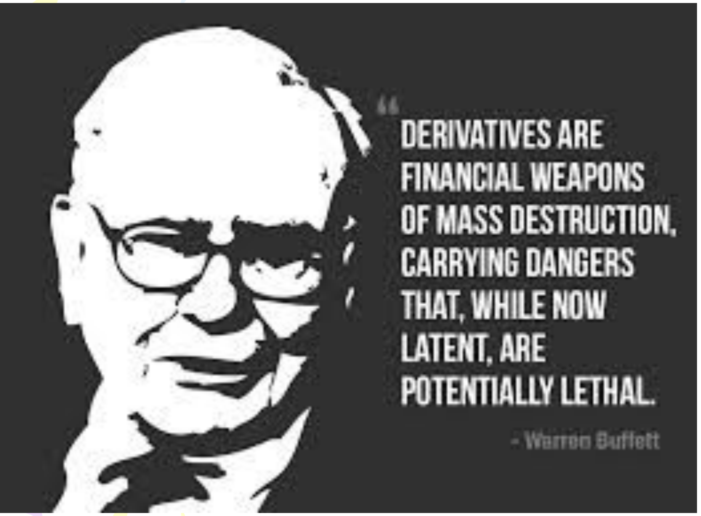
计算物理

Lecture 12

傅子文

fuziwen@scu.edu.cn



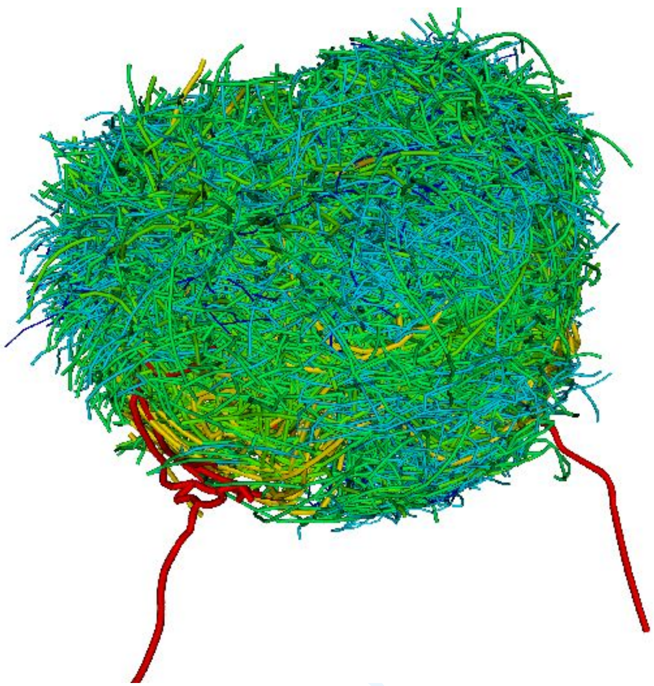
Today lecture

- Numerical Difference
- Introduction to ODE solvers
- Euler method

The example:

- Pollutant Transport-Chemistry Models

- Chemo-Taxis Problems from Mathematical
- Biology Like bacterial growth, tumor growth



Runge-Kutta Method for Advection-Diffusion-Reaction Equation

Numerical Differentiation

- Often possible to find derivatives given an analytic expression for a function
- But this is not always the case. In some cases, numerical determination of the derivative is the only alternative
  - Functions available only as a set of discrete data points
  - Determination of a function from non-linear differential equation and some initial conditions
- But there are some significant practical problems with numerical derivatives...

Simple Derivatives

Limit-based determination: $$\frac{df(x)}{dx} = \lim_{h\to 0}\frac{f(x+h)-f(x)}{h}$$

Another method of computing differences:

Forward Difference

$$D_h^+(f(x)) = \frac{f(x+h)-f(x)}{h}$$

Backward Difference

$$D_h^-(f(x)) = \frac{f(x-h)-f(x)}{h}$$

Forward and backward differences typically give about the same result with similar accuracy

Only a few special cases where one is preferred

- at a discontinuity
- at the boundary of bounded functions

Derivatives & Errors

Taylor Series Expansion:

$$f(x+h) = f(x) + h\frac{df(x)}{dx} + \frac{h^2}{2}\frac{d^2 f(x)}{dx^2} + \ldots$$

$O(h^2)$

Remianing Terms

Forward Difference

$$\left(\frac{f(x+h)-f(x)}{h}\right) = \frac{df(x)}{dx} + O(h)$$

Approximation error

$$\frac{h}{2}\left|f''(x)\right|$$

This implies that making h smaller, reduces the total error (Not TRUE)
Why?....... Round-off errors!

Forward Difference Error

$$\varepsilon = \varepsilon_c + \varepsilon_a$$

Roundoff error $\varepsilon_c = \dfrac{2cf(x)}{h}$

Approximation error $\varepsilon_a = \dfrac{h}{2}\left|f''(x)\right|$

$$\varepsilon = \frac{2c\left|f(x)\right|}{h} + \frac{h}{2}\left|f''(x)\right|$$

setting $\dfrac{d\varepsilon}{dh}=0$ to find the value of h which minimizes the error

$$h_{\text{best}} = \sqrt{4c\left|\frac{f(x)}{f''(x)}\right|}$$

$$\boxed{\varepsilon = h_{\text{best}}\left|f''(x)\right| = \sqrt{4c\left|f(x)f''(x)\right|}}$$

recall from numerical accuracy

$$x_c = x_{true}(1 \pm c)$$

$$f_c(x) = f(x) \pm cf(x)$$

$$D^+[f(x)] = \frac{f(x+h)-f(x)}{h} \pm \frac{2cf(x)}{h}$$

if f(x) & f''(x) are on the order 1,
we should choose a h on the order of 10^{-8}

Central Derivatives

Limit-based determination: $$\frac{df(x)}{dx} = \lim_{h\to 0}\frac{f(x+h)-f(x)}{h}$$

Another method of computing differences:

Central Difference

$$D_h^c(f(x)) = \frac{f(x+h/2)-f(x-h/2)}{h}$$

The Central Difference is overall more accurate

Central Difference Errors

Taylor Series Expansion:

$$f(x+h/2)=f(x)+\frac{h}{2}f'(x)+\frac{(h/2)^2}{2!}f''(x)+\frac{(h/2)^3}{3!}f'''(x)+\ldots$$

$$-\,f(x-h/2)=f(x)-\frac{h}{2}f'(x)+\frac{(h/2)^2}{2!}f''(x)-\frac{(h/2)^3}{3!}f'''(x)+\ldots$$

$$f(x+h/2)-f(x-h/2)=hf'(x)+\frac{h^3}{24}f'''(x)+\ldots$$

Central Difference

$$\left(\frac{f(x+h/2)-f(x-h/2)}{h}\right)=\frac{df(x)}{dx}+O(h^2)$$

Approximation error $\frac{h^2}{24}\left|f'''(x)\right|$

Truncation error term is of order in h^2

Central Difference Error

$$\varepsilon=\varepsilon_c+\varepsilon_a$$

Roundoff error $\varepsilon_c = \dfrac{2cf(x)}{h}$

Approximation error $\varepsilon_a = \dfrac{h^2}{24}\left|f'''(x)\right|$

$$\varepsilon = \frac{2c\left|f(x)\right|}{h} + \frac{h^2}{24}\left|f'''(x)\right|$$

setting $\dfrac{d\varepsilon}{dh}=0$ to find the value of h which minimizes the error

$$h_{\text{best}} = \left(2c\left|\frac{f(x)}{f'''(x)}\right|\right)^{1/3}$$

recall from numerical accuracy

$$x_c = x_{true}(1 \pm c)$$

$$f_c(x) = f(x) \pm cf(x)$$

$$D^+[f(x)] = \frac{f(x+h)-f(x)}{h} \pm \frac{2cf(x)}{h}$$

$$\boxed{\varepsilon = \frac{1}{8}h^2\left|f'''(x)\right| = \left(24c\left|f(x)f'''(x)\right|\right)^{1/3}}$$

if f(x) & f '''(x) are on the order 1,
we should choose a h on the order of 10^{-5}
but the error will be on the order of 10^{-10}

Central Difference Example

$$f(x) = x^3 \sin(5x)$$

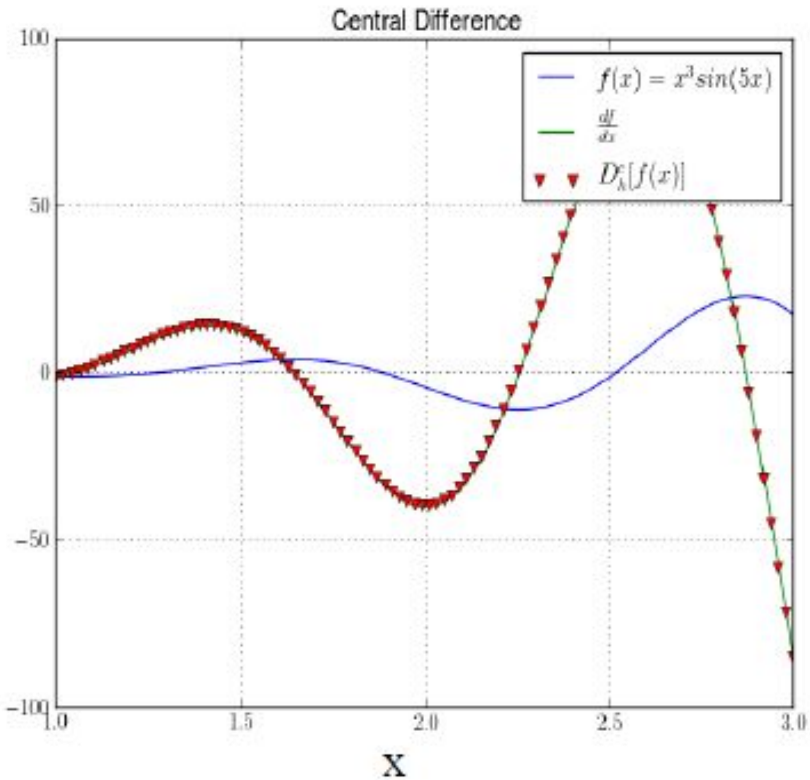
$$D_h^c[f(x)] = \frac{d\,f(x)}{dx} + O(h^2)$$

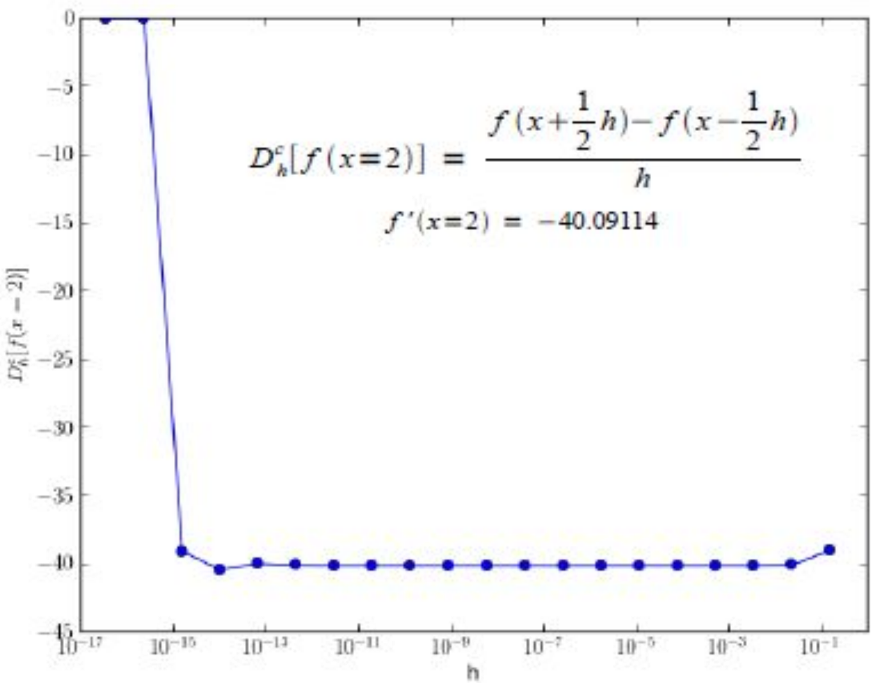
```
def F(x):
    return x**3 * np.sin(5*x)

def Dc(func, x, h=1e-5):
    return (func(x+0.5*h) - func(x-0.5*h)) / h

def dFdx(x):
    return  3*x**2 * np.sin(5*x) + 5*x**3 * cos(5*x)
```

centralDiff.py





Second Difference

calculate by applying the first-derivative formulas twice

$$f'(x+h/2) \approx \frac{f(x+h)-f(x)}{h}$$

$$f'(x-h/2) \approx \frac{f(x-h)-f(x)}{h}$$

The central difference for the second-derivative:

$$f''(x) \approx \frac{f'(x+h/2)-f'(x-h/2)}{h}$$

$$= \frac{[f(x+h)-f(x)]/h-[f(x)-f(x-h)]/h}{h}$$

2nd Central Difference

$$= \frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

2nd Central Difference Errors

Taylor Series Expansion:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + \ldots$$

$$+ \quad f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + \ldots$$

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12}f''''(x) + \ldots$$

2nd Central Difference

$$\left(\frac{f(x+h) - 2f(x) + f(x-h)}{h^2}\right) = \frac{d^2 f(x)}{dx^2} + \frac{h^2}{12}f''''(x)$$

Approximation error $\frac{h^2}{12}\left|f''''(x)\right|$

Truncation error term is of order in h^2

2nd Central Difference Errors

$$\varepsilon = \varepsilon_c + \varepsilon_a$$

Roundoff error $\varepsilon_c = \dfrac{4cf(x)}{h}$

Approximation error $\varepsilon_a = \dfrac{h^2}{12}\left|f'''(x)\right|$

$$\varepsilon = \frac{4c\left|f(x)\right|}{h} + \frac{h^2}{12}\left|f'''(x)\right|$$

setting $\dfrac{d\varepsilon}{dh}=0$ to find the value of h which minimizes the error

$$h_{\text{best}} = \left(48c\left|\frac{f(x)}{f'''(x)}\right|\right)^{1/4}$$

$$\boxed{\varepsilon = \frac{1}{6}h^2\left|f'''(x)\right| = \left(\frac{4}{3}c\left|f(x)f'''(x)\right|\right)^{1/2}}$$

if f(x) & f ''''(x) are on the order 1, we should choose a h on the order of 10^{-4} but the error will be on the order of 10^{-8}

Ordinary Differential Equations

- Equations which are composed of an unknown function and its derivatives are called ***differential equations.***

- Differential equations play a basic role in physics because many physical phenomena are best formulated mathematically in terms of their rate of change.

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

v - dependent variable

t - independent variable

Ordinary Differential Equations

- When a function involves **one dependent variable**, the equation is called an **ordinary differential equation (ODE).**

- **A partial differential equation (PDE)** involves **two or more independent variables**.

.

Ordinary Differential Equations

Differential equations are also classified as to their order:

A first order equation includes a first derivative as its highest derivative.

- Linear 1st order ODE

$$\frac{dy}{dx} + \alpha \cdot y = f(x)$$

- Non-Linear 1st order ODE

Where f(x,y) is nonlinear

$$\frac{dy}{dx} = f(x, y)$$

A second order equation includes a second derivative.

N^{th}-order Differential Equations

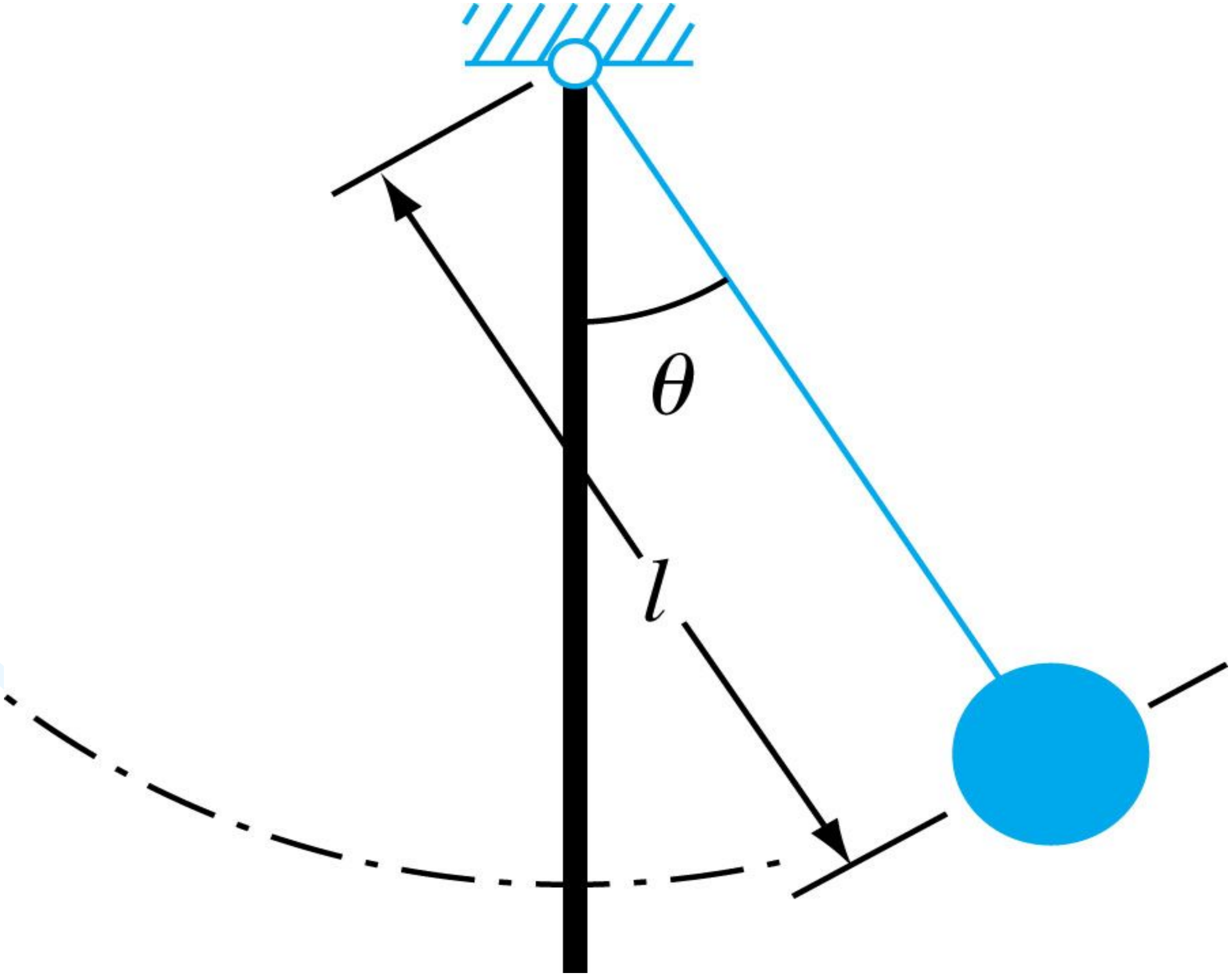
- Higher order equations can be reduced to a system of first order equations, by redefining a variable.

Problems Involving N^{th}-order Ordinary Differential Equations Can Always be Reduced to the Study of a set of 1^{st}-Order Differential Equations

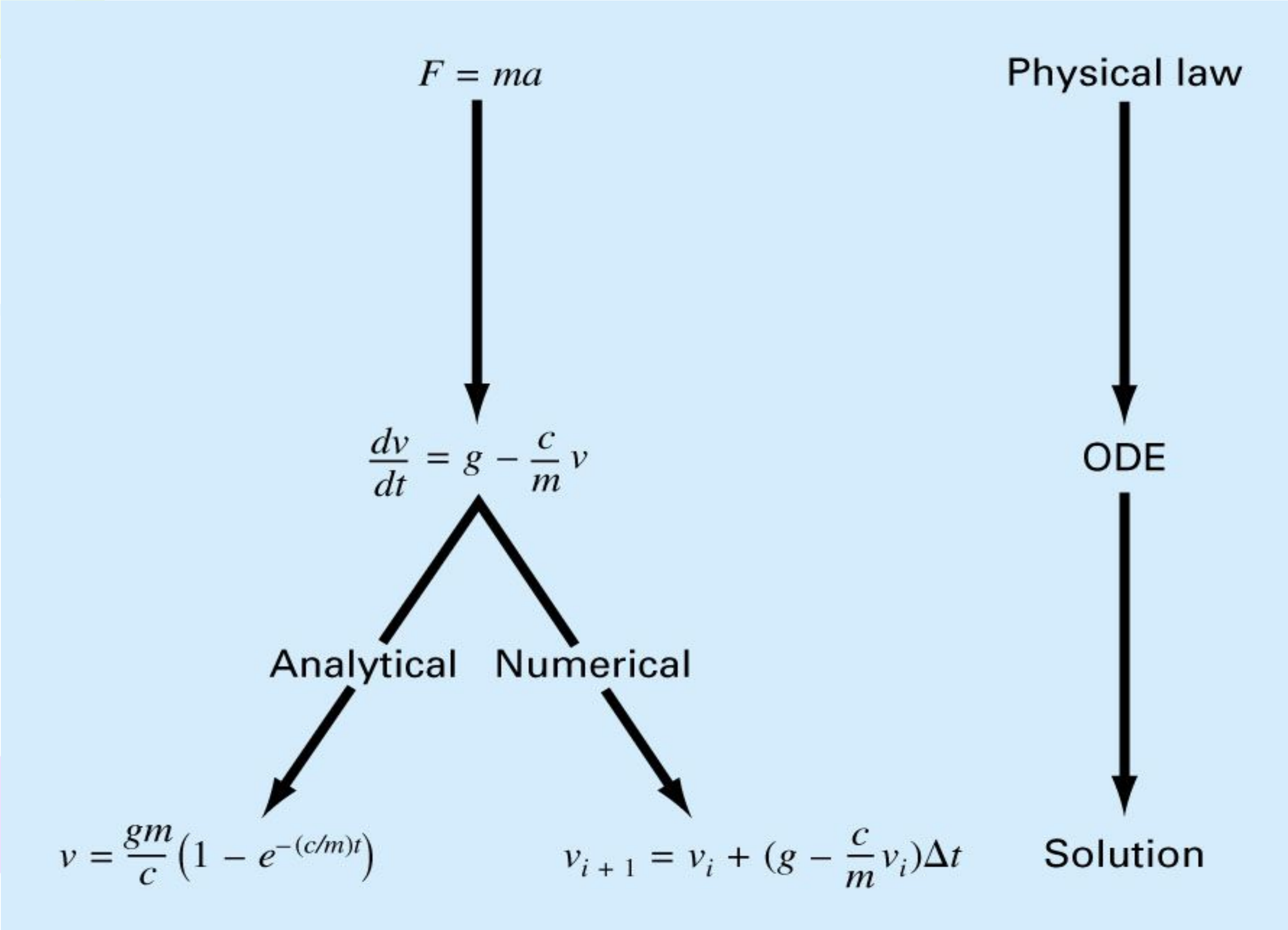
N^{th}-order ODE Transformed to N 1^{st}-order ODEs

$$\boxed{\frac{d^2y}{dt^2} = f(t)\frac{dy}{dt} = g(t)} \Rightarrow \boxed{\begin{aligned} \frac{dy}{dt} &= v(t) \\ \frac{dv}{dt} &= g(t) - f(t)v(t) \end{aligned}}$$

ODEs and Physical Practice



Ordinary Differential Equations



Simplest approach to ODEs

- To begin consider a general first order ordinary differential equation

$$\frac{dy}{dx} = y'(x) = f(x, y(x)) \qquad (1) \text{ with } y(x_0) = y_0$$

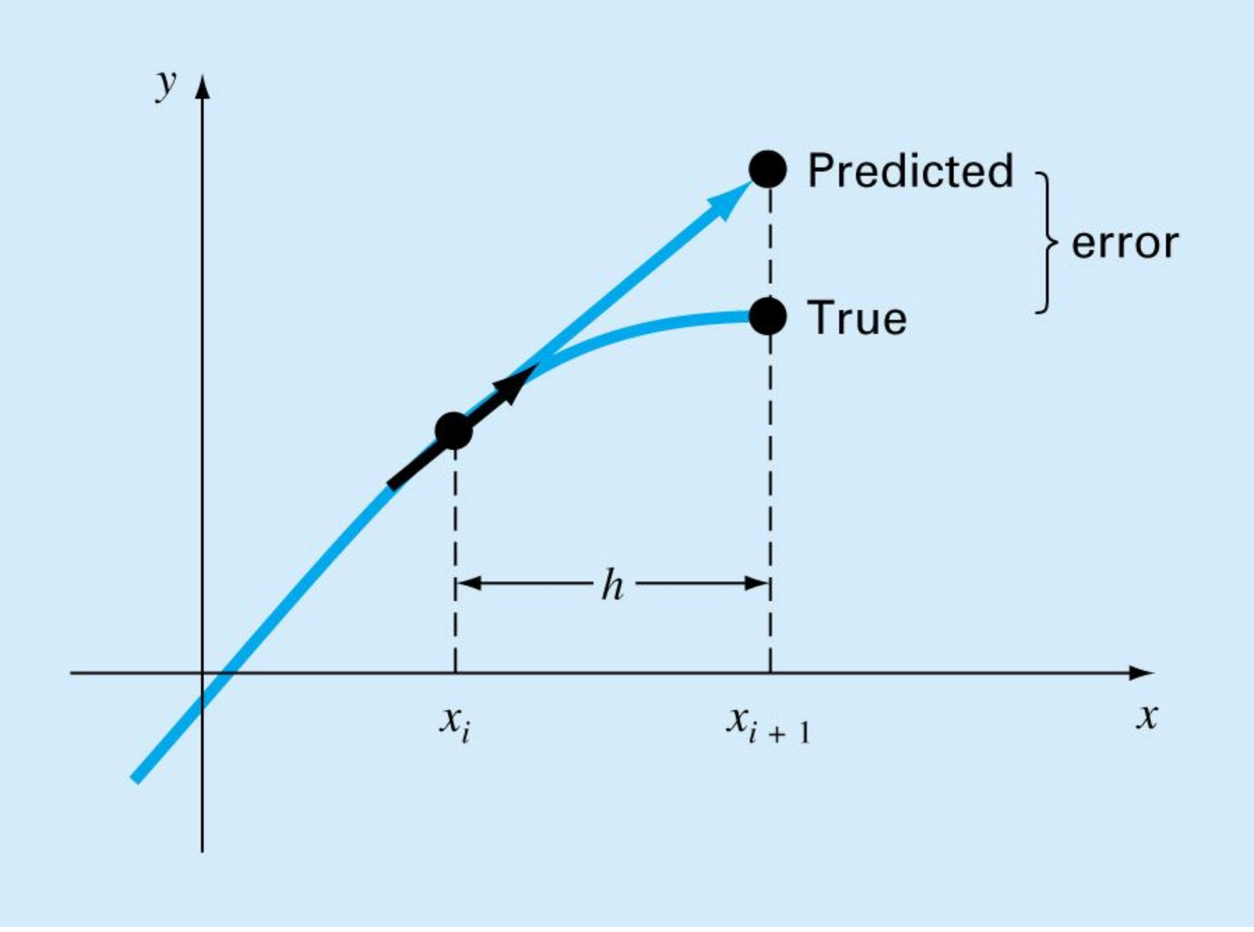
- Using a Taylor expansion of the solution $y(x)$

$$\begin{aligned} y(x) &= y(x_0) + (x - x_0)y'(x_0) + \cdots \\ &= y(x_0) + (x - x_0)f(x_0, y_0) + \cdots \\ &= y_0 + hf_0 + \cdots \end{aligned}$$

where $h = x - x_0$

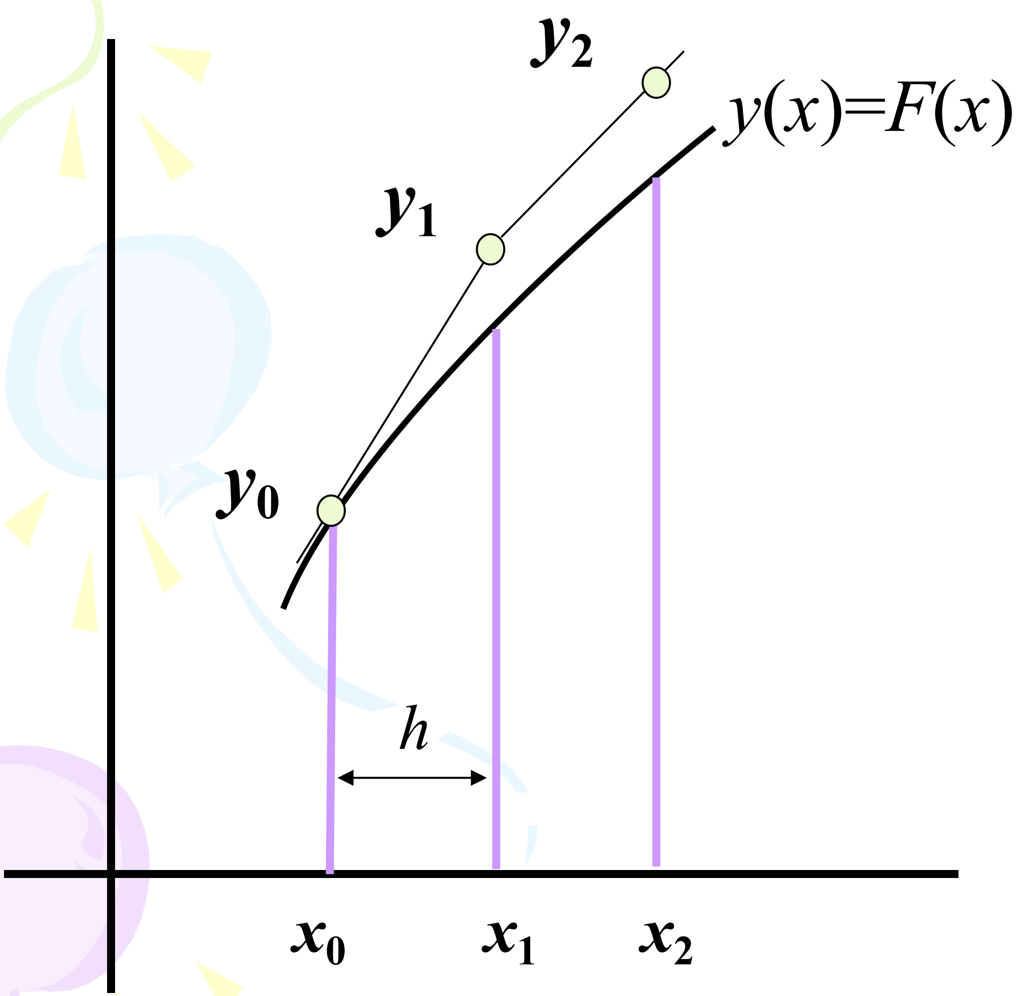
- Which suggests we predict forward function values from a starting point x_0, y_0

$$\frac{dy}{dx} = f(x, y)$$



$$\boxed{y_{i+1} = y_i + f(x_i, y_i) \cdot h}$$

Crude (forward) Euler solver graphically



Let $y_1 = y_0 + hf_0$,
where $f_0 = f(x_0, y_0)$
predict forward from y_1

$y_2 = y_1 + hf_1$,
where $f_1 = f(x_1, y_1)$

$y_3 = \ldots$

Useful notation

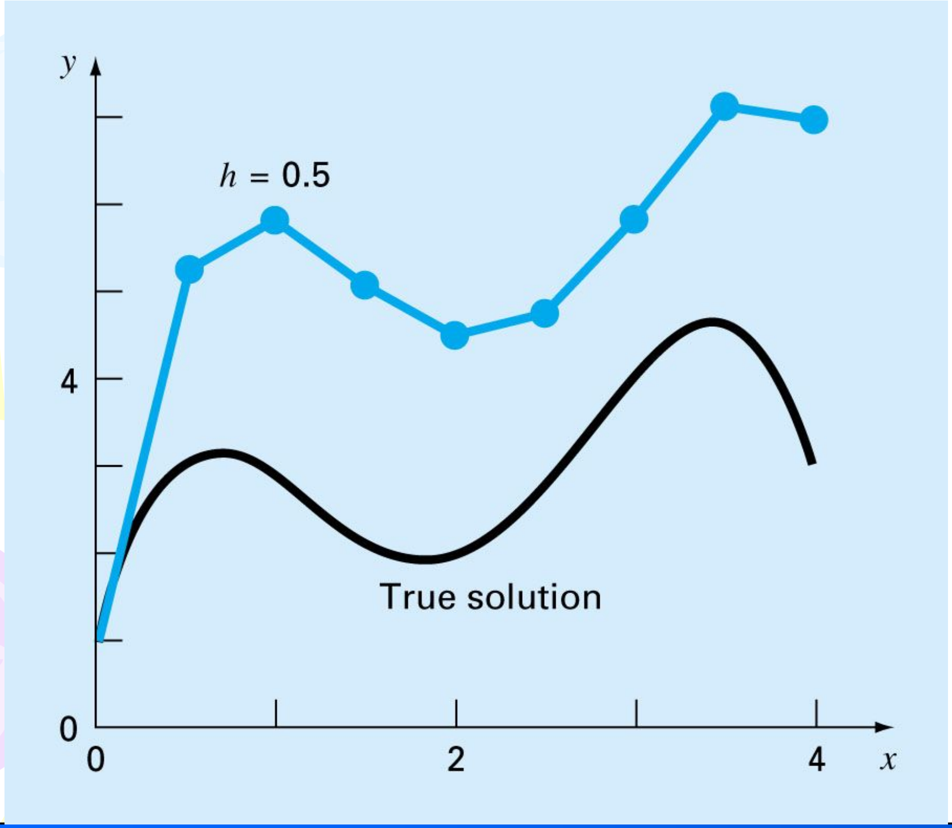
- n = step number
- Dx = width of interval
- $x_n = n \times \Delta x$
- $y_n = y(x_n)$
- $f_n = f(x_n, y_n)$

Example

$$\frac{dy}{dx} = f(x,y) = -2x^3 + 12x^2 - 20x + 8.5$$

$Starting \quad point \quad x_0 = 0, \quad y_0 = 1$

$$y_{i+1} = y_i + f(x_i, y_i)h = 1 + 8.5 * 0.5 = 5.25$$



Not good?

Numerical errors

- Discretization error:
  - Error resulting from the computation of quantities that have been calculated using an approximation to the true solution
- We may neglect higher order terms for example
  - This error is sometimes called truncation error
  - Unavoidable problem in numerical integration work
    - Would occur even in the presence of infinite precision
- Round-off error
  - Result of finite precision arithmetic

Discretization & round-off errors

- Suppose the exact solution at a given value of x_n is $(y=)F(x_n)$, the (accumulated) discretization error is defined as

$$E_n = F(x_n) - y_n$$

  - Caused by
    - approximate formula to estimate y_{n+1}
    - Input data at start of step do not necessarily correspond to exact soln

- Accumulated round-off error is defined as

$$R_n = y_n - Y_n$$

  - Where Y_n is the value we actually calculate after round-off rather than the true value y_n

- So the absolute value of the total error is given by the inequality

$$|F(x_n) - Y_n| \le |E_n| + |R_n|$$

Error Analysis for Euler's Method

Numerical solutions of ODEs involves two types of error:

- *Truncation* error
  - *Local truncation error*

$$E_a = \frac{f'(x_i, y_i)}{2!} h^2$$

$$E_a = O(h^2)$$

  - *Propagated truncation error*

  The sum of the two is the *total or global truncation error*

- *Round-off* errors

Error Analysis for Euler's Method

- The Taylor series provides a means of quantifying the error in Euler's method. However;
  - The Taylor series provides only an estimate of the local truncation error-that is, the error created during a single step of the method.
  - In actual problems, the functions are more complicated than simple polynomials. Consequently, the derivatives needed to evaluate the Taylor series expansion would not always be easy to obtain.
- In conclusion,
  - the error can be reduced by reducing the step size
  - If the solution to the differential equation is linear, the method will provide error free predictions as for a straight line the 2nd derivative would be zero.

Problems with forward Euler method

- This method relies upon the derivative at the *beginning* of each interval to predict forward to the end of each interval
- Any errors in the solution tend to get amplified quickly
- Calculated solution quickly diverges away from the true solution as the error grows
- We can precisely calculate the error in a single step as follows

Local discretization error in Euler Method

The easiest way to calculate the local discretization error is to use a Taylor expansion:

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!}\left.\frac{d^2 y}{dx^2}\right|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!}\left.\frac{d^3 y}{dx^3}\right|_{x_i, y_i} (x_{i+1} - x_i)^3 + \ldots$$

$$\boxed{y_{i+1} = y_i + f(x_i, y_i)(x_{i+1} - x_i)} + \frac{1}{2!} f'(x_i, y_i)(x_{i+1} - x_i)^2 + \frac{1}{3!} f''(x_i, y_i)(x_{i+1} - x_i)^3 + \ldots$$

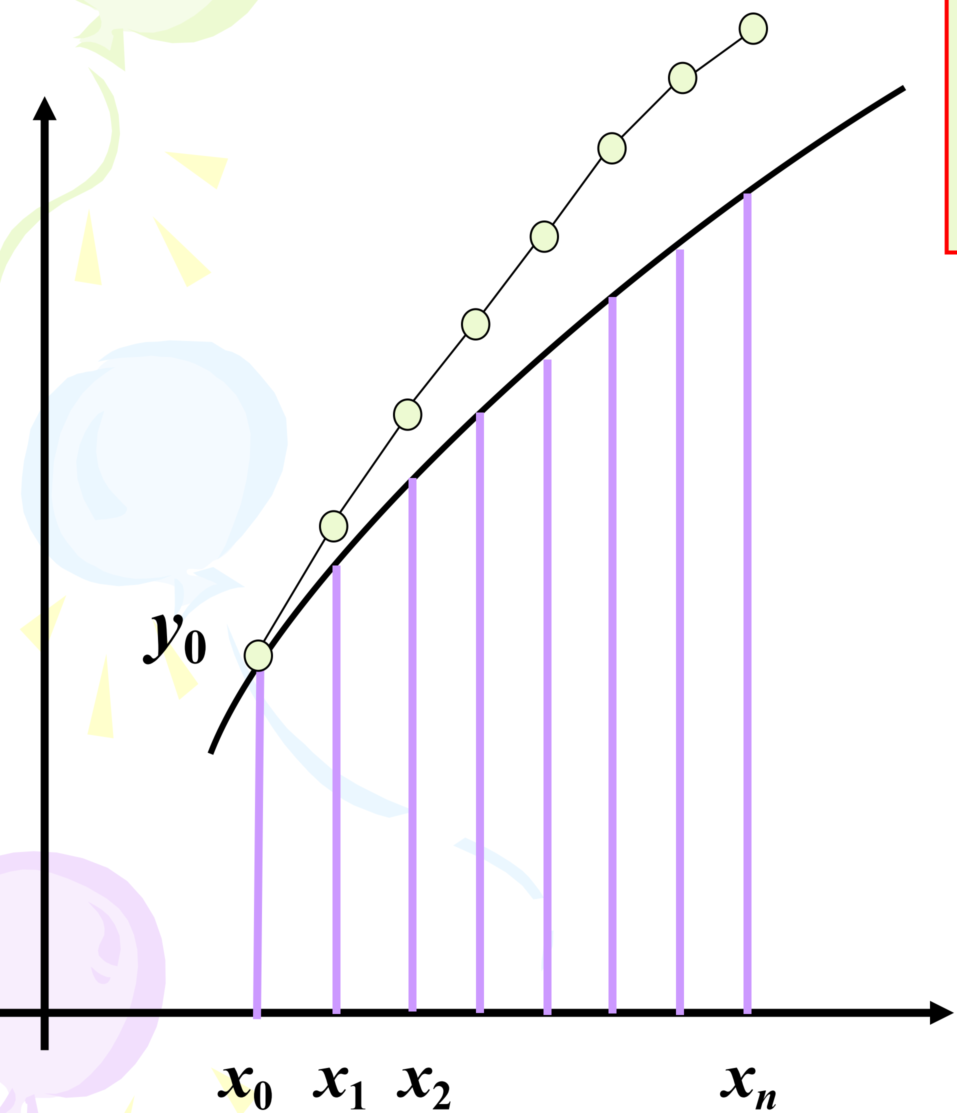
These **three** terms correspond to Euler's method -

$$y_{i+1} = y_i + f(x_i, y_i)h$$

Local discretization error in the approx. at one step is thus given by

$$e_i = \frac{f'(x_i, y_i)}{2!} h^2 + O(h^3) \qquad \therefore \boxed{e_i \propto h^2}$$

Error over a series of intervals



Be VERY careful about the distinction between the *local* discretization error e_i and the *global* error E_n accumulated over a series of intervals.

In many books/lectures a clear definition of what error is being discussed isn't always given.

Roughly speaking, if the local error is $O(h^n)$ then the global error will be $O(h^{n-1})$. This happens because $n=(x_n-x_0)/h$ and you sum over n intervals.

Unfortunately, calculating E_n usually requires fairly complicated derivations that we don't have time to do.

Euler's Method: Example

Obtain a solution between $x = 0$ to $x = 4$

with a step size of 0.5 for: $\dfrac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$

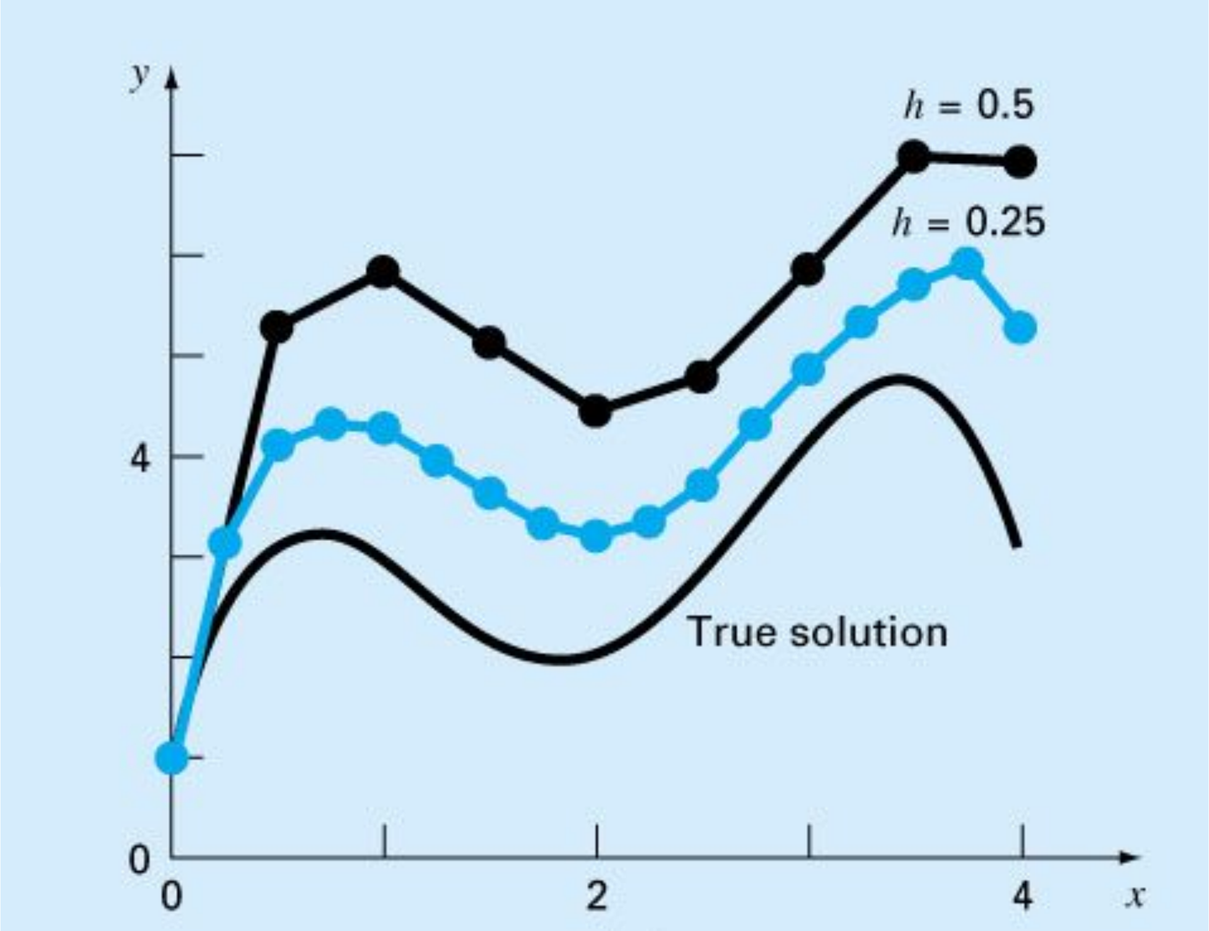
Initial conditions are: $x = 0$ to $y = 1$

Solution: $y_{i+1} = y_i + f(x_i, y_i) \cdot h$

$$y(0.5) = y(0) + f(0,1).(0.5)$$
$$= 1.0 + 8.5x0.5 = 5.25$$
$$y(1.0) = y(0.5) + f(0.5,5.25).(0.5)$$
$$= 5.25 + (-2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5).(0.5) = 5.875$$
$$y(2.0) = y(1.0) + f(1.0,5.875).(0.5)$$
$$= 5.25 + (-2(1.0)^3 + 12(1.0)^2 - 20(1.0) + 8.5).(0.5) = 5.125$$

Euler's Method: Example

- Although the computation captures the general trend solution, the error is considerable.
- This error can be reduced by using a smaller step size.



Improvements of Euler's method

- A fundamental source of error in Euler's method is that the derivative at the beginning of the interval is assumed to apply across the entire interval.

- Two simple modifications are available to circumvent this shortcoming:
  - The Midpoint (or Improved Polygon) Method
  - Heun's Method

Modified Euler Method
("extrapolate-integrate")

- The Euler method is flawed because we use the beginning of the interval to predict to the end
- If we could use the midpoint derivative that would usually be expected to be a better approximation
  - If the slope is changing rapidly across an interval using the midpoint slope usually gives us something closer to the average over the interval (of course it doesn't always have to be better, just on average)
- However since $y'_{mid} = f(x_{mid}, y_{mid})$ and we don't know y_{mid} (only y_0) & we have to estimate it

The Midpoint (or Improved Polygon) Method/

- Uses Euler's method t predict a value of *y* at the midpoint of the interval:

$$y_{i+1} = y_i + f(x_{i+1/2}, y_{i+1/2})h$$

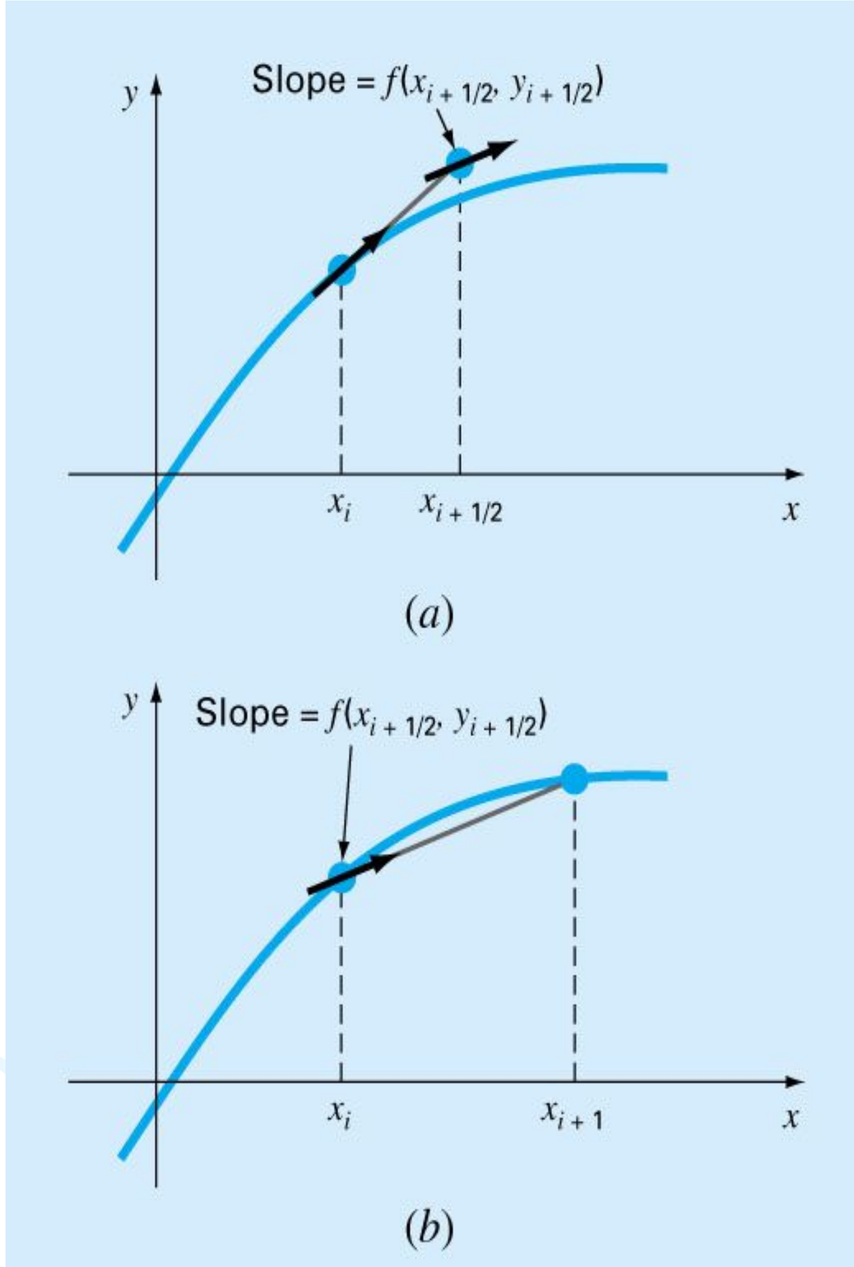


Figure 25.12

Modified Euler Method

- Let $y'(x) = f(x, y)$ and $y(x_0)=y_0$
- Let the step size be given by $h=x_1-x_0$, $f_0=f(x_0,y_0)$, $x_{1/2}=x_0+h/2$, $x_{3/2}=x_1+h/2$ *etc.*

Define $\tilde{y}_{1/2} = y_0 + \dfrac{h}{2} f_0$ *i.e.* extrapolate using Euler method to $x_{1/2}$

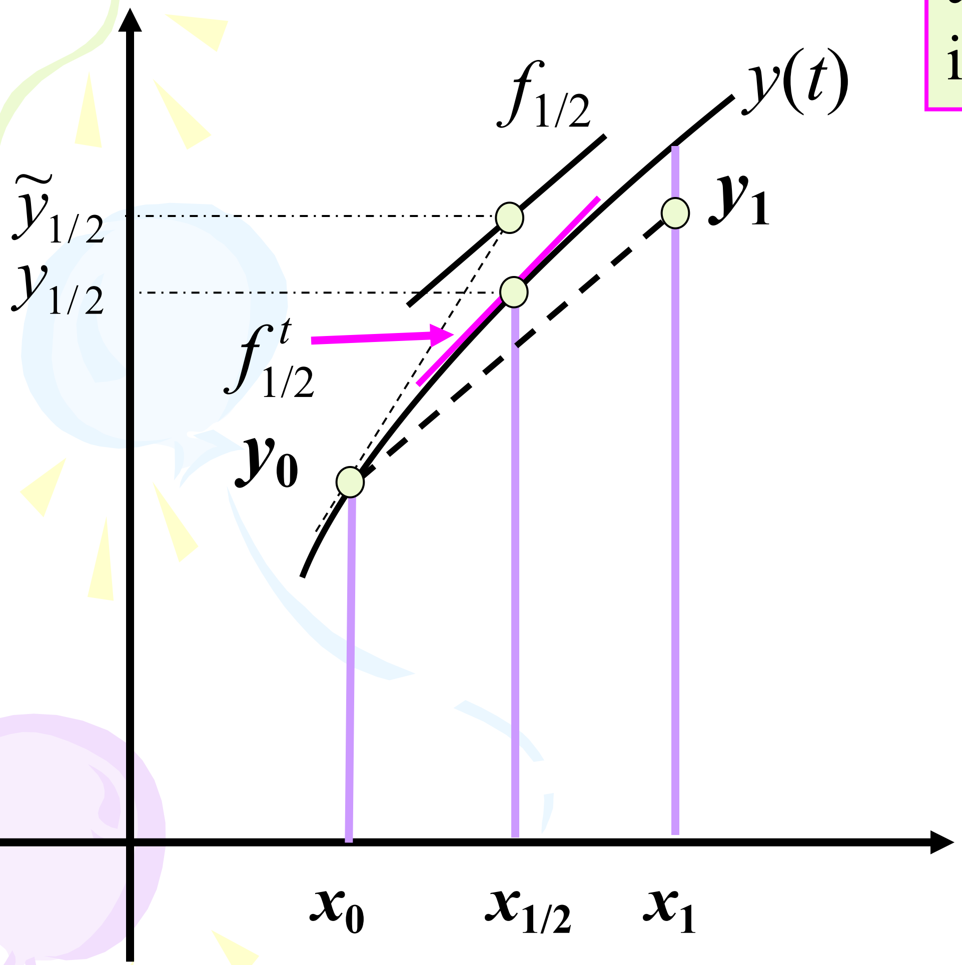
Then set $y_1 = y_0 + hf(x_{1/2},\tilde{y}_{1/2}) \equiv y_0 + hf_{1/2}$ *i.e.* integrate full step

Repeat extrapolation on half step :

Define $\tilde{y}_{3/2} = y_1 + \dfrac{h}{2} f(x_1, y_1) \equiv y_1 + \dfrac{h}{2} f_1$

Repeat integration : $y_2 = y_1 + hf(x_{3/2},\tilde{y}_{3/2}) \equiv y_1 + hf_{3/2}$ *etc...*

Modified Euler Method graphically



In this method the slope is estimated at the mid-point and the $y(x)$ is integrated forward using that slope.

Notice that at the predicted $\tilde{y}_{1/2}$ the slope $f_{1/2}$ is not necessarily equal to the true derivative $(f^t_{1/2})$ at the true y midpoint.
This is simply because $\tilde{y}_{1/2}$ does not have to be equal to $y_{1/2}$.
Even if we did know $f^t_{1/2}$ we would still not predict forward with perfect accuracy.

Can show that errors in this method are

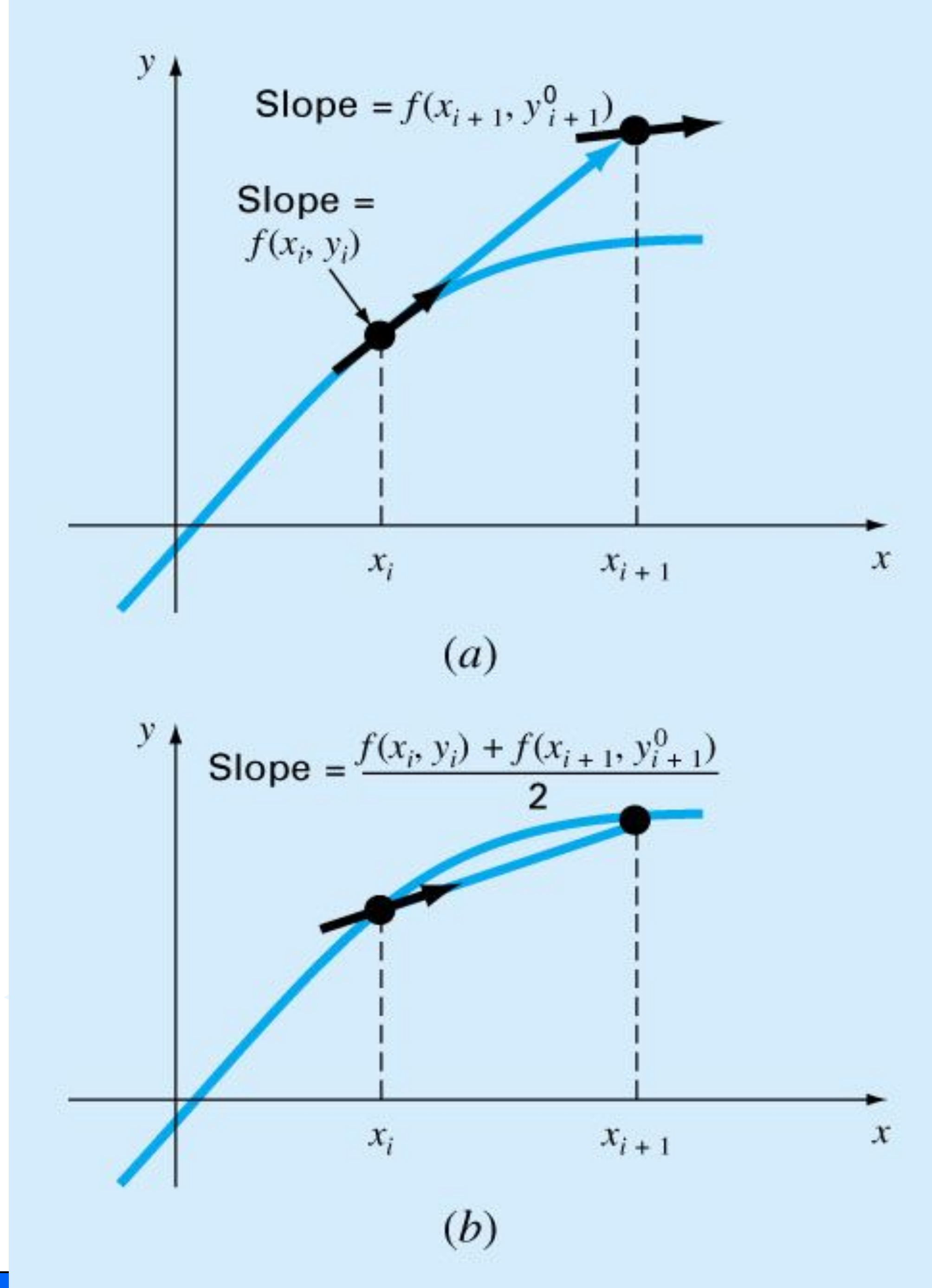
$$e_i \propto O(h^3) \quad \& \quad E_n \propto O(h^2)$$

Heun's Method

- One method to improve the estimate of the slope involves the determination of two derivatives for the interval:
  - At the initial point
  - At the end point
- The two derivatives are then averaged to obtain an improved estimate of the slope for the entire interval.

$$\text{Predictor}: \quad y_{i+1}^{0} = y_i + f(x_i, y_i)h$$

$$\text{Corrector}: \quad y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^{0})}{2} h$$


y
Slope = $f(x_{i+1}, y^0_{i+1})$
Slope = $f(x_i, y_i)$
x_i
x_{i+1}
x
(a)
y
Slope = $\frac{f(x_i, y_i) + f(x_{i+1}, y^0_{i+1})}{2}$
x_i
x_{i+1}
x
(b)

Improved Euler Method

- Similar in concept to the trapezoid rule in quadrature, by utilizing an average of the **start and end** point derivatives we can better approximate the change in *y* over the interval

$$\tilde{y}_1 = y_0 + hf(x_0, y_0), \quad \tilde{f}_1 = f(x_1, \tilde{y}_1) \quad \text{Prediction step}$$

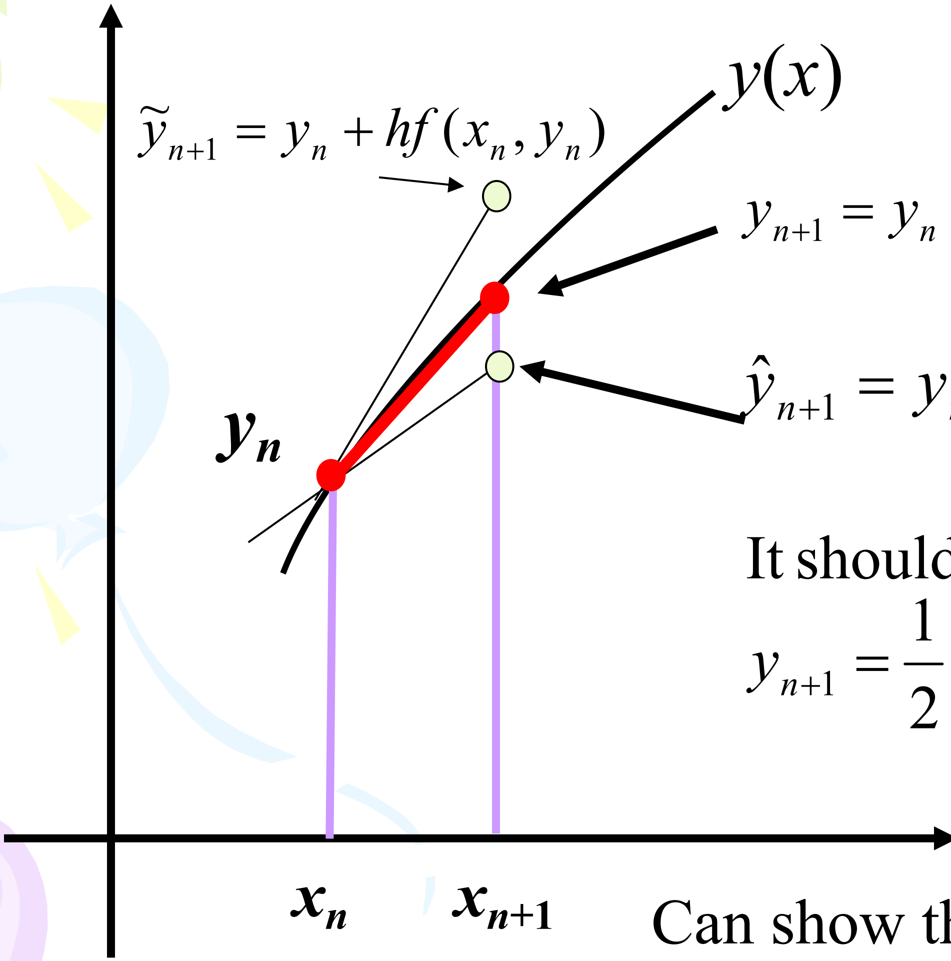
$$y_1 = y_0 + \frac{h}{2}\left(f_0 + \tilde{f}_1\right), \quad f_1 = f(x_1, y_1) \quad \text{Correction step}$$

$$\tilde{y}_2 = y_1 + hf_1, \quad \tilde{f}_2 = f(x_2, \tilde{y}_2) \quad \text{Prediction step}$$

$$y_2 = y_1 + \frac{h}{2}\left(f_1 + \tilde{f}_2\right), \quad f_2 = f(x_2, y_2) \quad \text{Correction step}$$

- This is the simplest example of so called "*Predictor-Corrector*" methods, (which includes Runge-Kutta methods)

Improved Euler method graphically



$$y_{n+1} = y_n + \frac{f(x_n, y_n) + f(x_{n+1}, \tilde{y}_{n+1})}{2} h$$

$$\hat{y}_{n+1} = y_n + f(x_{n+1}, \tilde{y}_{n+1})h$$

It should be clear that

$$y_{n+1} = \frac{1}{2}(\tilde{y}_{n+1} + \hat{y}_{n+1})$$

Can show that errors in this method are also

$$e_i \propto O(h^3) \quad \mathrm{E_n} \propto O(h^2)$$

Next lecture

- Continue to ODE solvers

Homework 12：05/29/2019

Problem 1: Let's compare solutions of the following system:

$$y' = 1 - x + 4y, y(0) = 1$$

a) Euler
b) Improved Euler
c) For the both methods, can we reach the error of 10^{-12} or higher? Please use data and formula answer it? (maybe some figs?)

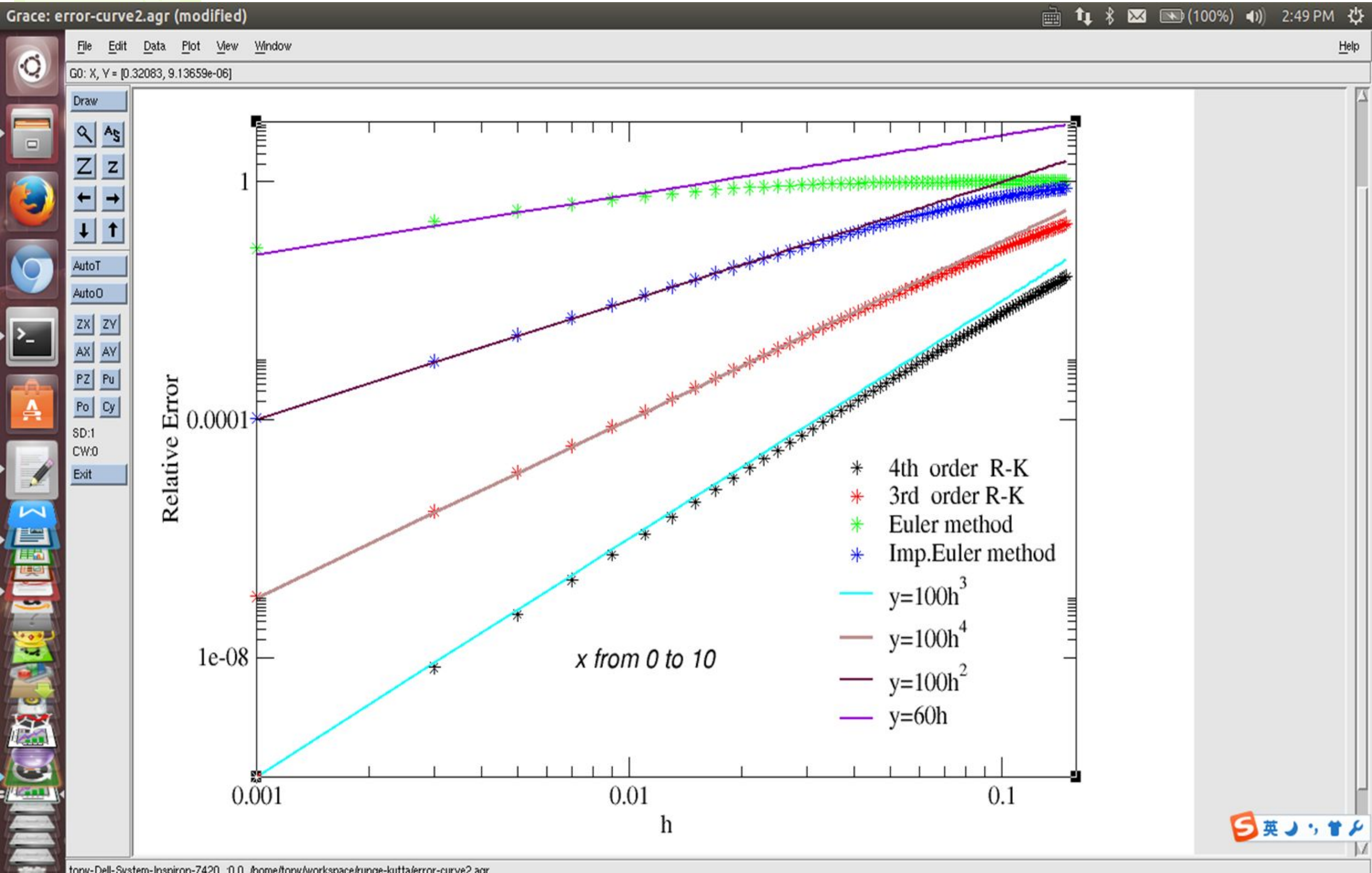
Hints:

1)Choose enough number of the step h, and fit the relative error E_r with h. For example: for Improved Euler, we should get

$$\mathrm{E_r} \propto O(h^2)$$

2) Can we consider the round error?

Thanks Tony (my student)



Problem 2: Difference Errors: Even when we can find the value of $f(x)$ for any value of x the forward difference can still be more accurate than the central difference for sufficiently large h. For what values of h will the approximation error on the forward difference be smaller than on the central difference?

Problem 3: Radioactive Decays: This problem is a straightforward application of a forward difference to numerically solve a differential equation. Given N(t) radioactive nuclei, they will decay randomly according to the following

$$\frac{dN}{dt} = -\frac{N(t)}{\tau}$$

By replacing dN/dt with **forward difference** $(N(t+h)-N(t))/h$, one obtains a numerical solution for $N(t+h)$. Given initial conditions (i.e. $N(t=0)$), one can obtain numerical values of $N(t)$ for all later times. This differential equation can be solved analytically as $N(t) = N(0)\exp(-t/\tau)$, where $N(0)$ is the initial number (or fraction) of radioactive nuclei. This solution allows one to compare our numerical results with the exact solution.

a) Write a program to numerically solve for the time dependence $N(t)$ from $0.0\ s \le t \le 15.0$ s assuming $N(0) = 100\%$ and $\tau = 2\ s$. Do this for the following values of h: 1.0s, 0.1s, and 0.01s. Graphically compare your results to the exact solution as a function of time. Also study the accuracy by plotting the fractional error vs. t. Overlay on one figure the graphs for the different values of h.

b) Using $h = 0.01\ s$, write another program to plot the time dependence of $N(t)$ for $\tau = 5.0s$, $3.0s$, $1.0s$, $0.1s$, and $0.01\ s$.

- Briefly discuss the accuracy of your results. If there are any problems explain.

c) Consider a system of a parent nucleus, ***P***, and a daughter nucleus, ***D*** both radioactive. The coupled equations which describe their decays are as follows:

$$\frac{dN_p}{dt} = -\frac{N_p(t)}{\tau_p} \qquad \frac{dN_D}{dt} = \frac{N_p(t)}{\tau_p} - \frac{N_D(t)}{\tau_D}$$

Write a program to numerically solve the above coupled equations and plot the time dependence of N_P and N_D for $\tau_P = 2.0s$ and $\tau_D = 0.02s$, $2.0s$ and $200.0s$. Assume you start out with 100% parent nuclei and no daughter nuclei. Graph all results overlaid on one figure.

- Qualitatively explain the behavior of N_D for situations in which $\tau_P \gg \tau_D$, $\tau_P \approx \tau_D$, and $\tau_P \ll \tau_D$.