Numerical Methods for Ordinary Differential Equations

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Ordinary Differential Equations

$$F\left(y, \frac{d}{dt} y(t), \frac{d^2}{dt^2} y(t), \ldots, \frac{d^n}{dt^n} y(t) \right) = 0$$

- **Ordinary:** only one independent variable
- **Differential:** unknown functions enter into the equation through its derivatives
- **Order:** highest derivative in F
- **Degree:** exponent of the highest derivative

$$\text{Example:} \left(\frac{d^2}{dt^2} y(t) \right)^3 - y(t) = 0$$

What is Solution of ODE?

$$y = y(t)$$

- **A problem involving ODE is not completely specified by its equation**
- **ODE has to be supplemented with boundary conditions:**

  - **Initial value problem:** y is given at some starting value t_i, and it is desired to find y at some final points t_f or at some discrete list of points (for example, at tabulated intervals).

  - **Two point bondary value problem:** Boundary conditions are specified at more than one t ; typically some of the conditions will be specified at t_i and some at t_f.

What is Numerical Solution to the Initial Value Problem?

$$\frac{dy(t)}{dt} = f\left(t, y(t)\right);\ y(t_0) = y_0$$

- A numerical solution to this problem generates sequence of values for the independent variable

$$t_1, t_2, \ldots, t_n$$

and a corresponding sequence of values of the dependent variable

$$y_1, y_2, \ldots, y_n$$

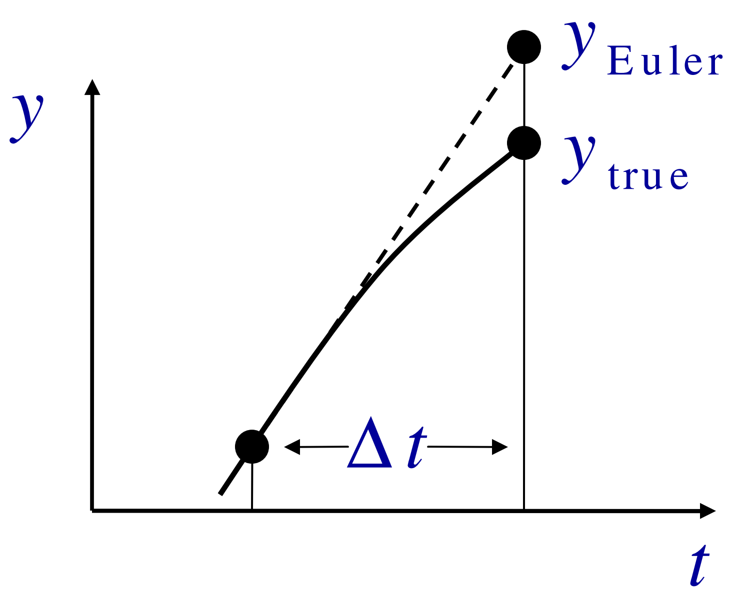
so that each y_n **approximates** solution at t_n :

$$y(t_n) \approx y_n, \quad n = 0, 1, \ldots$$

Euler Metod

- All finite difference methods start from the same conceptual idea: Add small increments to your function corresponding to derivatives (right-hand side of the equations) multiplied by the stepsize.

- Euler method is an implementation of this idea in the simplest and most direct form.



Single-Step Forward Propagation

Euler Algorithm for First-Order ODE

$$\frac{dy}{dt} = f(t, y) \longrightarrow \Delta y = f(t, y)\Delta t$$

initialize $t_1, y_1 \equiv y(t_1)$

do while $i \le n$

$$y_{i+1} = y_i + f(t_i, y)\Delta t$$

$$t_{i+1} = t_i + \Delta t$$

end do

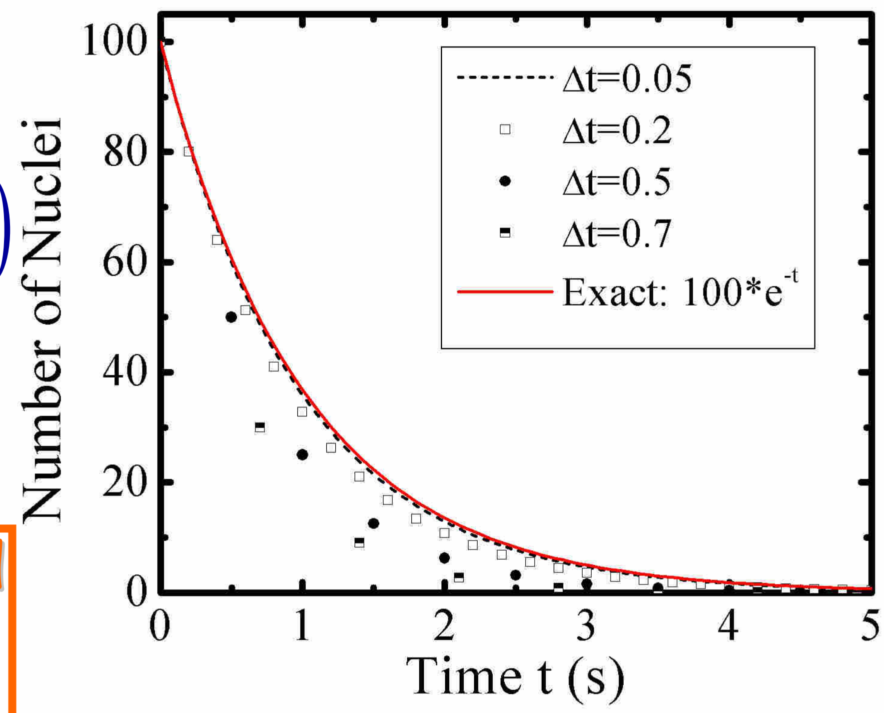
Step Size Effects in Radioactive Decay

Analytics: $$\frac{dN_U}{dt} = -\frac{N_U}{\tau} \Rightarrow N_U = N_U(t=0)e^{-\frac{t}{\tau}}$$

Numerics (Euler):

$$N_U(\Delta t) = N_U(0) + \frac{dN_U}{dt}\Delta t + O\left((\Delta t)^2\right)$$

$$N_{i+1} \approx N_i - \frac{N_i}{\tau}\Delta t$$



Numerical solution will depend on the step size

Δt

Stability of Euler Algorithm

- Step size if often limited by the **stability criterion**:

$$\frac{dy}{dt} = -ay \Rightarrow \; y(0) = 1, \; y = e^{-at}$$

After n Euler steps of size Δt:

$$y_{n+1} = y_n - ay_n \Delta t \Rightarrow \; y_n = (1 - a\Delta t)^n$$

Approximate solution will decay monotonically only if Δt is small enough:

$$\Delta t \le \Delta t_{\max} \equiv \frac{1}{a}$$

- For a single decaying exponential-like solution (i.e. if there is only one first order equation) the existence of a stability criterion is not a problem because Δt has to be small for the reasons of **accuracy**.

Accuracy: Discretization and Roundoff Errors

Integrate over interval: $L = t_f - t_0 \Rightarrow$ Full Error: $Ch^p + \frac{L\varepsilon}{h}$

Number of steps for roundoff error to be comparable with the discretization error: $N \approx L\left(\frac{C}{L\varepsilon}\right)^{\frac{1}{p+1}}$

- **Local:**

$$\left.\begin{aligned} \frac{du}{dt} &= f(u_n, t_n) \\ u_n(t_n) &= y_n \end{aligned}\right\} \Rightarrow LE_n = y_{n+1} - u_{n+1}(t_{n+1})$$

$$f = f(t) \Rightarrow y(t) = \int_{t_0}^{t_N} f(\tau)d\tau \approx \sum_{n=0}^{N-1} h_n f(t_n)$$

$$LE_n = h_n f(t_n) - \int_{t_n}^{t_{n+1}} f(\tau)d\tau$$

- **Global:**

$$GE_n = y_n - y(t_n)$$

$$GE_n = \sum_{n=0}^{N-1} h_n f(t_n) - \int_{t_0}^{t_N} f(\tau)d\tau$$

$$GE_n = \sum_{n=0}^{N-1} LE_n$$

- Method is of order **n** iff:

$$LE_n = O(h^{n+1}) \Leftrightarrow |LE_n| \le Ch^{n+1}$$

$$h = t_{n+1} - t_n \equiv \Delta t$$

Global Discretization Error Example

- Suppose we want to find the solution over the interval $[0,T]$ →Divide the interval into *n* equal steps so that $\Delta t = T/n$

$$y(T) = e^{-aT}, \quad y_n = \left(1 - a\frac{T}{n}\right)^n$$

$$y(T) = 1 - aT + \frac{(aT)^2}{2!} - \frac{(aT)^3}{3!} + \ldots$$

$$y_n = 1 - aT + \frac{n(n-1)}{n^2}\frac{(aT)^2}{2!} - \frac{n(n-1)(n-2)}{n^3}\frac{(aT)^3}{3!} + \ldots$$

$$y(T) - y_n = \frac{1}{n}\frac{(aT)^2}{2!} - \frac{3}{n}\frac{(aT)^2}{3!} + \ldots + O\left(\frac{1}{n^2}\right) \sim \frac{a\Delta t}{2} aTe^{-aT}$$

- This is a measure of the global truncation error, i.e., the error over a fixed range in *t*.
- It is proportional to the first power of the step size and hence the Euler method is a first order method (do not confuse this with the fact that we are applying it in this case to a first order equation).

Reducing Higher Order ODE to System of First Order ODE

- Solve **higher order ODEs** by splitting them into sets of **first order equations**:

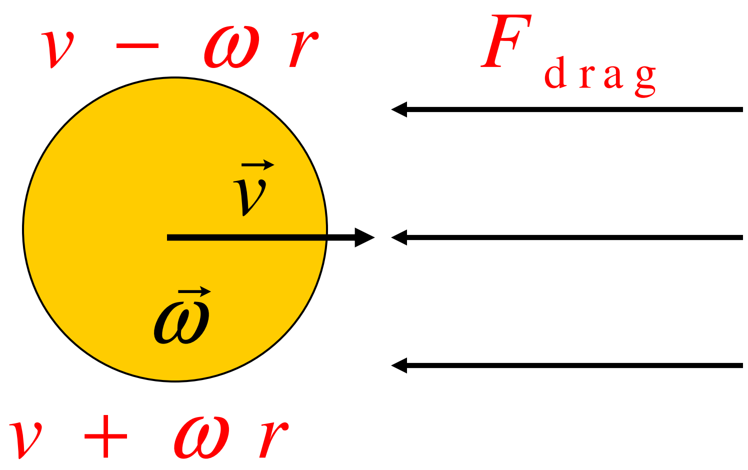
$$\frac{d^2y}{dt^2} + p(t)\frac{dy}{dt} + q(t)y = g(t)$$

$$z = \frac{dy}{dt} \Rightarrow \begin{cases} \dfrac{dz}{dt} = g(t) - p(t)z - q(t)y \\ \dfrac{dy}{dt} = z \end{cases}$$

There is no unique way to do this:

$$z = \frac{dy}{dt} + p(t)y \Rightarrow \begin{cases} \dfrac{dz}{dt} = g(t) + \left(\dfrac{dp(t)}{dt} - q(t)\right)y \\ \dfrac{dy}{dt} = z - p(t)y \end{cases}$$

Example: Realistic Motion of Baseball



$$m\frac{d^2\vec{r}}{dt^2} = m\vec{g} - B_2 v^2 \frac{\vec{v}}{v} + S_0 \vec{v} \times \vec{\omega}$$

initialize $t_1, \vec{y}(t_1)$

do while $i \le n$

$$\vec{y}_{i+1} = \vec{y}_i + f(t_i, \vec{y}_i)\Delta t$$

$$t_{i+1} = t_i + \Delta t$$

end do

$\Leftrightarrow$

$$x_{i+1} = x_i + v_i^x \Delta t$$

$$v_{i+1}^x = v_i^x - \frac{B_2}{m} v v_i^x \Delta t$$

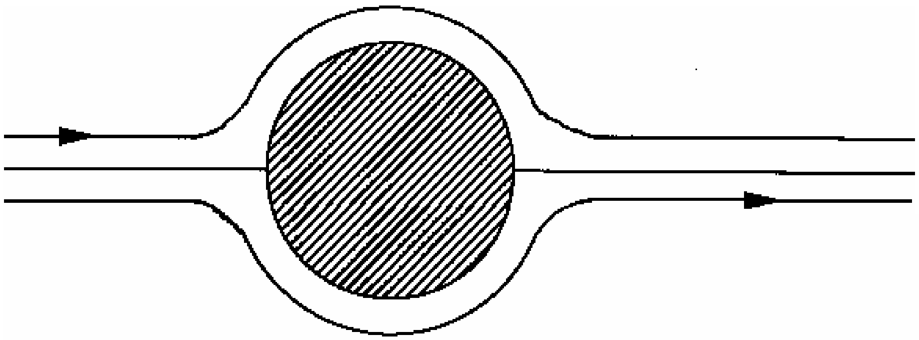
$$y_{i+1} = y_i + v_i^y \Delta t$$

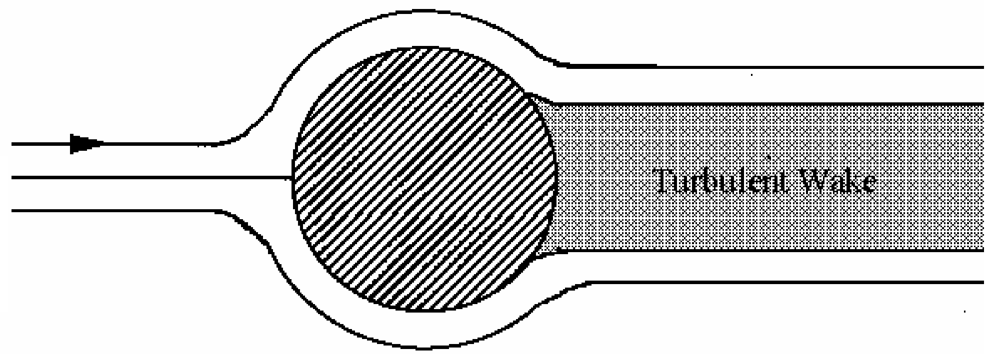
$$v_{i+1}^y = v_i^y - g\Delta t$$

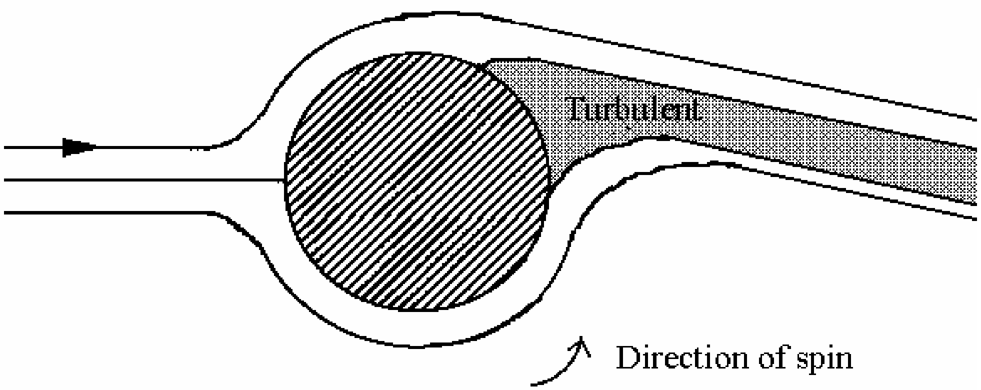
$$z_{i+1} = z_i + v_i^z \Delta t$$

$$v_{i+1}^z = v_i^z - \frac{S_0 v_x \omega}{m} \Delta t$$

More Realistic Modeling of Air Flow







ODE of Linear Harmonic Oscillator

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

$$\text{for small } \theta \Rightarrow \sin\theta \approx \theta$$

$$\frac{d^2\theta}{dt^2} + \frac{g}{l}\theta = 0, \quad \Omega = \sqrt{\frac{g}{l}}$$

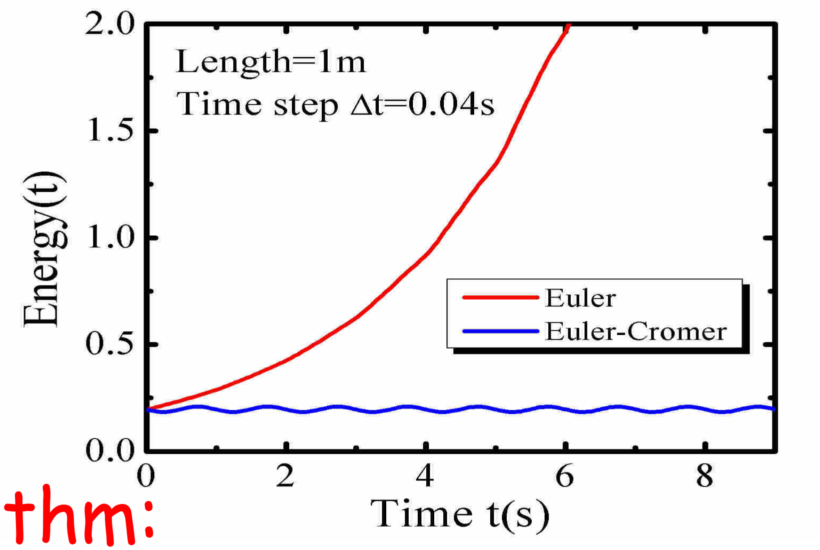
$$E_{total} = \frac{1}{2}ml^2\left(\frac{d\theta}{dt}\right)^2 + \frac{1}{2}mgl\theta^2 \text{ must be conserved!}$$

Euler Method for Linear Harmonic Oscillator

- Switch to **dimensionless** quantities:

$$\frac{d^2\theta}{dt^2}+\theta=0 \Rightarrow \theta=\theta_0\sin(\Omega t+\phi)$$

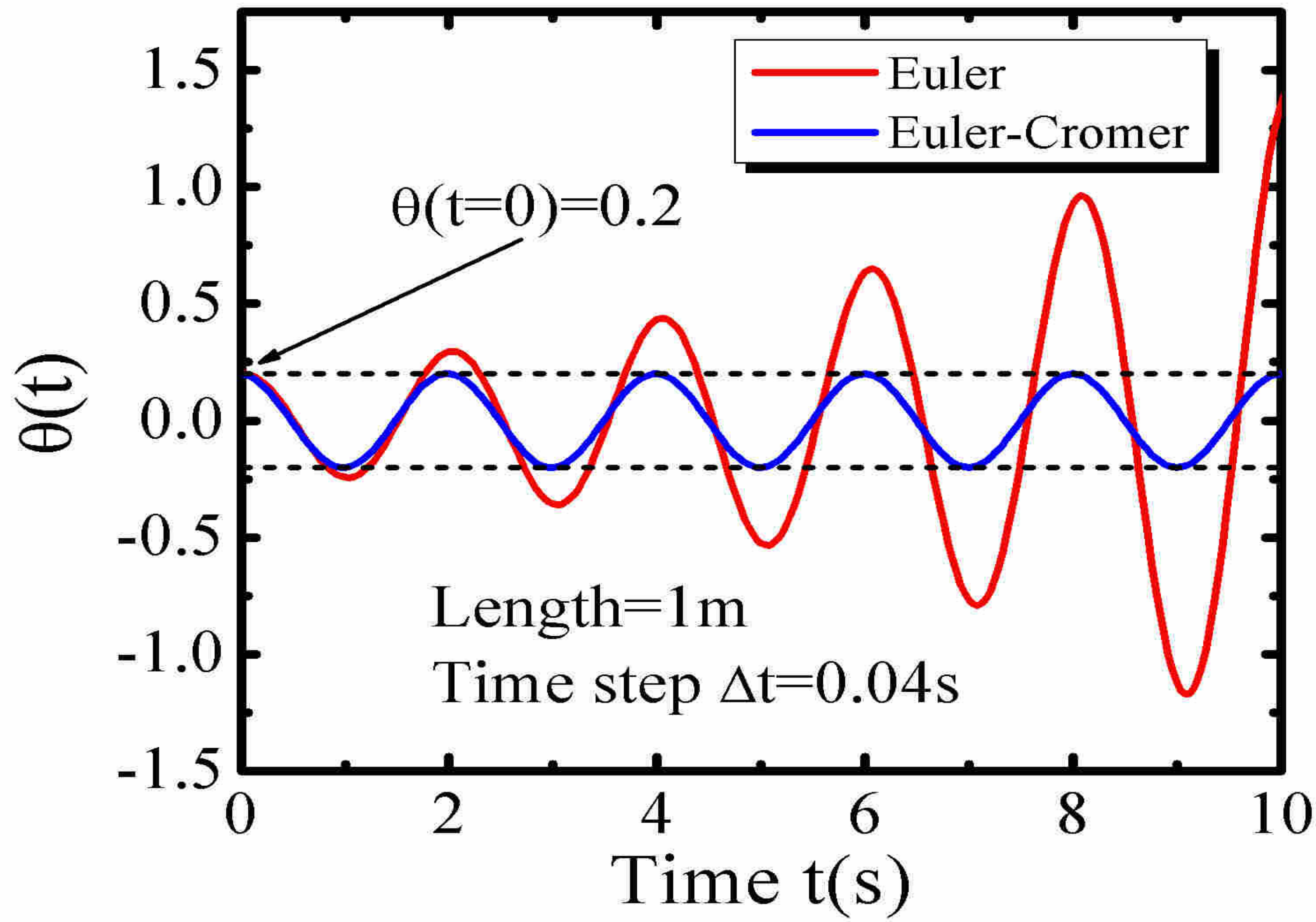
$$E_{total}=\frac{1}{2}\left(\frac{d\theta}{dt}\right)^2+\frac{1}{2}\theta^2$$



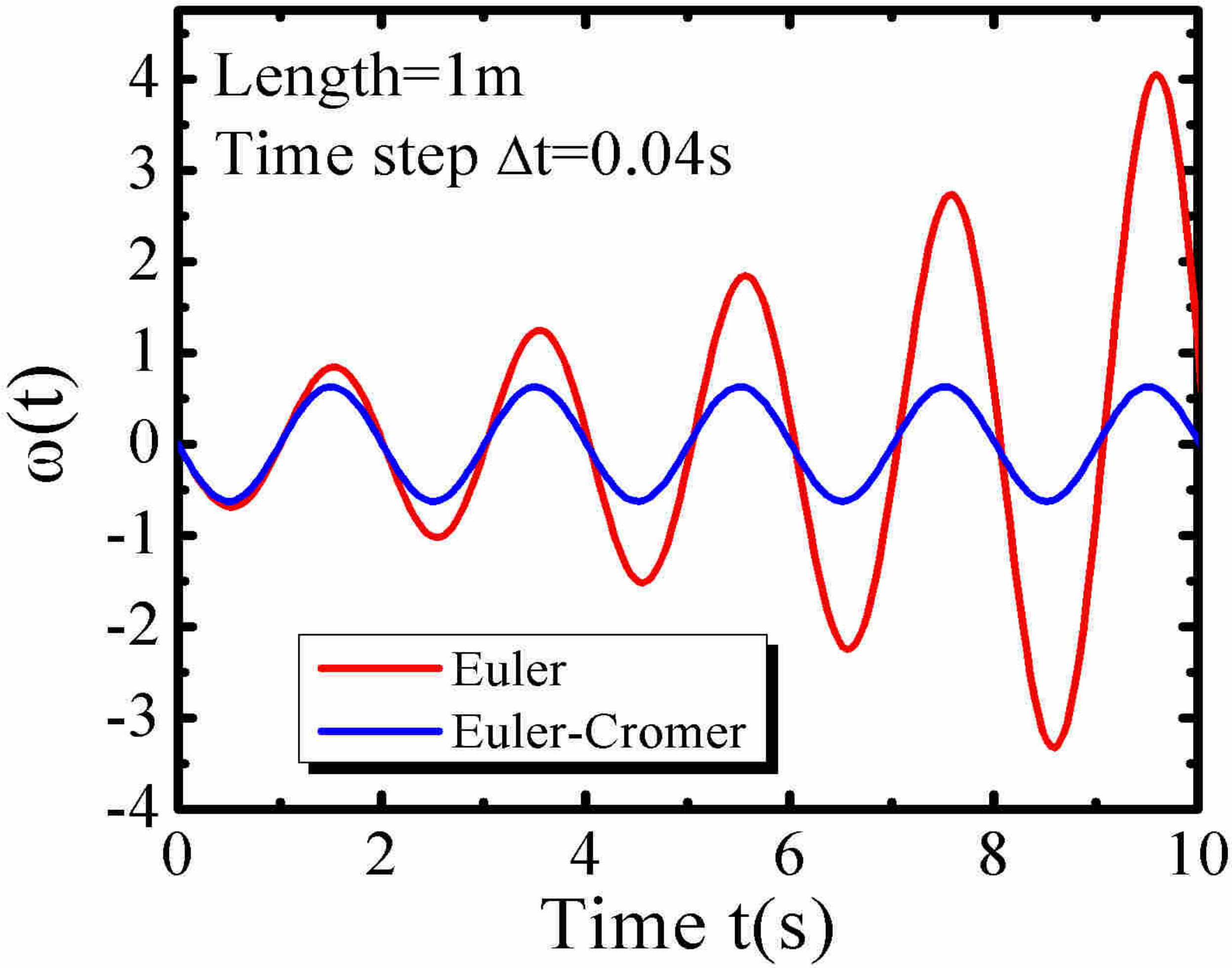
- Euler discretization algorithm:

$$\left.\begin{aligned}\omega_{n+1}&=\omega_n-\theta_n\Delta t\\ \theta_{n+1}&=\theta_n+\omega_n\Delta t\\ t_{n+1}&=t_n+\Delta t\end{aligned}\right\}\Rightarrow\left\{\begin{aligned}E_{total}&=\frac{1}{2}\left(\omega^2{}_{n+1}+\theta^2{}_{n+1}\right)\\ E_{total}&=E_n\left(1+\Delta t^2\right)\end{aligned}\right.$$

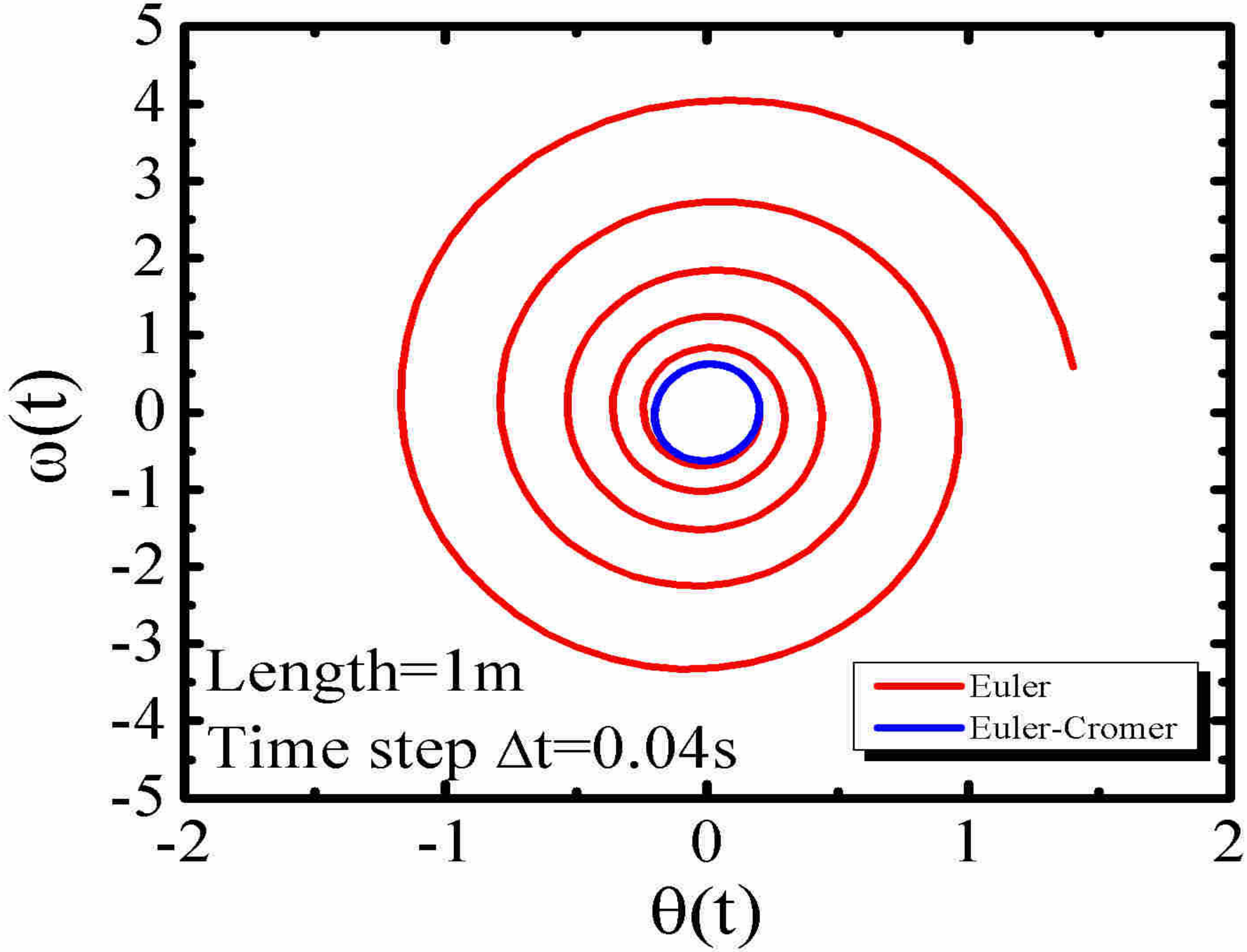
Euler Fails on $\theta(t)$



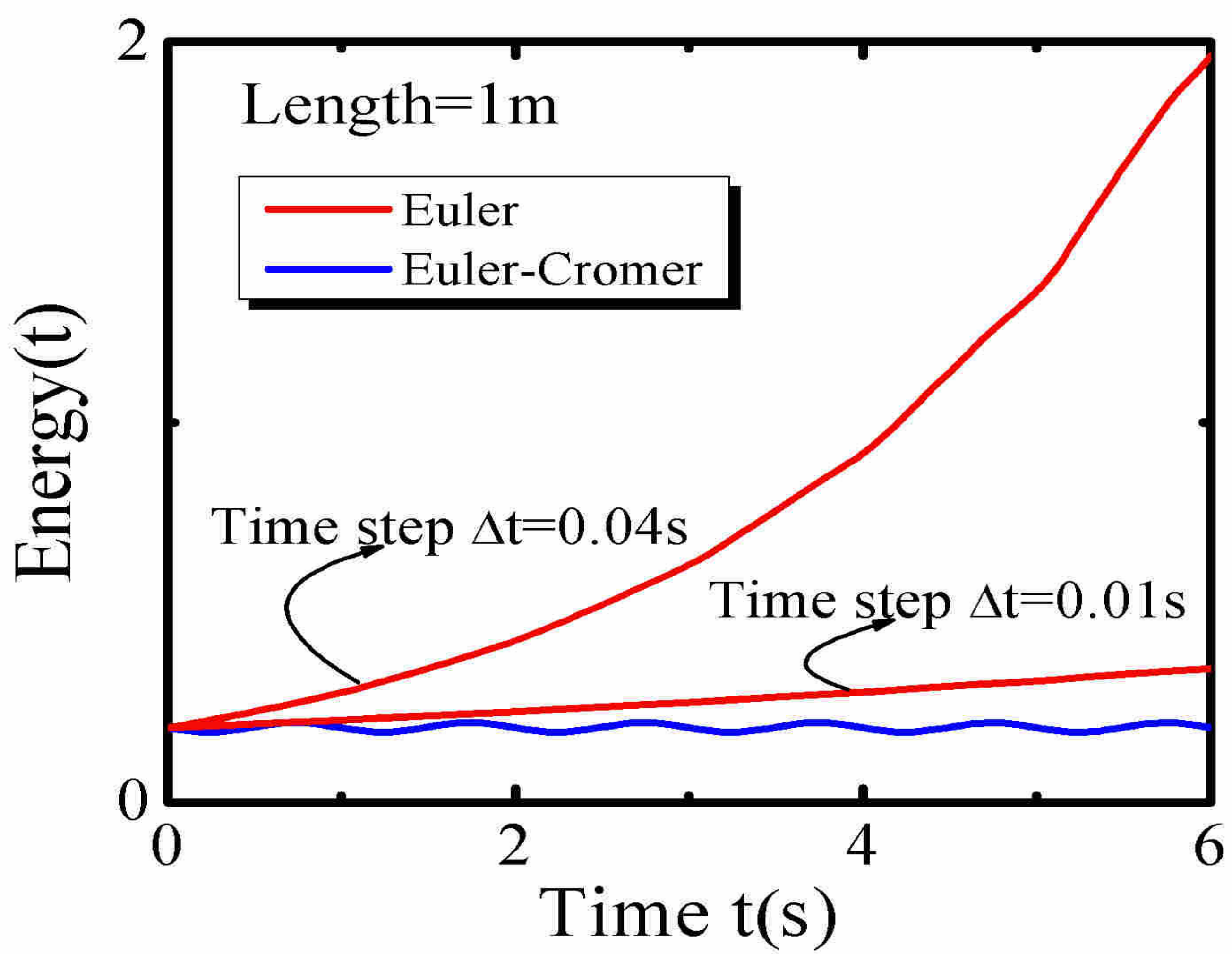
Euler Fails on $\omega(t)$



Euler Fails on Phase Space Trajectory



Can We Resurrect Euler by Using Smaller Step Size?



Cromer Fixed Euler Method for LHO

$$\omega_n \to \omega_{n+1} \Rightarrow \begin{cases} \omega_{n+1} = \omega_n - \theta_n \Delta t \\ \theta_{n+1} = \theta_n + \omega_{n+1} \Delta t \\ t_{n+1} = t_n + \Delta t \end{cases}$$

- Apparently trivial trick, but:

$$E_{n+1} = E_n + \frac{1}{2}\left(\omega_n^2 - \theta_n^2\right)\Delta t^2 + O\left(\Delta t^3\right)$$

$$\underbrace{\theta = \theta_0 \sin(t - t_0), \quad \omega = \theta_0 \cos(t - t_0)}_{\left\langle \omega^2 - \theta^2 = \theta_0^2 \cos 2(t - t_0) \right\rangle_{over\ a\ period} = 0}$$

From Euler to Higher Order Algorithms

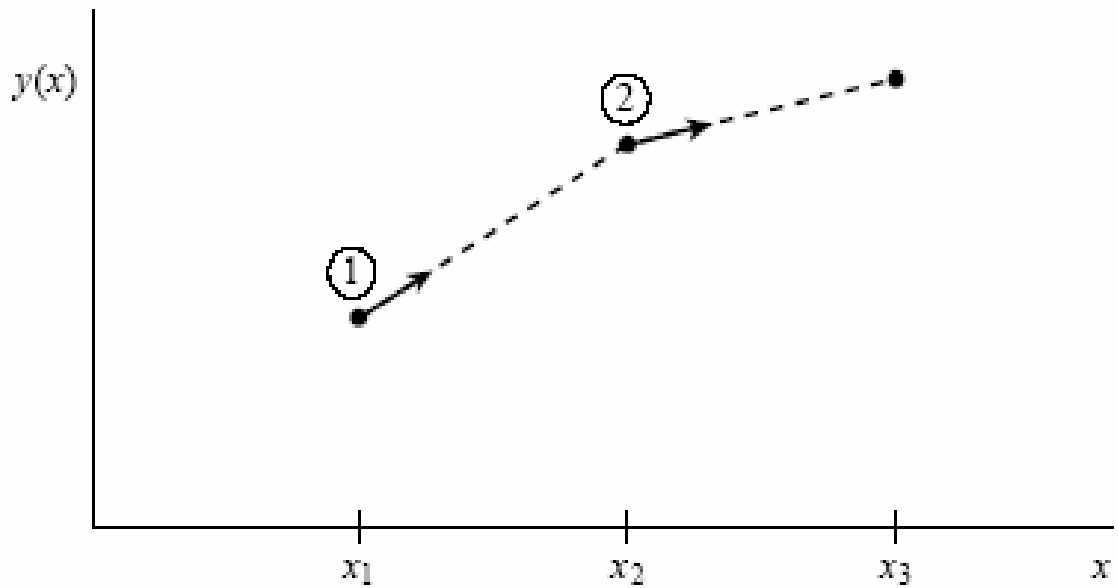


Figure 16.1.1. Euler's method. In this simplest (and least accurate) method for integrating an ODE, the derivative at the starting point of each interval is extrapolated to find the next function value. The method has first-order accuracy.

$$y_{n+1} = y_n + f(t_n, y_n)$$
$$t_{n+1} = t_n + h$$

vs.

Mean value theorem

$$y(t+\Delta t) \overset{exact}{=} y(t) + dy/dt\big|_{t_m} \Delta t$$

Midpoint Method: Second Order Runge-Kutta

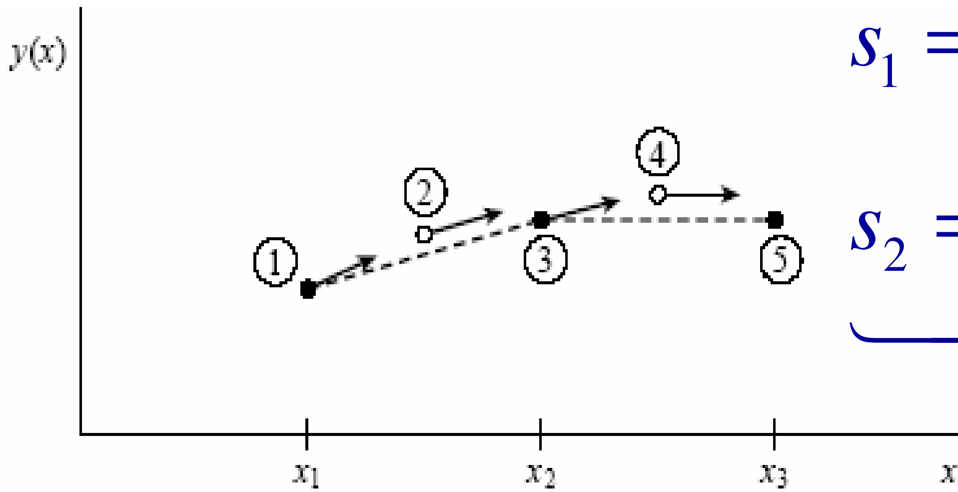


Figure 16.1.2. Midpoint method. Second-order accuracy is obtained by using the initial derivative at each step to find a point halfway across the interval, then using the midpoint derivative across the full width of the interval. In the figure, filled dots represent final function values, while open dots represent function values that are discarded once their derivatives have been calculated and used.

$$s_1 = f(t_n, y_n)$$

$$s_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} s_1\right)$$

$$y_{n+1} = y_n + h s_2 + O(h^3)$$

$$t_{n+1} = t_n + h$$

Classical Runge-Kutta

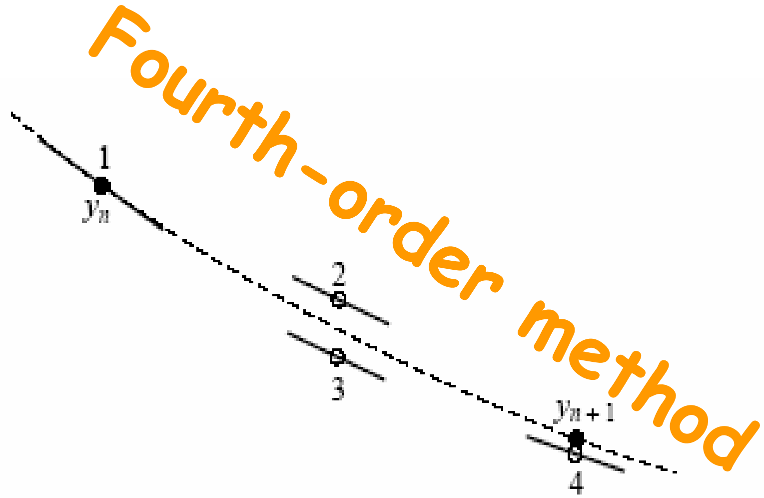


Figure 16.1.3. Fourth-order Runge-Kutta method. In each step the derivative is evaluated four times: once at the initial point, twice at trial midpoints, and once at a trial endpoint. From these derivatives the final function value (shown as a filled dot) is calculated. (See text for details.)

$$s_1 = f(t_n, y_n)$$

$$s_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} s_1\right)$$

$$s_3 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} s_2\right)$$

$$s_4 = f(t_n + h, y_n + h s_3)$$

$$y_{n+1} = y_n + \frac{h}{6}(s_1 + 2s_2 + 2s_3 + s_4) + O(h^5)$$

$$t_{n+1} = t_n + h$$

Classical Runge-Kutta F90 Subroutine

```
SUBROUTINE rk4(y,dydx,n,x,h,yout,derivs)
INTEGER n,NMAX
REAL h,x,dydx(n),y(n),yout(n)
EXTERNAL derivs
PARAMETER (NMAX=50)          Set to the maximum number of functions.
```

Given values for the variables y(1:n) and their derivatives dydx(1:n) known at x, use the fourth-order Runge-Kutta method to advance the solution over an interval h and return the incremented variables as yout(1:n), which need not be a distinct array from y. The user supplies the subroutine derivs(x,y,dydx), which returns derivatives dydx at x.

```
INTEGER i
REAL h6,hh,xh,dym(NMAX),dyt(NMAX),yt(NMAX)
hh=h*0.5
h6=h/6.
xh=x+hh
do 11 i=1,n                       First step.
    yt(i)=y(i)+hh*dydx(i)
enddo 11
call derivs(xh,yt,dyt)            Second step.
do 12 i=1,n
    yt(i)=y(i)+hh*dyt(i)
enddo 12
call derivs(xh,yt,dym)            Third step.
do 13 i=1,n
    yt(i)=y(i)+h*dym(i)
    dym(i)=dyt(i)+dym(i)
enddo 13
call derivs(x+h,yt,dyt)           Fourth step.
do 14 i=1,n                       Accumulate increments with proper weights.
    yout(i)=y(i)+h6*(dydx(i)+dyt(i)+2.*dym(i))
enddo 14
return
END
```

General Single-Step Methods

- Each of the k stages of the algorithm computes slope s_i by evaluating $f(t, y)$ for a particular value of t and a value of y obtained by taking linear combinations of the previous slopes:

$$s_i = f(t_n + \alpha_i h, y_n + h \sum_{j=1}^{i-1} \beta_{i,j} s_j), i = 1, \dots, k$$

- The proposed step is also a linear combination of the slopes:

$$y_{n+1} = y_n + h \sum_{i=1}^{k} \gamma_i s_i$$

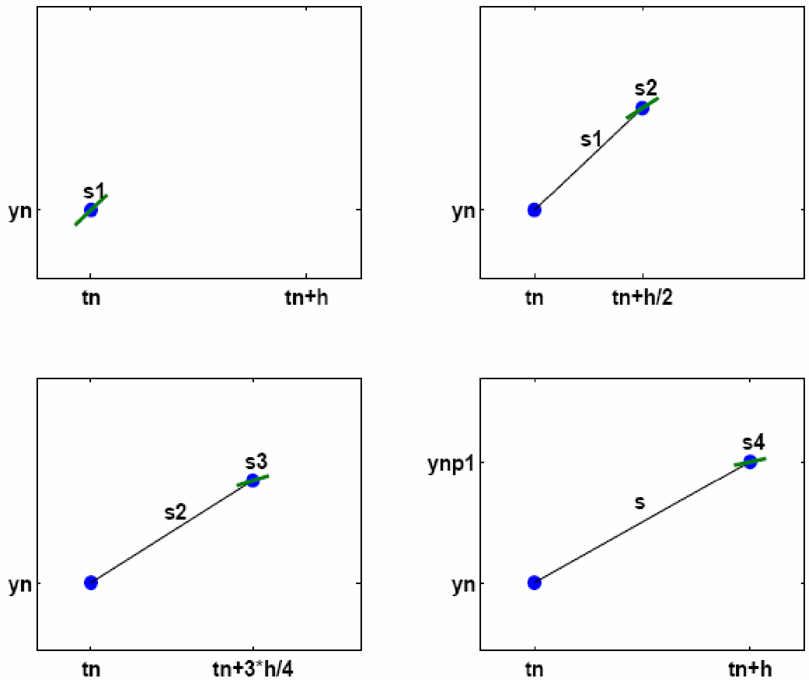
- Error is estimated from yet another linear combination of the slopes:

$$e_{n+1} = h \sum_{i=1}^{k} \delta_i s_i$$

- The parameters are determined by matching terms in the Taylor series expansion of the slopes → **the order** of the method is the exponent of the smallest power of h that cannot be matched.

- In MATLAB ODE numerical routines are named as odennxx, where nn indicates the order and xx is some special feature of the method.

Example: MATLAB ode23 Function (Bogacki and Shampine BS23 Algorithm)



$$s_1 = f(t_n, y_n)$$

$$s_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} s_1\right)$$

$$s_3 = f\left(t_n + \frac{3}{4} h, y_n + \frac{3}{4} h s_2\right)$$

$$y_{n+1} = y_n + \frac{h}{9}(2s_1 + 3s_2 + 4s_3)$$

$$t_{n+1} = t_n + h; \; s_4 = f(t_{n+1}, y_{n+1})$$

$$e_{n+1} = \frac{h}{72}(-5s_1 + 6s_2 + 8s_3 - 9s_4)$$

Beyond Runge-Kutta Methods

- **Runge-Kutta methods** propagates a solution over an interval by combining the information from several Euler-style steps (each involving one evaluation of the right-hand side f's), and then using the information obtained to match Taylor series expansion up to some higher order.
- **Richardson extrapolation** method used the powerful idea of extrapolating computed result to the value that would have been obtained if the stepsize had been very much smaller than it actually was. In particular, extrapolation to zero stepsize is the desired goal – implemented by **Burlich-Stoer algorithm**.
- **Predictor-corrector methods** store the solution along the way, and use those results to extrapolate the solution one step advanced; they correct the extrapolation using derivative information at the new point.

Stiff Systems of Differential Equations

❑**Stiffness** arises in systems of ODE where there are two or more very different scales of the independent variable:

$$\left.\begin{array}{l}\dfrac{du}{dt}=998u+1998v, \quad \dfrac{dv}{dt}=-999u-1999v \\ u(0)=1, \quad v(0)=0\end{array}\right\} \Rightarrow \begin{cases}u=2y-z\\ v=-y+z\end{cases} \Rightarrow \begin{cases}u=2e^{-t}-e^{-1000t}\\ v=-e^{-t}+e^{-1000t}\end{cases}$$

❑Follow the variation in the solution on the shortest length scale to maintain stability of the integration even though accuracy requirements allow for a much larger step size → use implicit methods:

$$y'=-cy, c>0 \overset{\text{explicit}}{\Rightarrow} y_{n+1}=y_n+\Delta t y'_n=(1-c\Delta t)y_n$$

$$\Delta t>2/c \Leftrightarrow |y_n| \to \infty \text{ as } n \to \infty$$

$$y'=-cy \overset{\text{implicit}}{\Rightarrow} y_{n+1}=y_n+\Delta t y'_{n+1} \Rightarrow y_{n+1}=\frac{y_n}{1+c\Delta t}$$

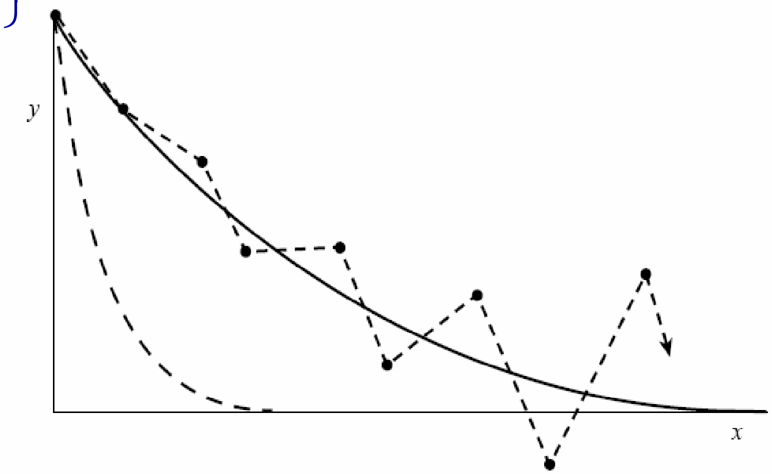


Figure 16.6.1. Example of an instability encountered in integrating a stiff equation (schematic). Here it is supposed that the equation has two solutions, shown as solid and dashed lines. Although the initial conditions are such as to give the solid solution, the stability of the integration (shown as the unstable dotted sequence of segments) is determined by the more rapidly varying dashed solution, even after that solution has effectively died away to zero. Implicit integration methods are the cure.

Solutions to Stiffness Beyond Implicit Euler

To improve higher-order (than Euler, which is first-order) methods use:

- **Generalizations of Runge-Kutta methods** → Rosenbrock methods and Kaps-Rentrop methods.
- **Burlich-Stoer algorithm** generalized to Bader-Deuflhard semi-implicit extrapolation method.
- **Predictor-corrector methods** generalized to Gear backward differentiation method.