : material constant

$\sigma = 5.67E-8 \left[J/\left(K^4 \cdot m^2 \cdot s\right)\right]$: Boltzmann's constant

Mass Diffusion Problems

- Fick's law of mass diffusion

$$f = -D\frac{d\rho}{dx}$$

$$F = -\frac{\mu A}{l}\left(\rho_0 - \rho\right)$$

Adolf Fick
(1829~1901)

$$\begin{cases} f : \text{mass flux } \left[kg/\left(m^2 \cdot s\right)\right] \\ D : \text{mass diffusivity } \left[m^2/s\right] \\ F : \text{mass flow } \left[kg/s\right] \\ \mu : \text{diffusivity } \left[m^2/s\right] \\ l : \text{thickness } \left[m\right] \end{cases}$$

Mechanical Moment Diffusion Problems

- Newton's law of viscosity

$$\tau_{xy} = -\mu \frac{dv_x}{dy} = -\nu \frac{d\left(\rho v_x\right)}{dy}$$

τ_{xy} : shear stress $\left[N/m^2\right]$

v_x : velocity along the x-axis and orthogonal to the y-axis $\left[m/s\right]$

$\mu\left(=\rho\nu\right)$: dynamic viscosity $\left[N \cdot s/m^2\right]$

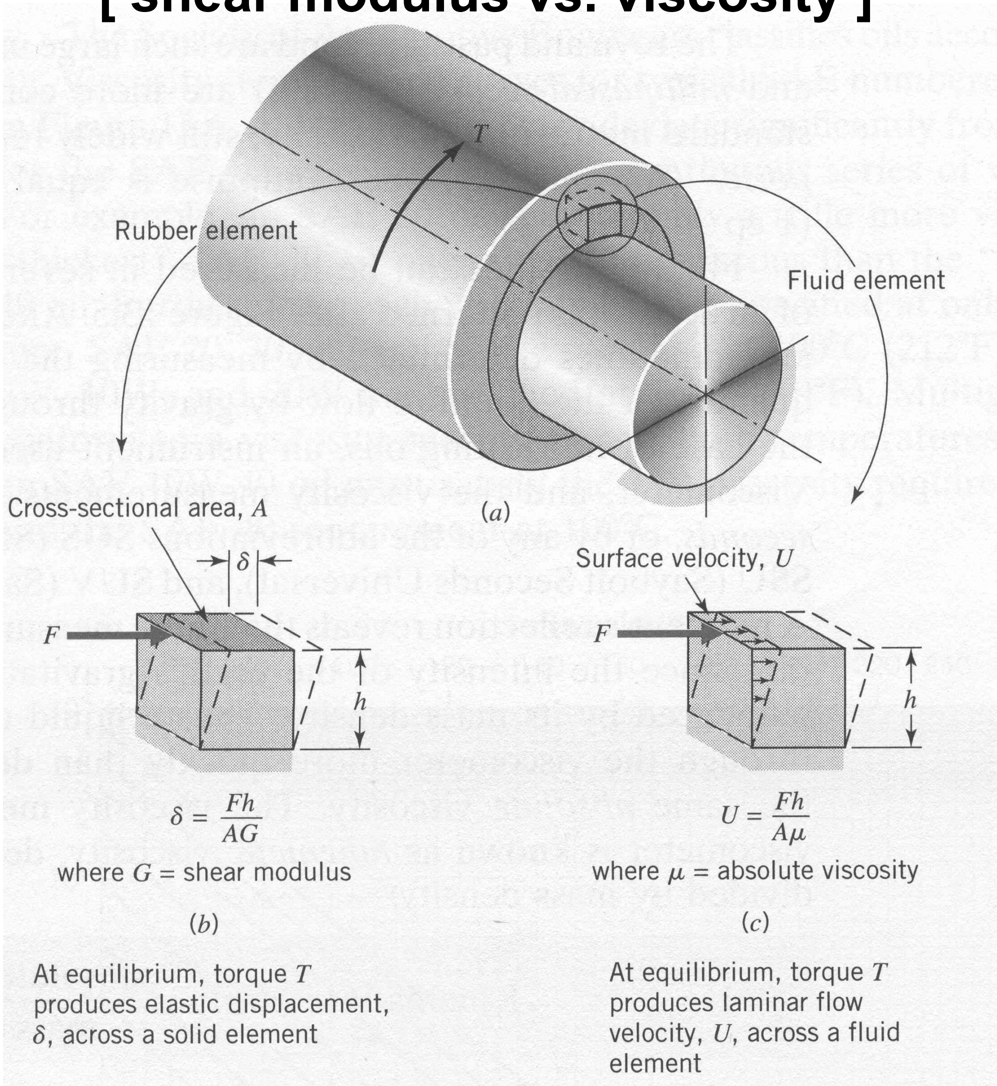
ν : kinematic viscosity $\left[m^2/s\right]$ (diffusion coefficient of the mechanical moment)

Viscosity

- Measure of a fluid's resistance to shear
  - Inversely with temperature, directly with pressure
- Absolute viscosity (μ)
  - calculation
- Kinematic viscosity (ν)
  - measurement

$$\nu = \frac{\mu}{\rho}$$

[shear modulus vs. viscosity]



Elastic Solid Mechanics Problems

- Hooke's law for an elastic bar

$$\sigma = E\varepsilon, \quad \varepsilon = \frac{du}{dx}$$

σ : stress $\left[N/m^2 \right]$

ε : strain $[\ ]$

u : displacemnt per unit length of the bar $[m]$

E : elasticity module $\left[N/m^2 \right]$ (Young's module)

Chemical Reaction Engineering Problems

- Mass action law in chemical kinetics

$$\text{reaction: } \alpha_1 A_1 + \cdots + \alpha_m A_m \rightarrow \beta_1 B_1 + \cdots + \beta_n B_n$$

$$r = k \prod_{i=1}^{m} c_i^{\alpha_i}, \quad k = A e^{-\frac{E}{RT}}$$

- General gas law

$$pV = nRT$$

Electrical Engineering Problems

- Ohm's law in electromagnetics

$$\boxed{\mathbf{j} = \sigma \mathbf{E}}$$

- Lorentz' law

$$\boxed{\mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)}$$

$\mathbf{j}$: electrical current density $\left[A/m^2\right]$

σ : conductivity $\left[A/(V \cdot m)\right]$

$\mathbf{E}$: electrical field strength $\left[V/m\right]$

$\mathbf{F}$: force $\left[N\right]$

q : electrical charge $\left[C\right]$

$\mathbf{B}$: magnetic field $\left[V \cdot s/m^2\right]$

$\mathbf{v}$: velocity $\left[m/s^2\right]$

$$\text{line} \xrightarrow{\text{curl}} \text{surface} \xrightarrow{\text{divergence}} \text{volume}$$

Electromagnetic Theory

electrostatic field: Gauss's law

$$(\text{Coulomb's force law}) \oint \mathbf{D} \cdot d\mathbf{S} = \int \rho_v dv \rightarrow \nabla \cdot \mathbf{D} = \rho_v$$

$$(\text{conservation}) \oint \mathbf{E} \cdot d\mathbf{l} = 0 \rightarrow \nabla \times \mathbf{E} = 0$$

$$\xrightarrow[\mathbf{E}=-\nabla V]{\mathbf{D}=\varepsilon\mathbf{E}} \nabla^2 V = -\frac{\rho_v}{\varepsilon} \xrightarrow{\rho_v=0} \nabla^2 V = 0$$

- $\mathbf{D}$: electric flux density $[coulombs/m^2]$
- ρ_v : volume charge density $[coulombs/m^3]$
- $\mathbf{E}$: electric field strength $[volts/m]$
- ε : dielectric permittivity $[farads/m]$(유전율)

magnetostatic field: Ampere's law

$$(\text{Biot-Savart law}) \oint_L \mathbf{H} \cdot d\mathbf{l} = \iint_S \mathbf{J}_e \cdot d\mathbf{S} \rightarrow \nabla \times \mathbf{H} = \mathbf{J}_e$$

$$(\text{conservation}) \oint_S \mathbf{B} \cdot d\mathbf{S} = 0 \rightarrow \nabla \cdot \mathbf{B} = 0$$

$$\xrightarrow[\nabla\times(\nabla\times\mathbf{A})=\nabla(\nabla\cdot\mathbf{A})-\nabla^2\mathbf{A}]{\mathbf{B}=\mu\mathbf{H}=\nabla\times\mathbf{A}} \nabla^2 \mathbf{A} = -\mu \mathbf{J}_e \xrightarrow{\mathbf{J}_e=0} \nabla^2 \mathbf{A} = 0$$

- $\mathbf{H}$: magnetic field intensity $[amperes/m]$
- $\mathbf{J}_e$: electric current density $[amperes/m^2]$
- $\mathbf{B}$: magnetic flux density $[tesla, vebers/m^2]$
- μ : permeability $[henries/m]$(투자율)

electric + magnetic field: Maxwell's equations

$$\begin{cases} \nabla \cdot \mathbf{D} = \rho_v \\ \nabla \cdot \mathbf{B} = 0 \\ \nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t} - \mathbf{J}_m \\ \nabla \times \mathbf{H} = \mathbf{J}_e + \dfrac{\partial \mathbf{D}}{\partial t} \end{cases}$$

Conservative Equations

- Based on the principle that physical quantities, such as mass, moment, and energy, are conserved in a system
  - Changes of some quantity in a control volume that is fixed in space → balance principle must hold for the quantity during a given time interval

$$\Delta Acc = In - Out + Prod - Cons$$

$$\begin{cases} \Delta Acc: \text{ change of amount of the accumulated quantity} \\ In: \text{ amount of the quantity that has flowed in} \\ Out: \text{ amount of the quantity that has flowed out} \\ Prod: \text{ amount of the quantity produced} \\ Cons: \text{ amount of the quantity consumed} \end{cases}$$

Conservative Equations

- Conservation principle leading to
  - ODE with time as independent variable: lumped model
  - PDE in time and space: distributed model

$$Q(t) = \frac{dM}{dt} \quad \text{where } M(t): \text{ amount of a quantity at time } t,\ Q(t): \text{ flow}$$

$$\rightarrow in(t) = \frac{d(In)}{dt}, out(t) = \frac{d(Out)}{dt}, prod(t) = \frac{d(Prod)}{dt}, cons(t) = \frac{d(Cons)}{dt}$$

$$\Delta Acc = \int_t^{t+\Delta t} \left(in(t) - out(t) + prod(t) - cons(t) \right) dt$$

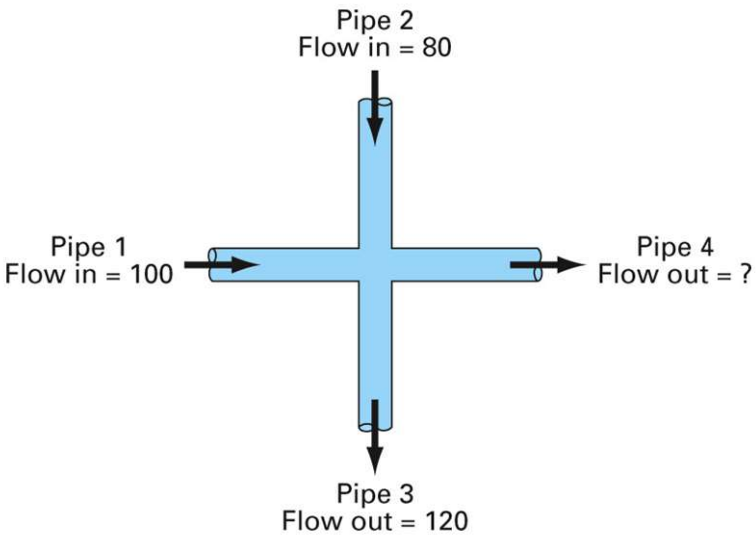
$$\lim_{\Delta t \to 0} \frac{\Delta Acc}{\Delta t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_t^{t+\Delta t} \left(in(t) - out(t) + prod(t) - cons(t) \right) dt$$

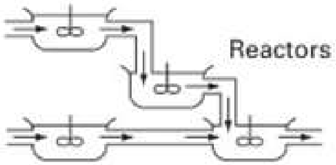
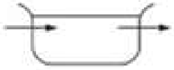
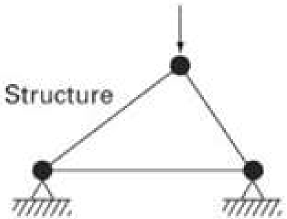
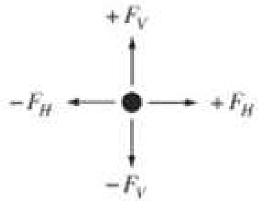
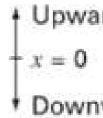
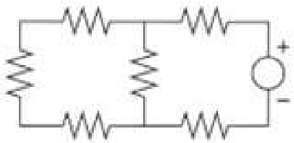
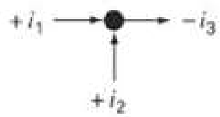
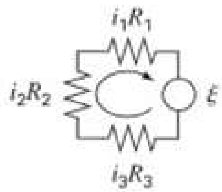
$$\frac{dAcc}{dt} = in - out + prod - cons \quad [\text{continuity equation}]$$

Conservation Laws and Engineering

- Change = increases – decreases
- Change implies changes with time (transient). If the change is nonexistent (steady-state),
- Increases = Decreases

  – Example: steady-state incompressible fluid flow



Field	Device	Organizing Principle	Mathematical Expression
Chemical engineering	 Reactors	Conservation of mass	Mass balance:  Input / Output Over a unit of time period Δmass = inputs − outputs
Civil engineering	 Structure	Conservation of momentum	Force balance:  $+F_V$, $-F_H$, $+F_H$, $-F_V$ At each node Σ horizontal forces (F_H) = 0 Σ vertical forces (F_V) = 0
Mechanical engineering	 Machine	Conservation of momentum	Force balance:  Upward force, $x = 0$, Downward force $m\dfrac{d^2x}{dt^2}$ = downward force − upward force
Electrical engineering	 Circuit	Conservation of charge	Current balance:  $+i_1$, $-i_3$, $+i_2$ For each node Σ current (i) = 0
		Conservation of energy	Voltage balance:  i_1R_1, i_2R_2, ξ, i_3R_3 Around each loop Σ emf's − Σ voltage drops for resistors = 0 $\Sigma \xi - \Sigma iR = 0$

Analogy

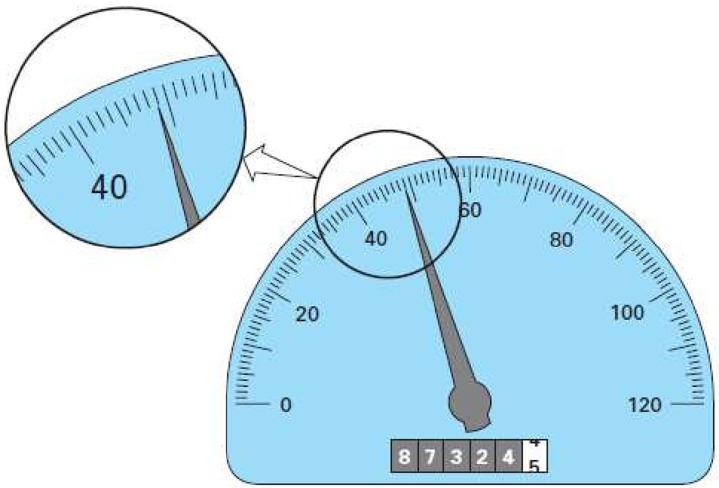
Linear		Torsional		Electrical	
Mass	m	Moment of inertia	I	Inductance	L
Stiffness	k	Torsional stiffness	k	1/Capacitance	1/C
Damping	c	Torsional damping	c	Resistance	R
Force	$P_0 \sin\omega t$	Torque	$T_0 \sin\omega t$	Voltage	$E_0 \sin\omega t$
Displacement	x	Angular displacement	φ	Condenser charge	Q
Velocity	$\dot{x} = v$	Angular velocity	$\dot{\varphi} = \omega$	Current	$\dot{Q} = i$

Approximations and Round-Off Errors

- For many engineering problems, we cannot obtain analytical solutions
- Numerical methods yield approximate results that are close to the exact analytical solution
- We cannot exactly compute the errors associated with numerical methods
  - input → algorithm → output
- How confident we are in our approximate result?
  - "how much error is present in our calculation and is it tolerable?"

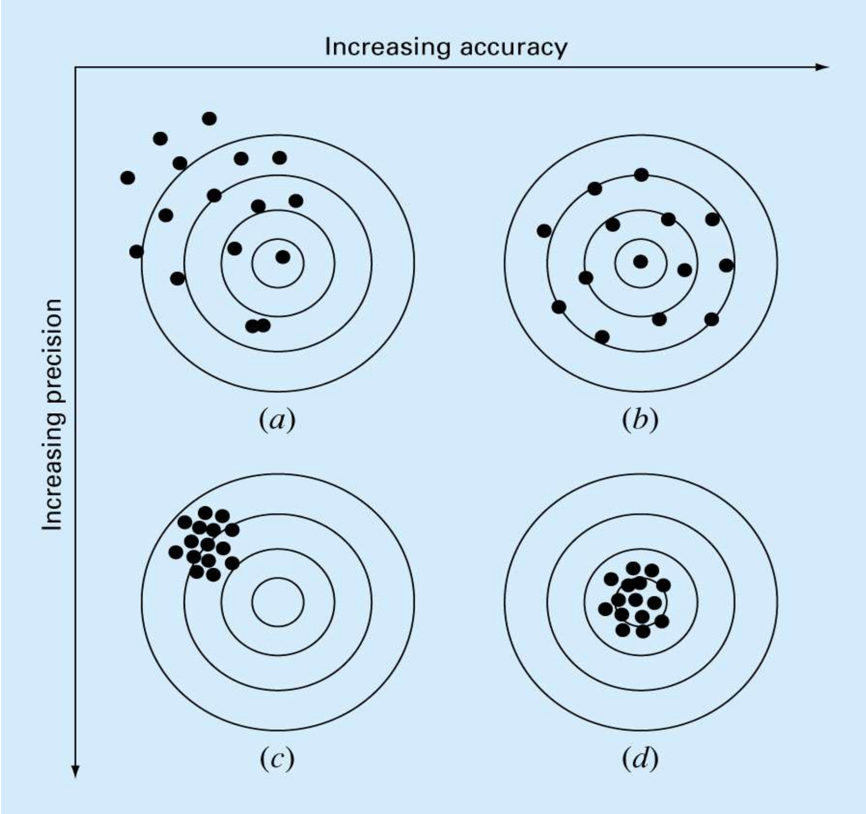
Significant Figures

- Number of significant figures indicates precision
  - Significant digits of a number are those that can be used with confidence
  - Number of certain digits plus one estimated digit
- How many significant figures?
  - 53,800?
    - Scientific notation: 5.38×10^4, 5.380×10^4 , 5.3800×10^4
  - Zeros?
    - 0.00001753, 0.0001753, 0.001753
  - Speedometer: 48.8
  - Odometer: 87324.45



Accuracy and Precision

- Accuracy
  - How close is a computed or measured value to the true value
- Precision (or reproducibility)
  - How close is a computed or measured value to previously computed or measured values
- Inaccuracy (or bias)
  - A systematic deviation from the actual value
- Imprecision (or uncertainty)
  - Magnitude of scatter



Error Definition (1)

- True Value = Approximation + Error
- True error: E_t = True value – Approximation (+/-)

$$\text{True fractional relative error} = \frac{\text{true error}}{\text{true value}}$$

$$\text{True percent relative error, } \varepsilon_t = \frac{\text{true error}}{\text{true value}} \times 100\%$$

- For numerical methods, true value?
  - only when we solve functions analytically (simple systems)
- In real world applications, no answer a priori

$$\underbrace{\varepsilon_a}_{(+/-)} = \frac{\text{approximate error}}{\text{approximation}(a)} \times 100\% = \frac{\text{current\_a} - \text{previous\_a}}{\text{current\_a}} \times 100\%$$

Error Definition (2)

- Use absolute value
- Computations are repeated until stopping criterion is satisfied

$$|\varepsilon_a| < \varepsilon_s$$

Pre-specified % tolerance based on the knowledge of your solution

- Correct result to at least n significant figures if

$$\varepsilon_s = (0.5 \times 10^{(2-n)})\%$$

Example

Problem Statement. Suppose that you have the task of measuring the lengths of a bridge and a rivet and come up with 9999 and 9 cm, respectively. If the true values are 10,000 and 10 cm, respectively, compute (*a*) the true error and (*b*) the true percent relative error for each case.

E_t = 1 cm, ε_t =?

Problem Statement. In mathematics, functions can often be represented by infinite series. For example, the exponential function can be computed using

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!} \tag{E3.2.1}$$

Thus, as more terms are added in sequence, the approximation becomes a better and better estimate of the true value of e^x. Equation (E3.2.1) is called a *Maclaurin series expansion.*

Starting with the simplest version, $e^x = 1$, add terms one at a time to estimate $e^{0.5}$. After each new term is added, compute the true and approximate percent relative errors with Eqs. (3.3) and (3.5), respectively. Note that the true value is $e^{0.5} = 1.648721\ldots$. Add terms until the absolute value of the approximate error estimate ε_a falls below a prespecified error criterion ε_s conforming to three significant figures.

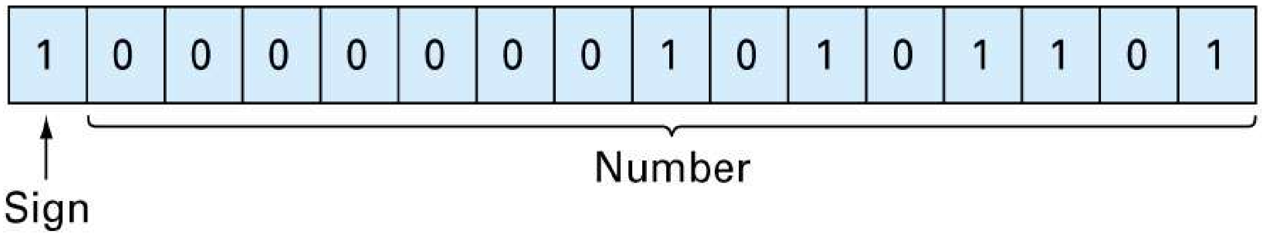
Round-off Errors

- Limitations of a computer's number system
- Arithmetic manipulations of computer numbers

- Numbers such as π, e, or $\sqrt{7}$ cannot be expressed by a fixed number of significant figures
- Computers use a base-2 representation, they cannot precisely represent certain exact base-10 numbers

Integer Representation

- Signed magnitude method
- Limitation
  - Capability to represent integers
  - storage, manipulation of fractional quantities



-173

Problem Statement. Determine the range of integers in base-10 that can be represented on a 16-bit computer.

32767(2^{15}-1): -32768~+32767 why? (+0/-0)

Floating-Point Representation

- Fractional quantities are typically represented in computer using “floating point” form
  - Take ore room and longer to process than integer numbers

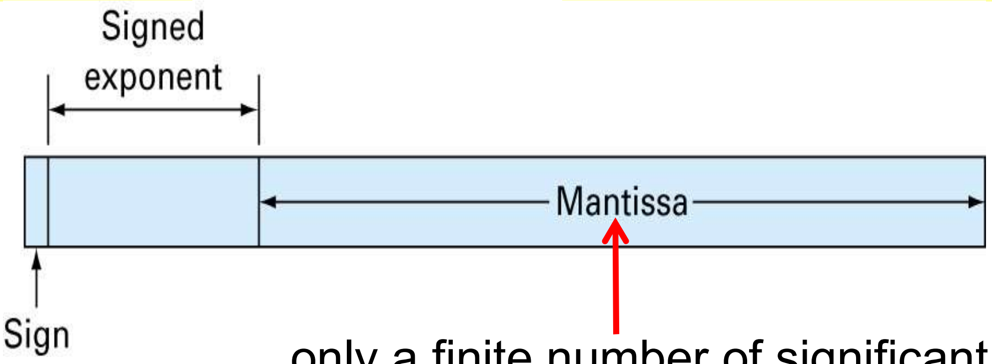
$$m \cdot b^e$$

Integer part

exponent

Mantissa (假數)

Base of the number system used



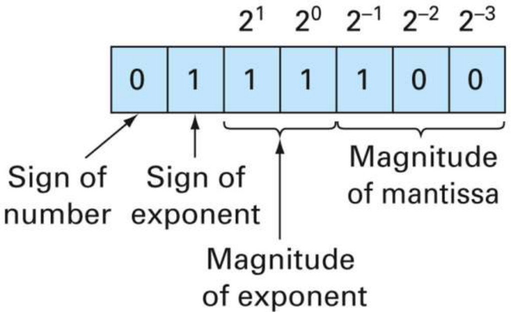
only a finite number of significant figures
→ round-off error

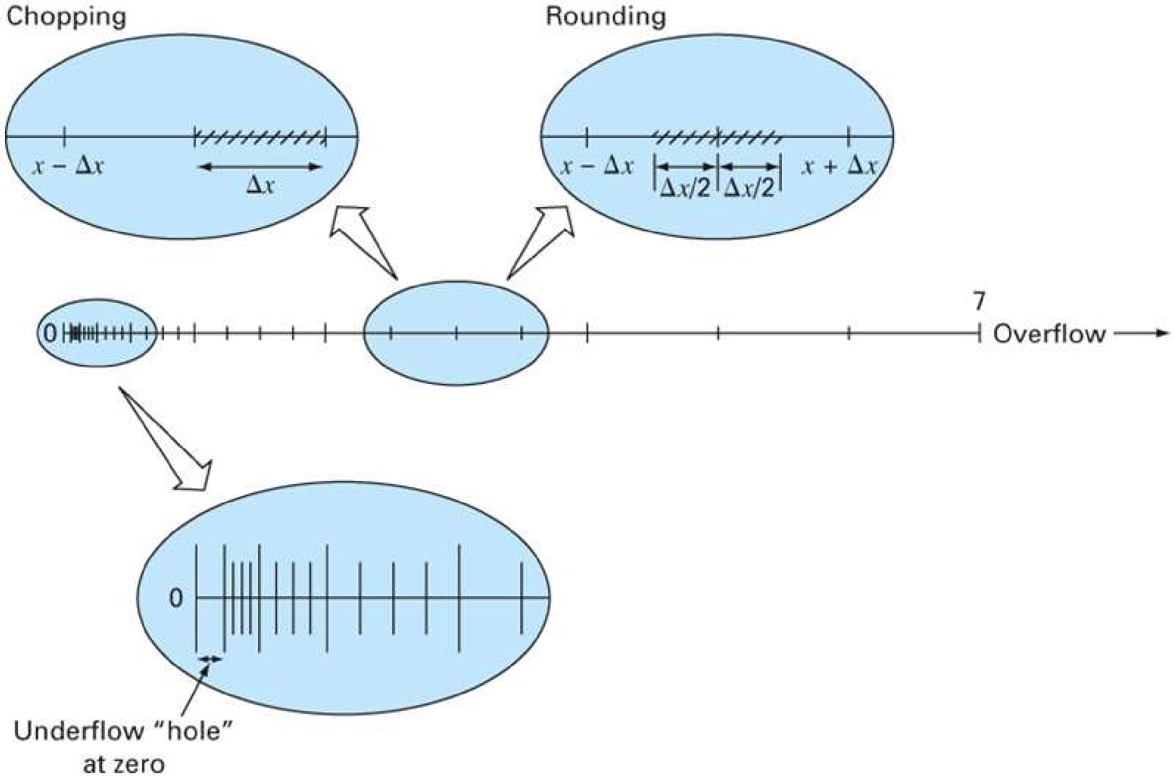
$$156.78 \rightarrow 0.15678 \times 10^3$$

$$\frac{1}{34} = 0.029411765 \xrightarrow{\text{4 decimal places}} 0.0294 \times 10^0 \xrightarrow[\text{normalized}]{\frac{1}{b} \le |m| < 1} 0.2941 \times 10^{-1}$$

Example

Problem Statement. Create a hypothetical floating-point number set for a machine that stores information using 7-bit words. Employ the first bit for the sign of the number, the next three for the sign and the magnitude of the exponent, and the last three for the magnitude of the mantissa (Fig. 3.8).





Limitations

- Limited range of quantities that may be represented
  - Overflow error, underflow hole
- Only a finite number of quantities that can be represented within the range (quantizing error)
  - Chopping
  - Rounding
  - Example: π(3.1415926**5**) 7-bit
- Interval between numbers, Δx, increases as the numbers grow in magnitude

$$\begin{cases} \text{chopping: } \dfrac{|\Delta x|}{|x|} \le \varepsilon \\ \text{rounding: } \dfrac{|\Delta x|}{|x|} \le \dfrac{\varepsilon}{2} \end{cases} \qquad \begin{cases} \varepsilon = b^{1-t} \\ \varepsilon : \text{machine epsilon} \\ b : \text{number base} \\ t : \text{number of significant digits} \end{cases}$$

Arithmetic Manipulations

- Common arithmetic operations
  - Addition, subtraction, multiplication, division
- Large computations
- Adding a large and a small number
- Subtractive cancellation
- Smearing
  - the individual terms in a summation are larger than the summation itself.
- Inner products

Examples

$0.1557 \cdot 10^1 + 0.4381 \cdot 10^{-1}$

$$\begin{array}{l} 0.1557 \quad \cdot 10^1 \\ 0.004381 \cdot 10^1 \\ \hline 0.160081 \cdot 10^1 \end{array}$$

$0.1600 \cdot 10^1$

subtracting 26.86 from 36.41

$$\begin{array}{r} 0.3641 \cdot 10^2 \\ -\ 0.2686 \cdot 10^2 \\ \hline 0.0955 \cdot 10^2 \end{array} \qquad \begin{array}{r} 0.7642 \cdot 10^3 \\ -\ 0.7641 \cdot 10^3 \\ \hline 0.0001 \cdot 10^3 \end{array}$$

$0.9550 \cdot 10^1 = 9.550 \qquad 0.1000 \cdot 10^0 = 0.1000$

$0.1363 \cdot 10^3 \times 0.6423 \cdot 10^{-1} = 0.08754549 \cdot 10^2$

$0.08754549 \cdot 10^2 \rightarrow 0.8754549 \cdot 10^1$

$0.8754 \cdot 10^1$

$$\begin{array}{l} 0.4000 \quad\quad \cdot 10^4 \\ 0.0000001 \cdot 10^4 \\ \hline 0.4000001 \cdot 10^4 \end{array}$$

$$y = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots$$

$$\sum_{i=1}^{n} x_i y_i = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n$$

$$\begin{matrix} x_1 \\ x_2 \end{matrix} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$b^2 \gg 4ac,$$

$$\begin{matrix} x_1 \\ x_2 \end{matrix} = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$

```
PROGRAM fig0312
IMPLICIT none
INTEGER::i
REAL::sum1, sum2, x1, x2
DOUBLE PRECISION::sum3, x3
sum1=0.
sum2=0.
sum3=0.
x1=1.
x2=1.e-5
x3=1.d-5
DO i=1,100000
   sum1=sum1+x1
   sum2=sum2+x2
   sum3=sum3+x3
END DO
PRINT *, sum1
PRINT *, sum2
PRINT *, sum3
END
output:
100000.000000
        1.000990
  9.99999999980838E-001
```

Truncation Errors and Taylor Series

- Truncation errors
  - Errors that result from using an approximation in place of an exact mathematical procedure
- Taylor series
  - Any smooth function can be approximated as a polynomial
  - means to predict the value of a function at one point in terms of the function value and its derivatives at another point

Taylor Series Expansion

$$\begin{cases} f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \dfrac{f''}{2!}(x_{i+1} - x_i)^2 + \cdots + \dfrac{f^{(n)}}{n!}(x_{i+1} - x_i)^n + R_n \\ R_n = \dfrac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{(n+1)} \end{cases}$$

$$\xrightarrow{h = x_{i+1} - x_i} \begin{cases} f(x_{i+1}) \cong f(x_i) + f'(x_i)h + \dfrac{f''}{2!}h^2 + \cdots + \dfrac{f^{(n)}}{n!}h^n + R_n \\ R_n = \dfrac{f^{(n+1)}(\xi)}{(n+1)!}h^{(n+1)} = O\left(h^{(n+1)}\right) \end{cases}$$

ξ is not known exactly, lies somewhere between $x_i < \xi < x_{i+1}$

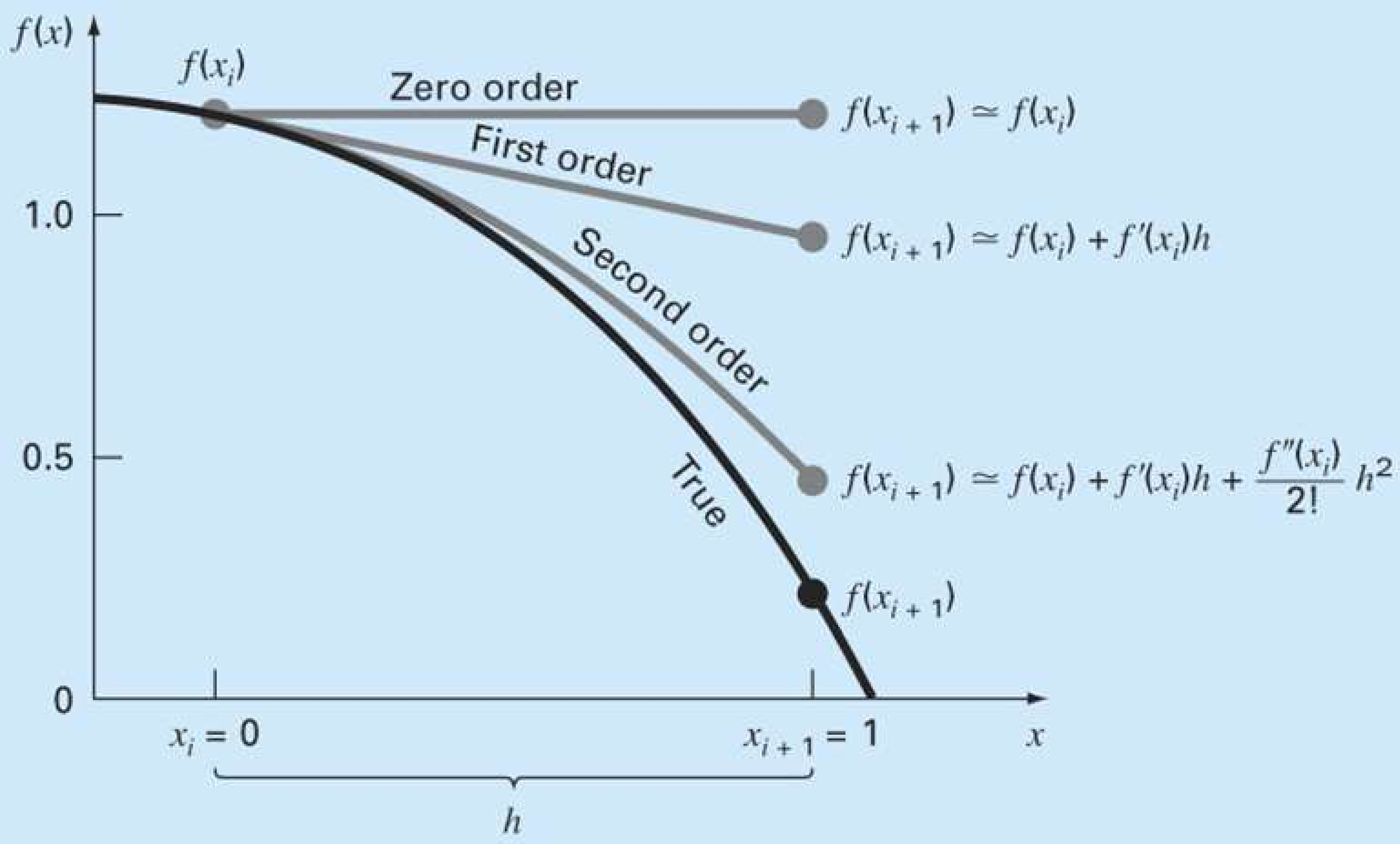
Need to determine $f^{(n+1)}(x)$, to do this you need $f'(x)$

If we knew $f(x)$, we don't need to perform the Taylor series expansion

Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

$x_i = 0$, predict the function's value at $x_{i+1} = 1$



Example

Approximate $f(x) = \cos x$ at $x_{i+1} = \pi/3$

on the basis of the value of $f(x)$ and its derivatives at $x_i = \pi/4$

Order *n*	$f^{(n)}(x)$	$f(\pi/3)$	ε_t
0	$\cos x$	0.707106781	−41.4
1	$-\sin x$	0.521986659	−4.4
2	$-\cos x$	0.497754491	0.449
3	$\sin x$	0.499869147	2.62×10^{-2}
4	$\cos x$	0.500007551	-1.51×10^{-3}
5	$-\sin x$	0.500000304	-6.08×10^{-5}
6	$-\cos x$	0.499999988	2.44×10^{-6}

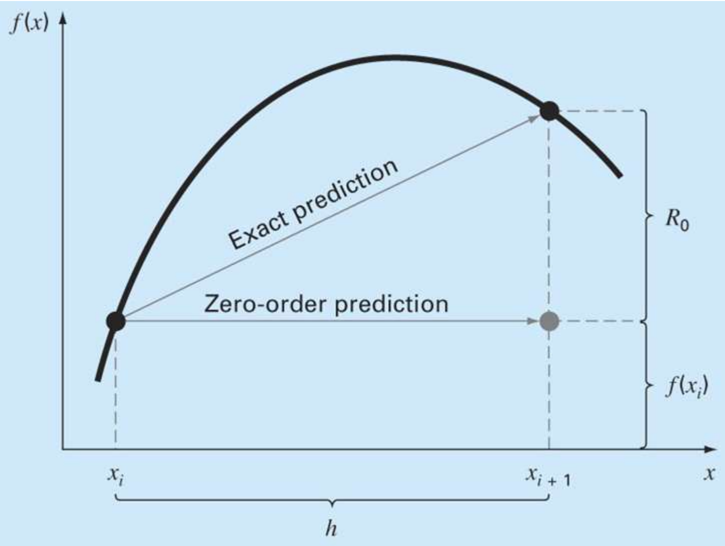
Remainder for the Taylor Series Expansion

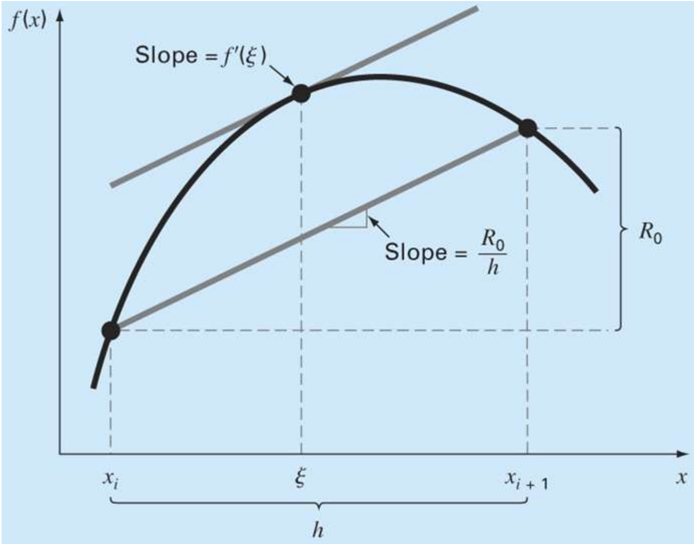
$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''}{2!}h^2 + \cdots \rightarrow f(x_{i+1}) \cong f(x_i)$$

$$R_0 = f'(x_i)h + \frac{f''}{2!}h^2 + \cdots \rightarrow R_0 \cong f'(x_i)h$$

$$\left[\text{derivative mean-value theorem}\right] f'(\xi) = \frac{R_0}{h} \rightarrow R_0 = f'(\xi)h \rightarrow R_1 \cong \frac{f''(\xi)}{2!}h^2$$

$$R_n = \int_{x_i}^{x_{i+1}} \frac{\left(x_{i+1}-t\right)^n}{n!} f^{(n+1)}\left(t\right)dt \xrightarrow[g(t)=f^{(n+1)}(t),\,h(t)=\frac{(x_{i+1}-t)^n}{n!}]{\int_a^x g(t)h(t)dt = g(\xi)\int_a^x h(t)dt} R_n = \frac{f^{(n+1)}\left(\xi\right)}{\left(n+1\right)!}\left(x_{i+1}-x_i\right)^{n+1}$$





Estimate Truncation Errors

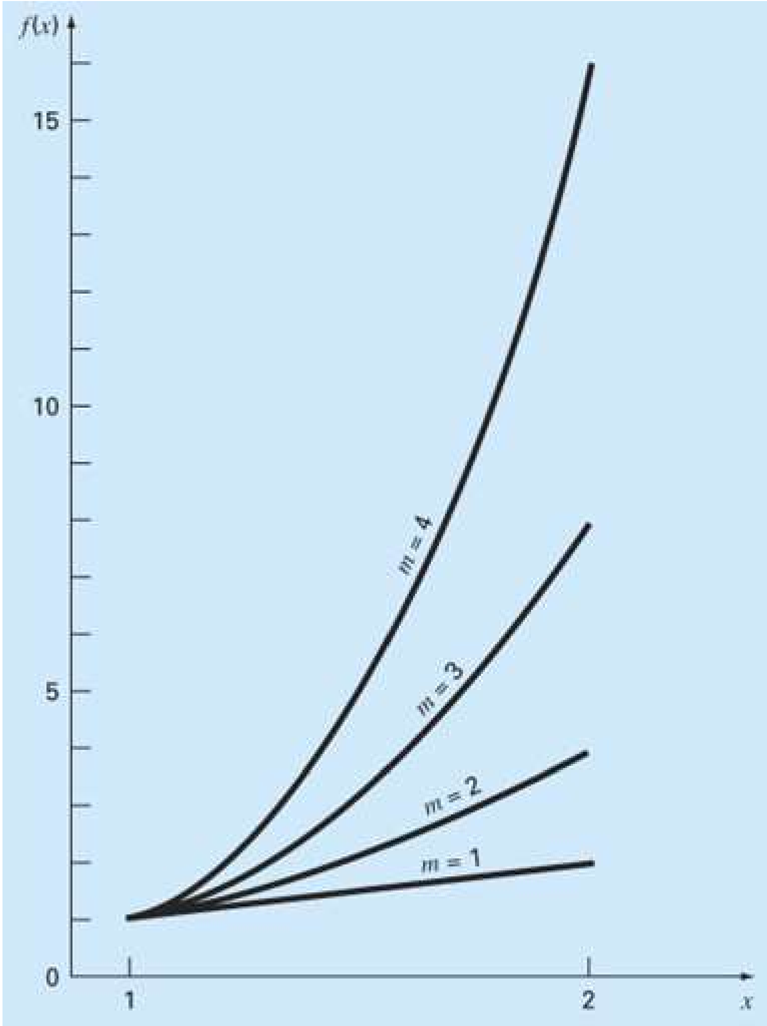
$$v(t_{i+1}) = v(t_i) + v'(t_i)(t_{i+1} - t_i) + R_1$$

$$\rightarrow v'(t_i) = \underbrace{\frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}}_{\text{first-order approximation}} - \underbrace{\frac{R_1}{t_{i+1} - t_i}}_{\text{truncation error}}$$

$$\frac{R_1}{t_{i+1} - t_i} = \frac{v''(\xi)}{2!}(t_{i+1} - t_i) = O(t_{i+1} - t_i)$$

– Example: effect of nonlinearity and step size

$$f(x) = x^m$$



Numerical Differentiation

- Forward difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)\underbrace{(x_{i+1}-x_i)}_{h} + \frac{f''(x_i)}{2!}\underbrace{(x_{i+1}-x_i)}_{h}^2 + \cdots \rightarrow f'(x_i) = \frac{f(x_{i+1})-f(x_i)}{h} + \underbrace{\frac{f''(x_i)}{2}h + \cdots}_{O(h)}$$

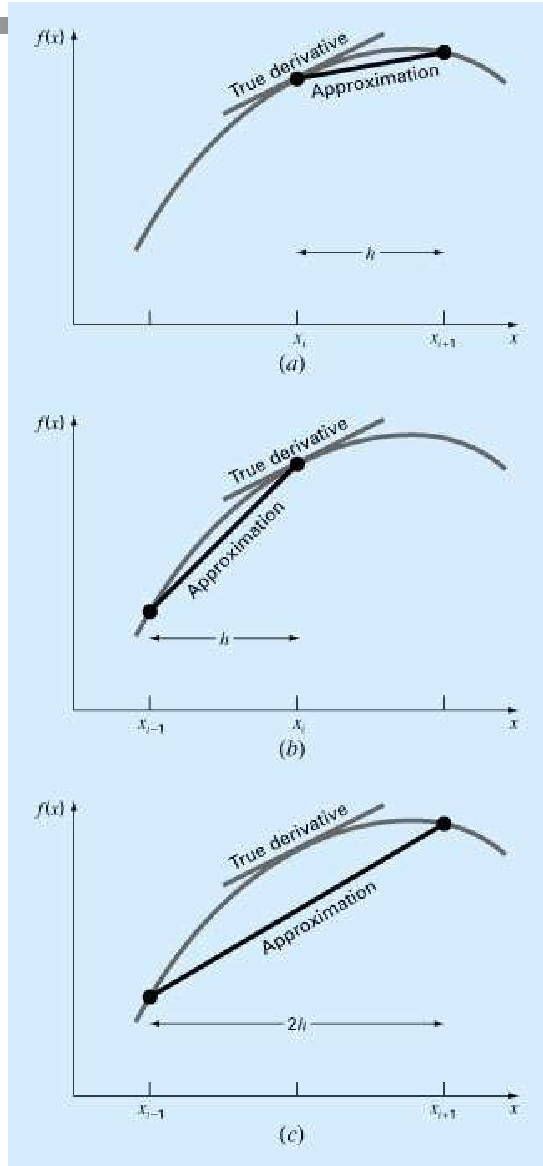
- Backward difference

$$f(x_{i-1}) = f(x_i) + f'(x_i)\underbrace{(x_{i-1}-x_i)}_{-h} + \frac{f''(x_i)}{2!}\underbrace{(x_{i-1}-x_i)}_{-h}^2 + \cdots \rightarrow f'(x_i) = \frac{f(x_i)-f(x_{i-1})}{h} + \underbrace{\frac{f''(x_i)}{2}h + \cdots}_{O(h)}$$

- Central difference
  - Error↓ # of function evaluation ↑
  - Perturbation?
  - If the function is not too nonlinear, $h = 0.01|x_i|$

$$\begin{cases} f(x_{i+1}) = f(x_i) + f'(x_i)\underbrace{(x_{i+1}-x_i)}_{h} + \frac{f''(x_i)}{2!}\underbrace{(x_{i+1}-x_i)}_{h}^2 + \frac{f'''(x_i)}{3!}\underbrace{(x_{i+1}-x_i)}_{h}^3 + \cdots \\ f(x_{i-1}) = f(x_i) + f'(x_i)\underbrace{(x_{i-1}-x_i)}_{-h} + \frac{f''(x_i)}{2!}\underbrace{(x_{i-1}-x_i)}_{-h}^2 + \frac{f'''(x_i)}{3!}\underbrace{(x_{i-1}-x_i)}_{-h}^3 + \cdots \end{cases}$$

$$\rightarrow f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{f'''(x_i)}{3}h^3 \rightarrow f'(x_i) = \frac{f(x_{i+1})-f(x_{i-1})}{2h} + O(h^2)$$



Error Propagation

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x-\tilde{x}) + \frac{f''(\tilde{x})}{2}(x-\tilde{x})^2 + \cdots$$

$$f(x) - f(\tilde{x}) \cong f'(\tilde{x})(x-\tilde{x})$$

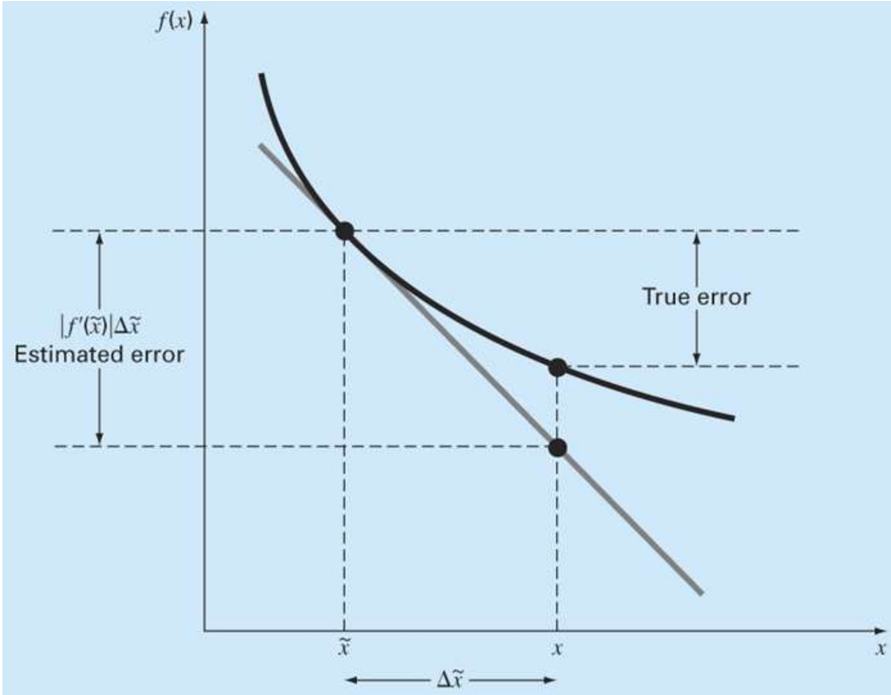
$$\rightarrow \underbrace{\left|f(x)-f(\tilde{x})\right|}_{\Delta f(\tilde{x})} = \left|f'(\tilde{x})\right| \underbrace{\left|x-\tilde{x}\right|}_{\Delta\tilde{x}}$$

$$\left.\begin{array}{l}\text{relative error of } f(x): \dfrac{f(x)-f(\tilde{x})}{f(\tilde{x})} \cong \dfrac{f'(\tilde{x})(x-\tilde{x})}{f(\tilde{x})} \\ \text{relative error of } x: \dfrac{x-\tilde{x}}{\tilde{x}}\end{array}\right\}$$

$$\rightarrow \text{condition number} = \frac{\text{relative error of } f(x)}{\text{relative error of } x} = \frac{\tilde{x}f'(\tilde{x})}{f(\tilde{x})}$$

: sensitivity, stability

$$\Delta f(\tilde{x}_1,\ldots,\tilde{x}_n) \cong \left|\frac{\partial f}{\partial x_1}\right|\Delta\tilde{x}_1 + \cdots + \left|\frac{\partial f}{\partial x_n}\right|\Delta\tilde{x}_n$$



Operation		Estimated Error
Addition	$\Delta(\tilde{u}+\tilde{v})$	$\Delta\tilde{u} + \Delta\tilde{v}$
Subtraction	$\Delta(\tilde{u}-\tilde{v})$	$\Delta\tilde{u} + \Delta\tilde{v}$
Multiplication	$\Delta(\tilde{u}\times\tilde{v})$	$\lvert\tilde{u}\rvert\Delta\tilde{v} + \lvert\tilde{v}\rvert\Delta\tilde{u}$
Division	$\Delta\left(\frac{\tilde{u}}{\tilde{v}}\right)$	$\frac{\lvert\tilde{u}\rvert\Delta\tilde{v} + \lvert\tilde{v}\rvert\Delta\tilde{u}}{\lvert\tilde{v}\rvert^2}$

Total Numerical Error

centered difference approximation

$$\underbrace{f'(x_i)}_{\text{true value}} = \underbrace{\frac{f(x_{i+1}) - f(x_{i-1})}{2h}}_{\text{finte-difference approximation}} \underbrace{- \frac{f^{(3)}(\xi)}{6} h^2}_{\text{truncation error}}$$

$$f(x_{i-1}) = \underbrace{\tilde{f}(x_{i-1})}_{\text{rounded function value}} + \underbrace{e_{i-1}}_{\substack{\text{associated} \\ \text{round-off error}}}$$

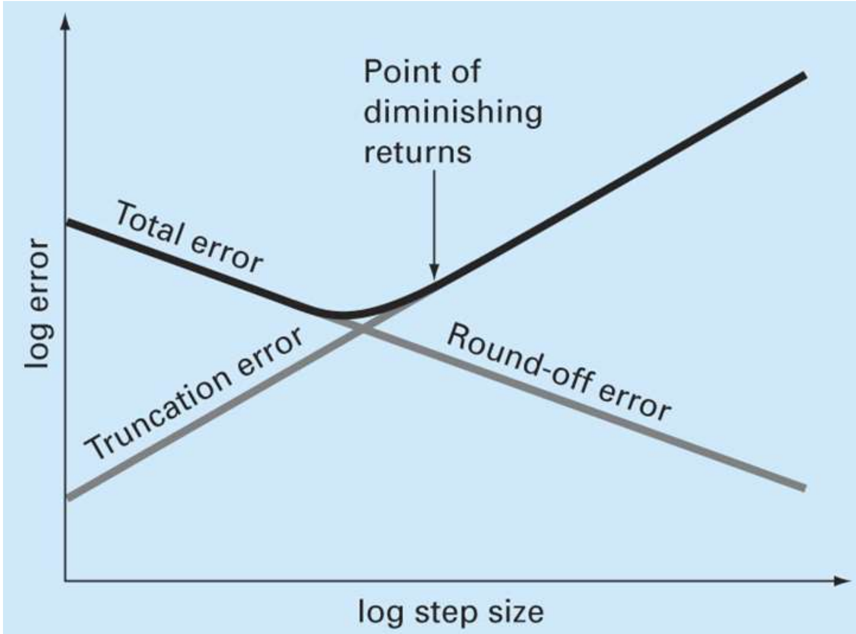
$$f(x_{i+1}) = \tilde{f}(x_{i+1}) + e_{i+1}$$

$$\rightarrow f'(x_i) = \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} + \frac{e_{i+1} - e_{i-1}}{2h} - \frac{f^{(3)}(\xi)}{6} h^2$$

$$\text{Total error} = \left| f'(x_i) - \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} \right|$$

$$\xrightarrow{|e| \le \varepsilon,\ |f^{(3)}(x)| \le M} \le \frac{\varepsilon}{h} + \frac{h^2 M}{6}$$

$$h_{opt} = \sqrt[3]{\frac{3\varepsilon}{M}}$$

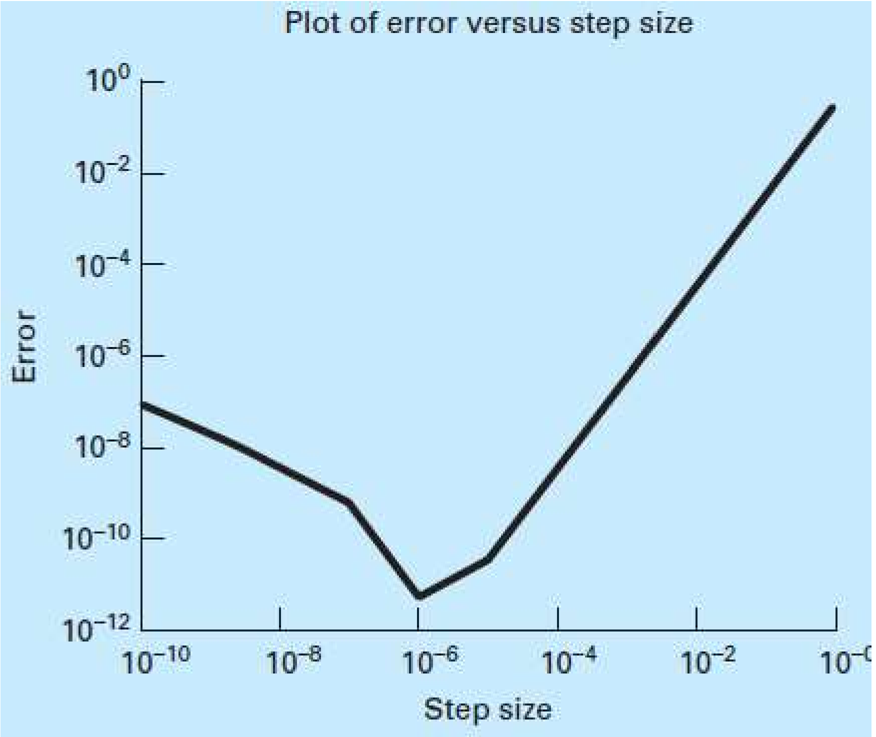


Example

Problem Statement. In Example 4.4, we used a centered difference approximation of $O(h^2)$ to estimate the first derivative of the following function at $x = 0.5$,

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

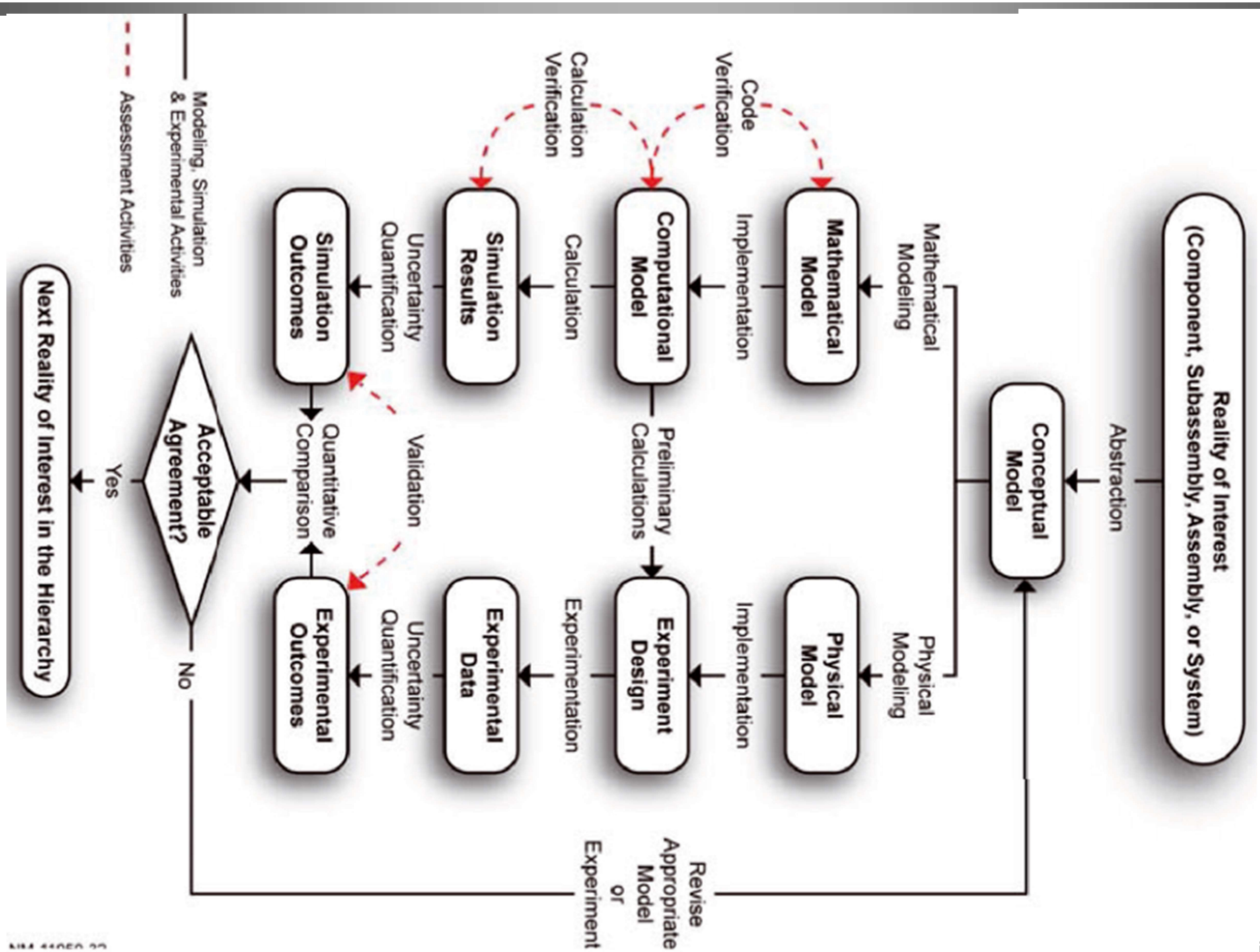
Perform the same computation starting with $h = 1$. Then progressively divide the step size by a factor of 10 to demonstrate how round-off becomes dominant as the step size is reduced. Relate your results to Eq. (4.31). Recall that the true value of the derivative is -0.9125.



Control of Numerical Errors

- No systematic and general approaches to evaluate numerical errors
  - Avoid subtracting two nearly equal numbers, or use extended-precision arithmetic
  - Sort the numbers and work with the smallest numbers first
  - Perform numerical experiments to increase your awareness of computational errors and possible ill-conditioned problems
- Source of errors
  - Blunder
  - Formulation error
  - Data uncertainty

What is Verification and Validation ?



Engineering Simulation

- Three types of models
  - Conceptual
  - Mathematical
  - Computational
- Verification: domain of mathematics
  - Process of determining that a computational model accurately represents the underlying mathematical model and its solution
- Validation: domain of physics
  - Process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

Verification

- Code verification
  - Mathematical model and solution algorithms are working correctly
  - Domain of software developers: Software Quality Assurance techniques along with testing of each released version
  - To compare code outputs with analytical solutions
- Calculation verification
  - Discrete solution of the mathematical model is accurate
  - Domain of user of the software
  - Estimating the errors in the numerical solution due to discretization
  - Mesh-to-mesh comparison: to determine the rate of convergence of the solution

Validation

- Answering the adequacy of the selected models for representing the reality of interest
  - Mechanics (physics) included in the models sufficient to provide reliable answers to the questions posed in the problem statement

- Interaction between mathematics and physics in V&V process
  - Close cooperation among modelers and experimentalist
  - ‘cross-talk’ activity to model the same conceptual model, e.g., fixed-end condition
  - Segregation of the outcomes
- Role of uncertainty quantification (UQ)
  - Different experimental results
  - Distributed numerical and physical parameters

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