In the name of $\mathcal{GOD}$

Computational Physics

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Outline

- Fortran-90 Programming
- Numerical calculus
- Approximation of a function
- Numerical methods for matrices
- Ordinary differential equations
- Partial differential equations
- Monte Carlo simulations
- Molecular dynamics simulations

Ordinary differential equations

In general, we can classify ordinary differential equations into three major categories:

(1) initial-value problems, which involve time-dependent equations with given initial conditions;

(2) boundary-value problems, which involve differential equations with specified boundary conditions;

(3) eigenvalue problems, which involve solutions for selected parameters (eigenvalues) in the equations.

Initial-value problems

$$\begin{cases} \dfrac{dv}{dt} = \dfrac{f(x,\dot{x},t)}{m} \\ \dfrac{dx}{dt} = v \end{cases}, \qquad \begin{aligned} v(0) &= v_0 \\ x(0) &= x_0 \end{aligned}$$

The Euler methods

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

$y(t) \longrightarrow$ known

$y(t+\delta t) \longrightarrow$ unknown

$$y(t+\delta t) = y(t) + \delta t\left(\frac{dy}{dt}\right)_t + O(\delta t^2) \xrightarrow{\frac{dy}{dt}=f(y,t)} \boxed{y(t+\delta t) = y(t) + \delta t\ f(y(t),t)}$$

$$y(t),\ f(y(t),t) \rightarrow y(t+\delta t)$$

$$t_n = n\,\delta t$$

$$y(t_n) = y(n\,\delta t)$$

$$y(t_{n+1}) = y(t_n + \delta t) = y((n+1)\,\delta t)$$

$$y(0)$$

$$y(\delta t) = y(0) + \delta t\ f\,(y(0),0)$$

$$y(\delta t)$$

$$y(2\delta t) = y(\delta t) + \delta t\ f\,(y(\delta t),\delta t)$$

$$\vdots$$

$$y(n\delta t)$$

$$y((n+1)\delta t) = y(n\delta t) + \delta t\ f\,(y(n\delta t), n\delta t)$$

$$\vdots$$

$$\begin{cases} \dfrac{dv}{dt} = \dfrac{f(x,v,t)}{m} = a(x,v,t) \\ \dfrac{dx}{dt} = v \end{cases} , \qquad \begin{aligned} v(0) &= v_0 \\ x(0) &= x_0 \end{aligned}$$

$v(t) \longrightarrow$ known
$x(t) \longrightarrow$ known

$x(t+\delta t) \longrightarrow$ unknown
$v(t+\delta t) \longrightarrow$ unknown

$$v(t+\delta t) = v(t) + \delta t \left(\frac{dv}{dt}\right)_t + O(\delta t^2) \xrightarrow{\frac{dv}{dt}=a(x,v,t)} v(t+\delta t) = v(t) + \delta t\, a(y(t), v(t), t)$$

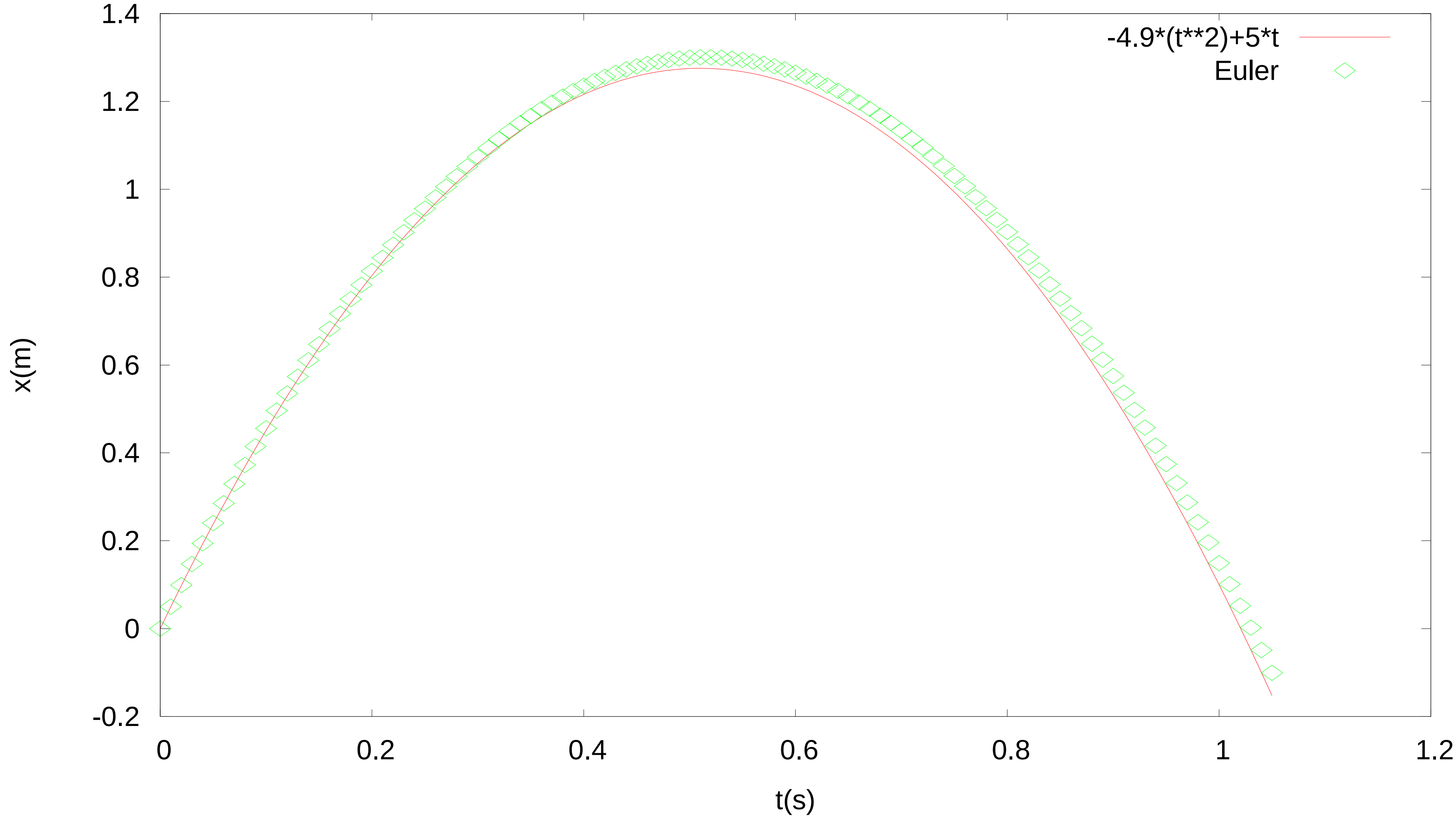
$$x(t+\delta t) = x(t) + \delta t \left(\frac{dx}{dt}\right)_t + O(\delta t^2) \xrightarrow{\frac{dx}{dt}=v(x,t)} x(t+\delta t) = x(t) + \delta t\, v(x(t), t)$$

$$v(\delta t) = v(0) + \delta t\, a(y(0), v(0), 0)$$
$$x(\delta t) = x(0) + \delta t\, v(x(0), 0)$$

$$v(2\delta t) = v(\delta t) + \delta t\, a(y(\delta t), v(\delta t), \delta t)$$
$$x(2\delta t) = x(\delta t) + \delta t\, v(x(\delta t), \delta t)$$

$$v(n\delta t + \delta t) = v(n\delta t) + \delta t\, a(y(n\delta t), v(n\delta t), n\delta t)$$
$$x(n\delta t + \delta t) = x(n\delta t) + \delta t\, v(x(n\delta t), n\delta t)$$

$$x(0) = 0 \quad , \quad v(0) = 5\,m/s$$



The Picard methods

$$\frac{dy}{dt} = f(y,t) \Rightarrow y_{i+1} = y_i + \int_{t_i}^{t_{i+1}} f(y,t)dt$$

use the rectangular approximation:

The Euler method

$$y_{i+1} = y_i + f(y_{i+1}, t_{i+1})\tau + O(\tau^2)$$

The Picard method

use the trapezoid rule:

$$y_{i+1} = y_i + \frac{f(y_{i+1}, t_{i+1}) + f(y_i, t_i)}{2}\tau + O(\tau^3)$$

The Picard methods

$$\begin{cases} \dfrac{dv}{dt} = \dfrac{f(x,v,t)}{m} = a(x,v,t) \\ \dfrac{dx}{dt} = v \end{cases} , \qquad \begin{array}{l} v(0) = v_0 \\ x(0) = x_0 \end{array}$$

$v(t) \longrightarrow$ known

$x(t) \longrightarrow$ known

$x(t+\delta t) \longrightarrow$ unknown

$v(t+\delta t) \longrightarrow$ unknown

Euler:

$$\boxed{v(t+\delta t) = v(t) + \delta t\, a(y(t), v(t), t)} \Rightarrow v(t+\delta t) \longrightarrow \text{known}$$

Picard:

$$\boxed{x(t+\delta t) = x(t) + \delta t \frac{v(t) + v(t+\delta t)}{2}} \Rightarrow x(t+\delta t) \longrightarrow \text{known}$$

Verlet algorithm

$$\begin{cases} x(t+\delta t) = x(t) + \delta t\,\dot{x}(t) + \dfrac{\delta t^2}{2!}\ddot{x}(t) + O(\delta t^3) & \text{①} \\ x(t-\delta t) = x(t) - \delta t\,\dot{x}(t) + \dfrac{\delta t^2}{2!}\ddot{x}(t) + O(\delta t^3) & \text{②} \end{cases}$$

$$\xrightarrow{\text{①} + \text{②}} x(t+\delta t) = 2x(t) - x(t-\delta t) + \delta t^2 a(t) + O(\delta t^4)$$

$$\xrightarrow{\text{①} - \text{②}} v(t) = \frac{x(t+\delta t) - x(t-\delta t)}{2\delta t}$$

Verlet algorithm

$$x(0) = x_0 \quad , \quad v(0) = v_0$$

Euler algorithm:

$$\boxed{x(\delta t) = x(0) + \delta t\, v(x(0),0)}$$

$x(\delta t)$

Verlet algorithm:

$$x(2\delta t) = 2x(\delta t) - x(0) + \delta t^2 a(\delta t)$$

$$v(\delta t) = \frac{x(2\delta t) - x(0)}{2\delta t}$$

$x(2\delta t)$

$v(\delta t)$

Verlet algorithm:

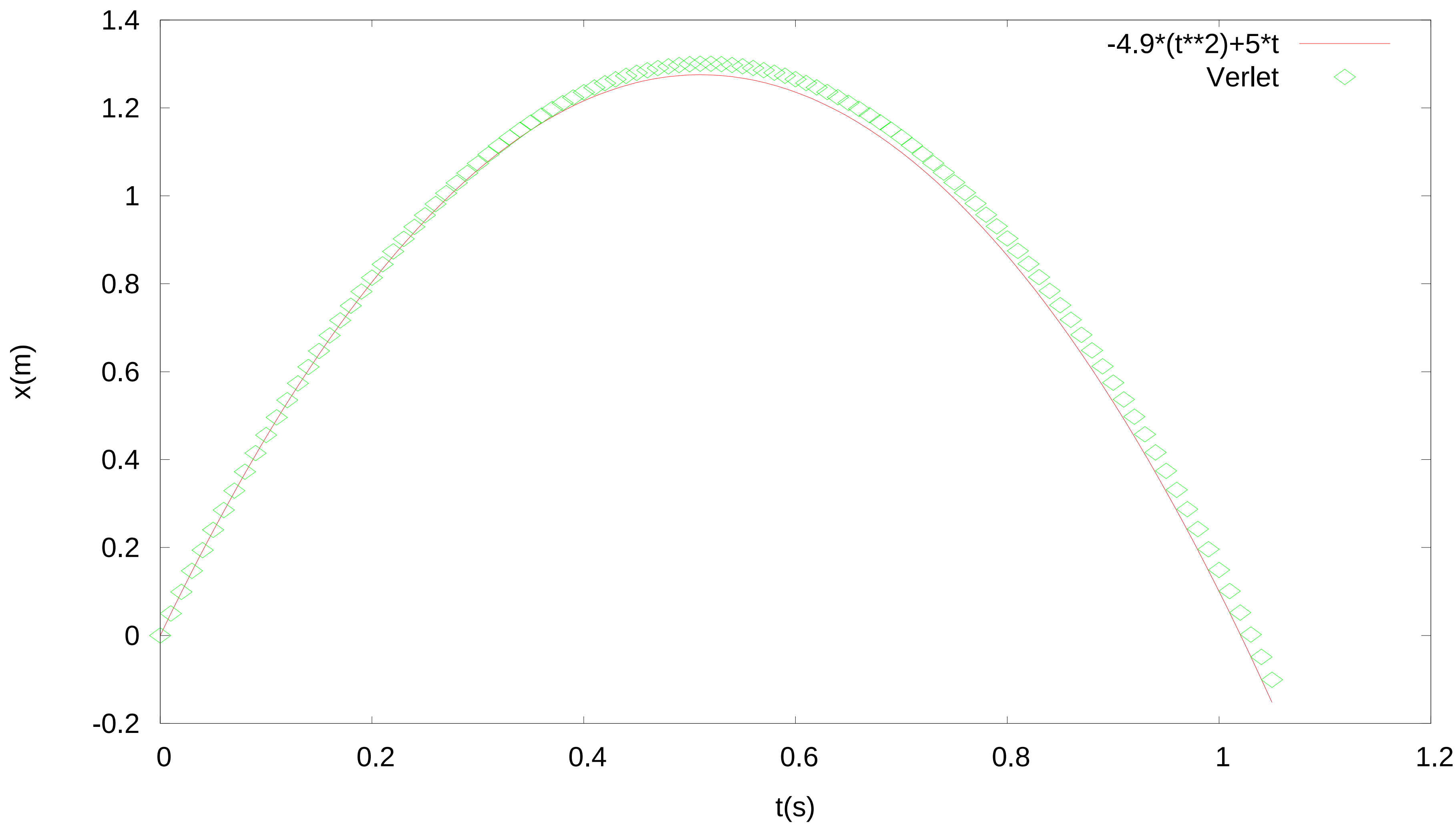
$$x(3\delta t) = 2x(2\delta t) - x(\delta t) + \delta t^2 a(2\delta t)$$

$$v(2\delta t) = \frac{x(3\delta t) - x(\delta t)}{2\delta t}$$

$x(3\delta t)$

$v(2\delta t)$

$$x(0) = 0 \quad , \quad v(0) = 5\, m/s$$



Leap-frog algorithm

$$v(t+\frac{\delta t}{2}) = v(t-\frac{\delta t}{2}) + \delta t\, a(t)$$

$$x(t+\delta t) = x(t) + \delta t\, v(t+\frac{\delta t}{2})$$

$$v(t) = \frac{1}{2}\left(v(t-\frac{\delta t}{2}) + v(t+\frac{\delta t}{2}) \right)$$

Leap-frog algorithm

$$\begin{cases} v(t+\frac{\delta t}{2}) = v(t-\frac{\delta t}{2}) + \delta t\, a(t) \\ \boxed{x(t+\delta t) = x(t) + \delta t\, v(t+\frac{\delta t}{2})} \end{cases}$$

$$v(t) = \frac{1}{2}\left(v(t-\frac{\delta t}{2}) + v(t+\frac{\delta t}{2}) \right)$$

$$\begin{cases} v(t-\frac{\delta t}{2}) + v(t+\frac{\delta t}{2}) = 2v(t) \\ v(t+\frac{\delta t}{2}) - v(t-\frac{\delta t}{2}) = \delta t\, a(t) \end{cases} \Rightarrow \boxed{v(t+\frac{\delta t}{2}) = \frac{2v(t)+\delta t\, a(t)}{2}}$$

Leap-frog algorithm

$$
\begin{cases}
v(t+\frac{\delta t}{2}) = \frac{2v(t)+\delta t\, a(t)}{2} \\
x(t+\delta t) = x(t)+\delta t\, v(t+\frac{\delta t}{2})
\end{cases}
$$

$$
x(t+\delta t) = x(t)+\delta t\, v(t)+\frac{\delta t^2}{2}a(t)
$$

Leap-frog algorithm

$$x(0) = x_0 \quad , \quad v(0) = v_0$$

$$v(\frac{\delta t}{2}) = \delta t\, a(0)$$

$$x(\delta t) = x(0) + \delta t\, v(\frac{\delta t}{2})$$

$$v(\delta t) = \frac{1}{2}\left(v(\frac{\delta t}{2}) \right)$$

$$v(\frac{3\delta t}{2}) = v(\frac{\delta t}{2}) + \delta t\, a(\delta t)$$

$$x(2\delta t) = x(\delta t) + \delta t\, v(\frac{3\delta t}{2})$$

$$v(2\delta t) = \frac{1}{2}\left(v(\frac{\delta t}{2}) + v(\frac{3\delta t}{2}) \right)$$

$$v(\frac{5\delta t}{2}) = v(\frac{3\delta t}{2}) + \delta t\, a(2\delta t)$$

$$x(3\delta t) = x(2\delta t) + \delta t\, v(\frac{5\delta t}{2})$$

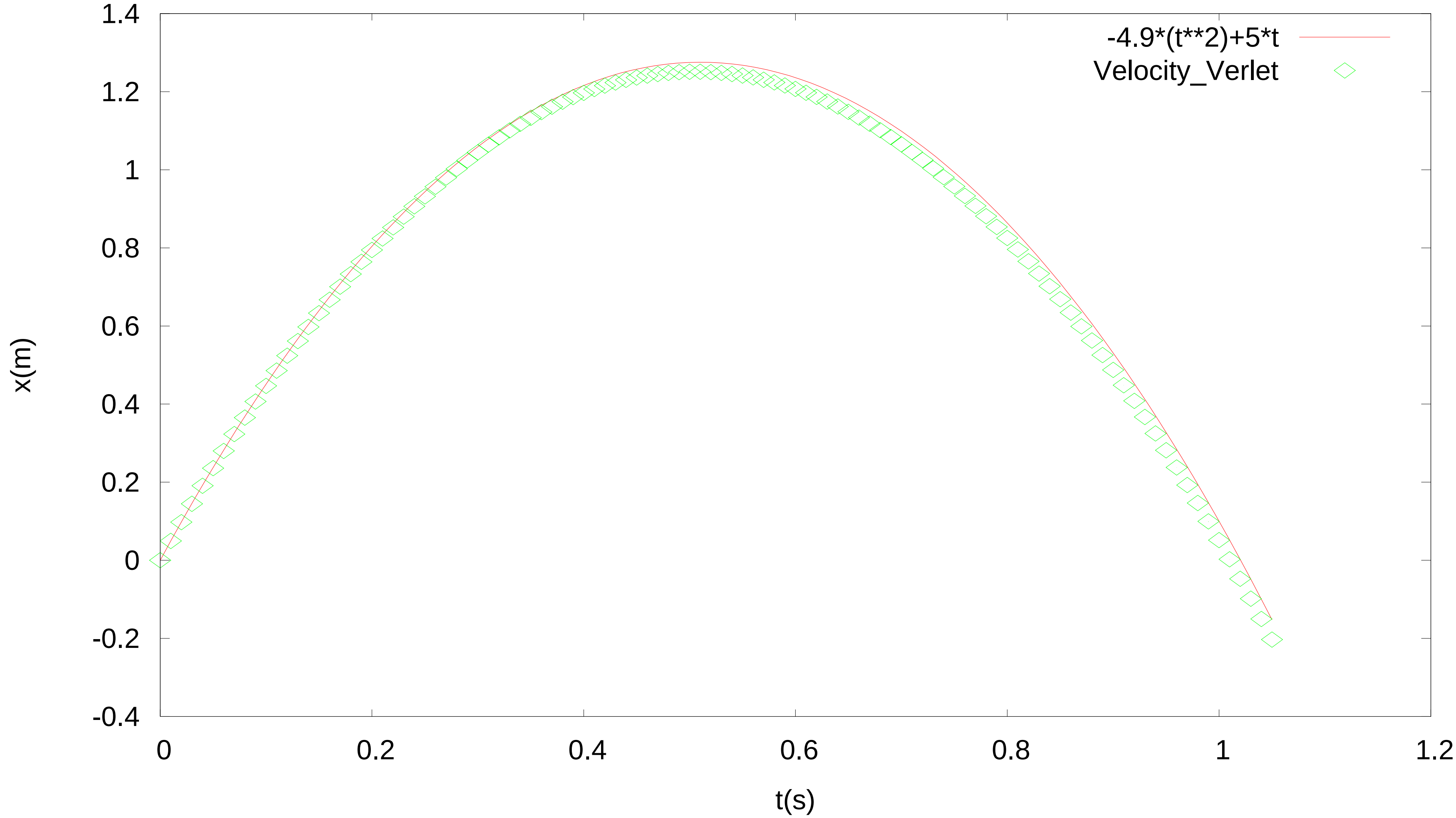
$$v(3\delta t) = \frac{1}{2}\left(v(\frac{3\delta t}{2}) + v(\frac{5\delta t}{2}) \right)$$

Velocity-Verlet algorithm

$$x(0) = x_0 \quad , \quad v(0) = v_0$$

$$\begin{cases} x(t+\delta t) = x(t) + \delta t\, v(t) + \dfrac{1}{2}\delta t^2\, a(t) \\ v(t+\delta t) = v(t) + \dfrac{1}{2}\delta t\left[a(t+\delta t) + a(t)\right] \end{cases}$$

$$x(0) = 0 \quad , \quad v(0) = 5\,m/s$$



Runge-Kutta Methods

Second order

$$\frac{dx}{dt} = f(x,t)$$

$$\boxed{\begin{aligned} x_{n+1} &= x_n + ak_1 + bk_2 \\ k_1 &= \delta t\, f(x_n, t_n) \\ k_2 &= \delta t\, f(x_n + \alpha k_1, t_n + \beta \delta t) \end{aligned}}$$

$$x_{n+1} = x_n + a\delta t\, f(x_n, t_n) + b\delta t\, f(x_n + \alpha k_1, t_n + \beta \delta t)$$

$$f(x_n + \alpha k_1, t_n + \beta \delta t) = f(x_n, t_n) + \alpha k_1 f_x(x_n, t_n) + \beta \delta t\, f_t(x_n, t_n)$$

$$f(x_n + \alpha k_1, t_n + \beta \delta t) = f(x_n, t_n) + \alpha \delta t\, f(x_n, t_n)\, f_x(x_n, t_n) + \beta \delta t\, f_t(x_n, t_n)$$

1

$$\boxed{x_{n+1} = x_n + (a+b)\delta t\, f(x_n, t_n) + b\delta t^2 (\alpha\, f(x_n, t_n)\, f_x(x_n, t_n) + \beta\, f_t(x_n, t_n))}$$

Runge-Kutta Methods

Second order

$$\frac{dx}{dt} = f(x,t)$$

$$x_{n+1} = x_n + \delta t\, f(x_n, t_n) + \frac{\delta t^2}{2} f'(x_n, t_n) + \cdots$$

$$d\,f = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} dx \xrightarrow{\frac{1}{dt}} \frac{d\,f}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} f$$

$$\frac{d\,f}{dt} = f_t + f_x f$$

2

$$\boxed{x_{n+1} = x_n + \delta t\, f(x_n, t_n) + \frac{\delta t^2}{2}\left(f_t(x_n, t_n) + f_x(x_n, t_n) f(x_n, t_n)\right)}$$

$$a + b = 1 \qquad b\beta = \frac{1}{2} \qquad b\alpha = \frac{1}{2}$$

$$a = \frac{1}{2} \quad : \quad b = \frac{1}{2}, \alpha = 1, \beta = 1$$

Runge-Kutta Methods

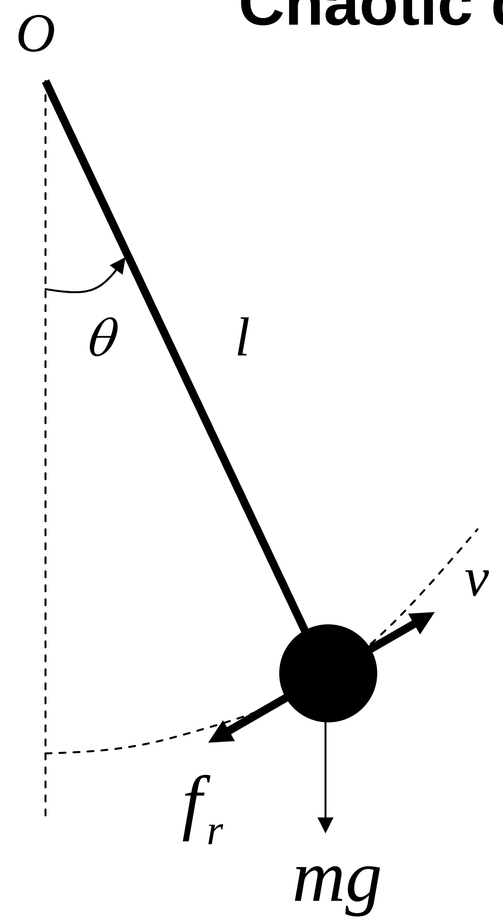
fourth order

$$x_{n+1} = x_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$\boxed{\begin{aligned}
k_1 &= \delta t\, f(x_n, t_n) \\
k_2 &= \delta t\, f(x_n + k_1, t_n + \frac{1}{2}\delta t) \\
k_3 &= \delta t\, f(x_n + \frac{1}{2}k_2, t_n + \frac{1}{2}\delta t) \\
k_4 &= \delta t\, f(x_n + k_3, t_n + \delta t)
\end{aligned}}$$

Write program

Chaotic dynamics of a driven pendulum



$$ma_t = f_g + f_d + f_r$$

$$f_g = -mgSin\theta$$

$$f_d = f_0 Cos\omega_0 t$$

$$f_r = -\kappa v$$

$$a_t = l\frac{d^2\theta}{dt^2} \quad , \quad v = l\frac{d\theta}{dt}$$

Chaotic dynamics of a driven pendulum

$$ma_t = f_g + f_d + f_r$$

$$ma_t = -mgSin\theta + f_0 Cos\omega_0 t - \kappa v$$

$$ml\frac{d^2\theta}{dt^2} = -mgSin\theta + f_0 Cos\omega_0 t - \kappa l\frac{d\theta}{dt}$$

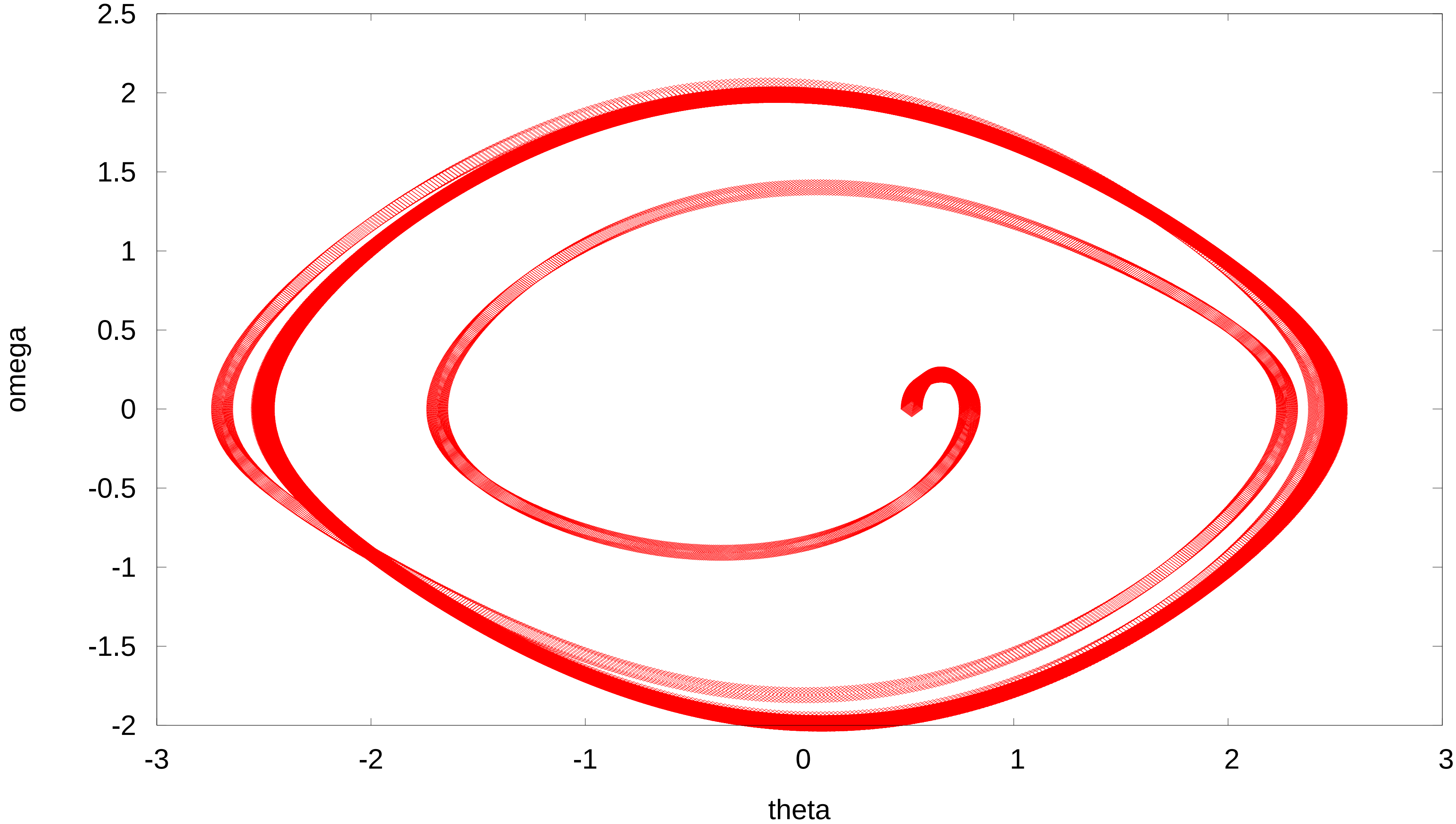
$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}Sin\theta + \frac{f_0}{ml}Cos\omega_0 t - \frac{\kappa}{m}\frac{d\theta}{dt}$$

$$\boxed{\frac{d^2\theta}{dt^2} + \frac{\kappa}{m}\frac{d\theta}{dt} + \frac{g}{l}Sin\theta = \frac{f_0}{ml}Cos\omega_0 t}$$

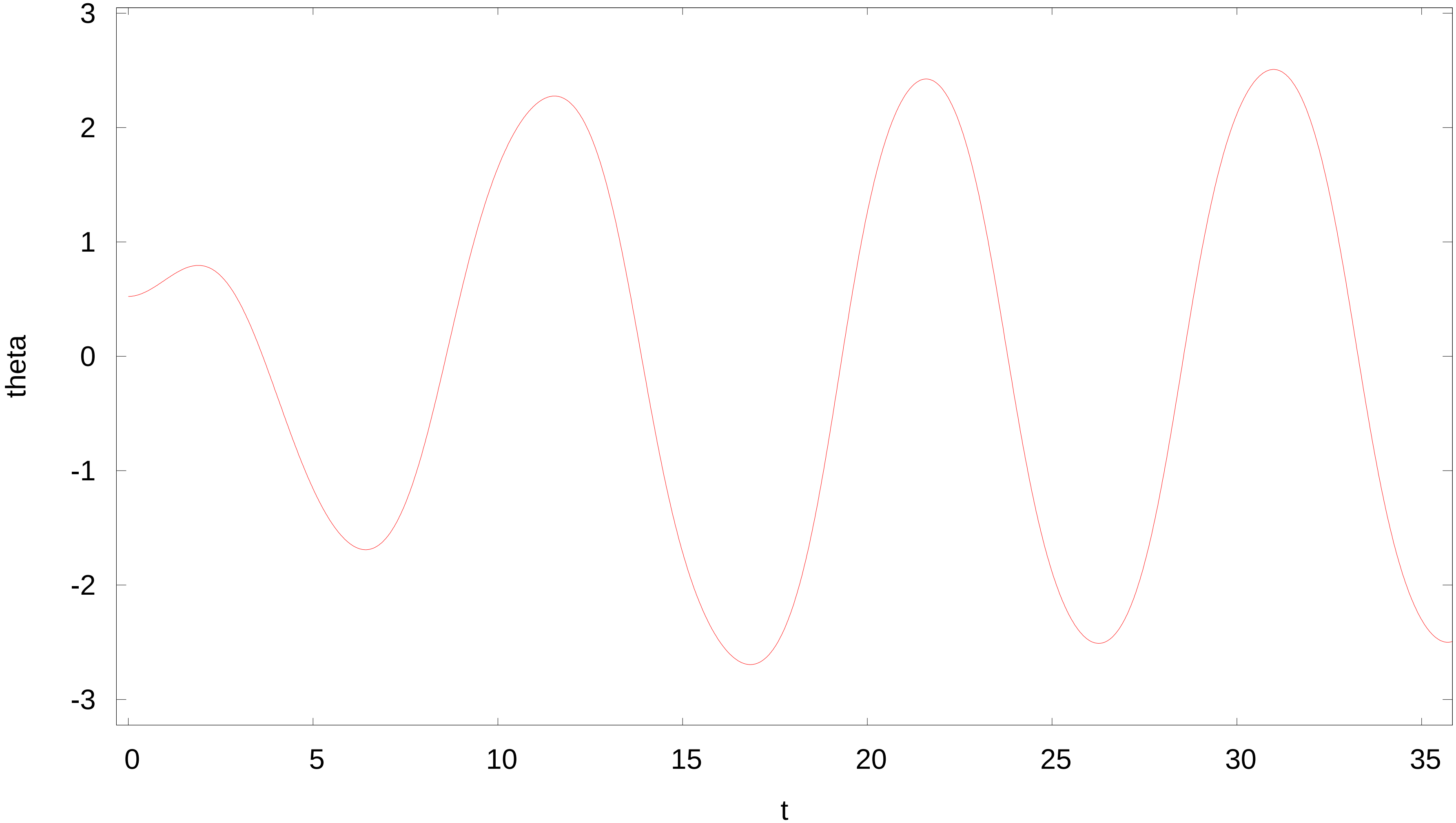
Chaotic dynamics of a driven pendulum

$$\frac{d^2\theta}{dt^2} + \frac{\kappa}{m}\frac{d\theta}{dt} + \frac{g}{l} Sin\theta = \frac{f_0}{ml} Cos\omega_0 t$$

$$\begin{cases} \dfrac{\kappa}{m} = 0.5 \\ \dfrac{g}{l} = 1.0 \\ \dfrac{f_0}{ml} = 0.9 \\ \omega_0 = \dfrac{2}{3} \end{cases} \qquad\qquad \begin{cases} \dfrac{\kappa}{m} = 0.5 \\ \dfrac{g}{l} = 1.0 \\ \dfrac{f_0}{ml} = 1.15 \\ \omega_0 = \dfrac{2}{3} \end{cases}$$



omega
theta
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-3
-2
-1
0
1
2
3



theta
3
2
1
0
-1
-2
-3
0
5
10
15
20
25
30
35
t

2D

$$f_x = 0$$

$$f_y = -g = 9.8\, m/s^2$$

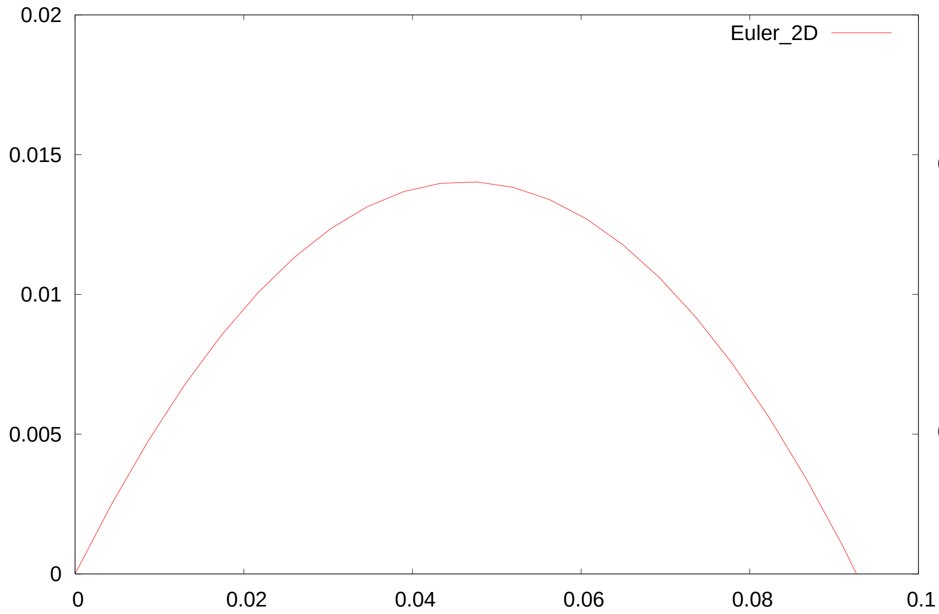
$$m\frac{d^2x}{dt^2} = 0$$

$$m\frac{d^2y}{dt^2} = f_y$$

$$\begin{cases} x(t=0) = 0.0 \\ y(t=0) = 0.0 \end{cases}$$

$$\begin{cases} v_0 = 1.0 \\ \theta = 30^\circ \end{cases}$$

$$\begin{cases} v_x = v_0 Cos\theta \\ v_y = v_0 Sin\theta \end{cases}$$


Euler_2D
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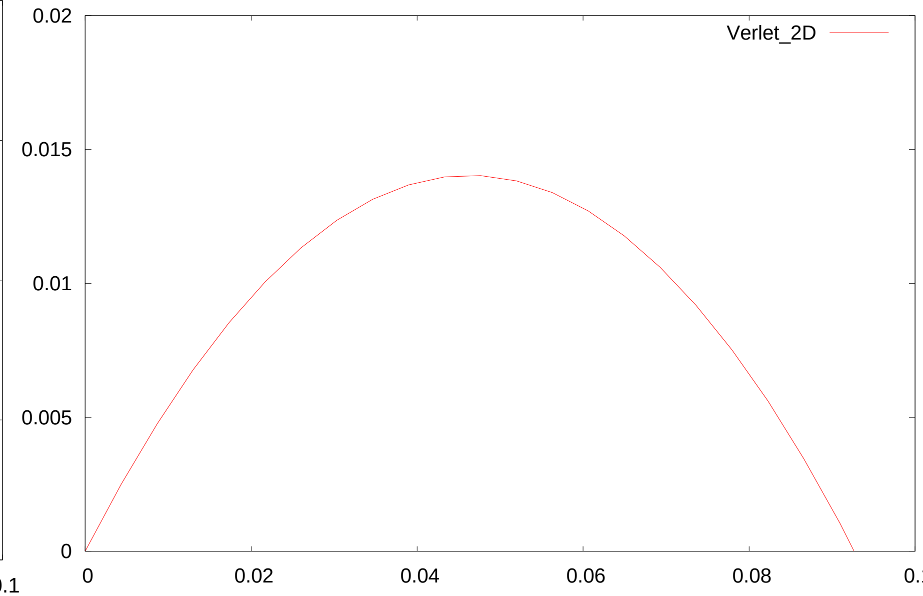
0.015
0.01
0.005
0
0
0.02
0.04
0.06
0.08
0.1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0.015
0.01
0.005
0
0
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0.04
0.06
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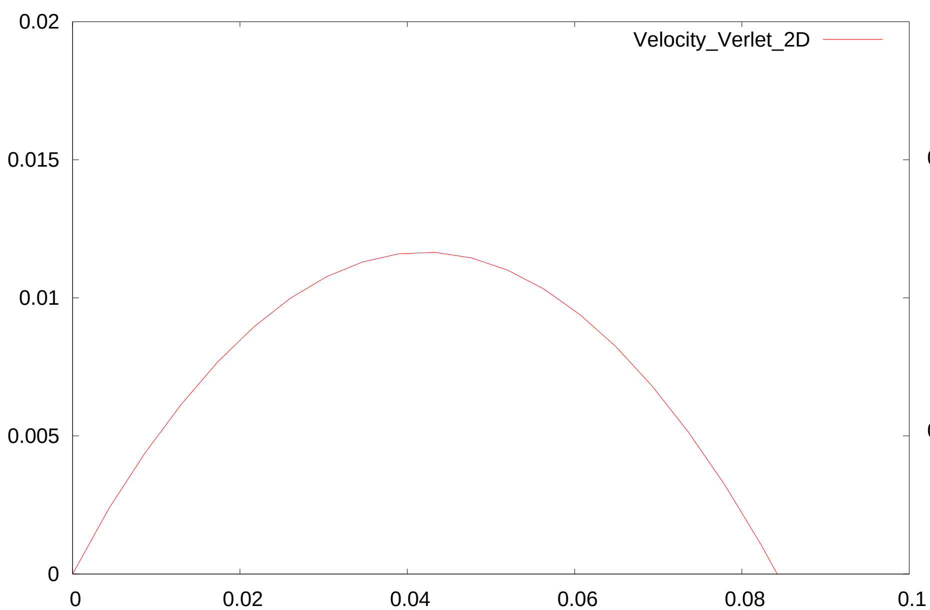
0.1


Velocity_Verlet_2D
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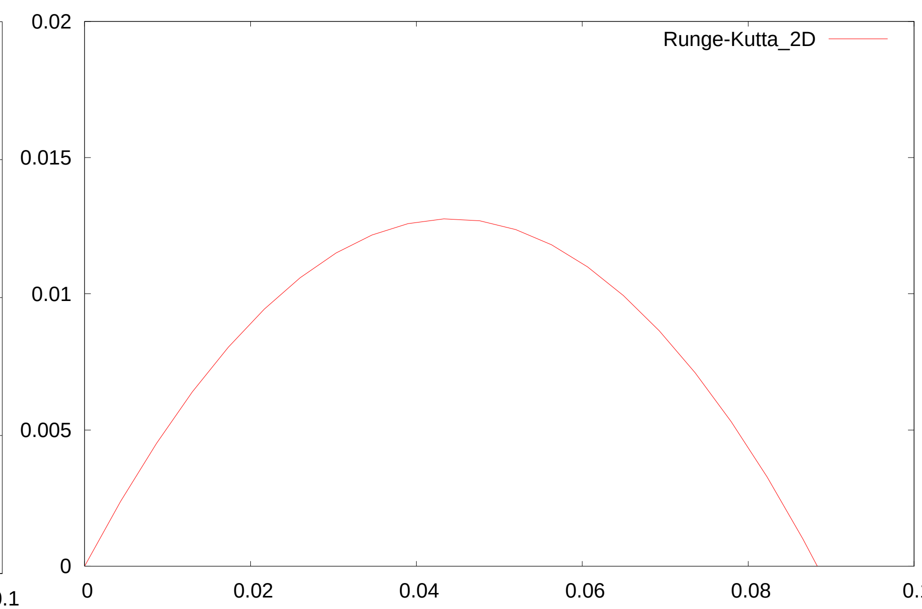
0.015
0.01
0.005
0
0
0.02
0.04
0.06
0.08
0.1


Runge-Kutta_2D
0.02
0.015
0.01
0.005
0
0
0.02
0.04
0.06
0.08
0.1

2D

$$f_x = -k_x x$$

$$f_y = -k_y y$$

$$m\frac{d^2x}{dt^2} = f_x \Rightarrow m\frac{d^2x}{dt^2} = -k_x x \Rightarrow \frac{d^2x}{dt^2} + \frac{k_x}{m}x = 0$$

$$m\frac{d^2y}{dt^2} = f_y \Rightarrow m\frac{d^2y}{dt^2} = -k_y y \Rightarrow \frac{d^2y}{dt^2} + \frac{k_y}{m}y = 0$$

$$(x_0, y_0) \quad , \quad (v_{x0}, v_{y0})$$

2D

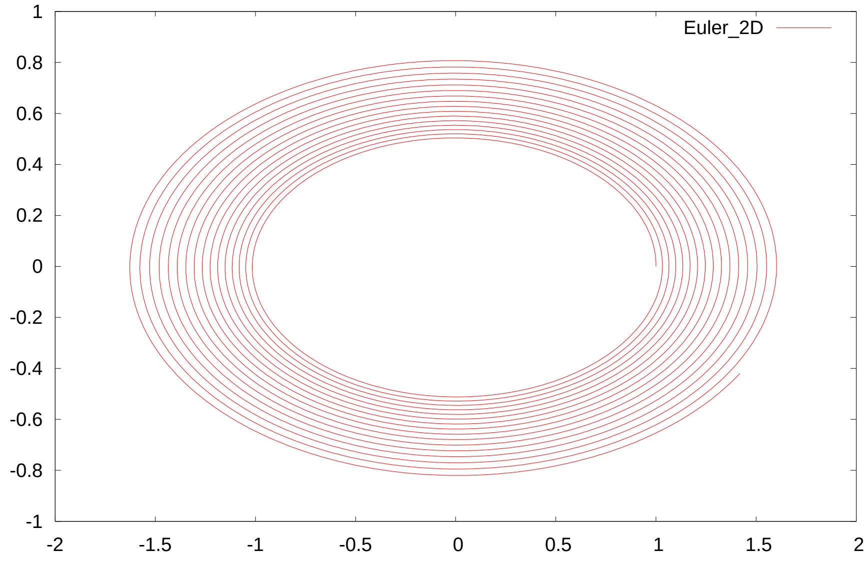
$$\boxed{\begin{aligned} f_x &= -1.0x \\ f_y &= -1.0y \end{aligned}}$$

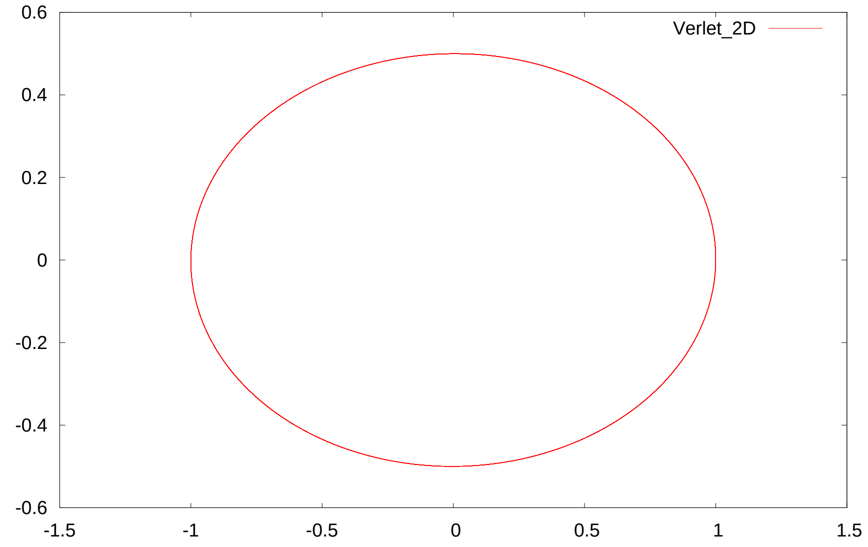
$$m = 1$$

$$\begin{cases} x(t=0) = 1.0 \\ y(t=0) = 0.0 \end{cases}$$

$$\begin{cases} v_0 = 0.5 \\ \theta = 90^\circ \end{cases}$$

$$\begin{cases} v_x = v_0 Cos\theta \\ v_y = v_0 Sin\theta \end{cases}$$


Euler_2D
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2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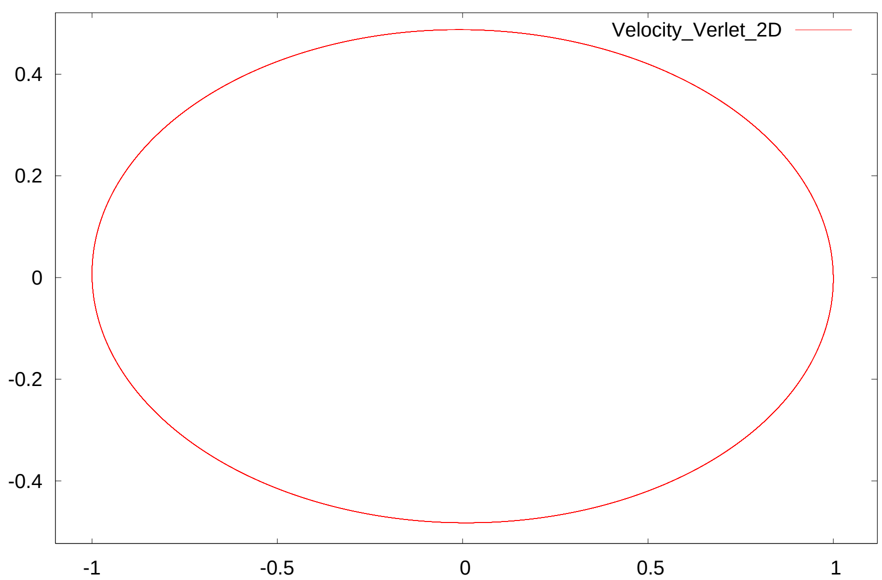
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-1.5
-1
-0.5
0
0.5
1
1.5


Velocity_Verlet_2D
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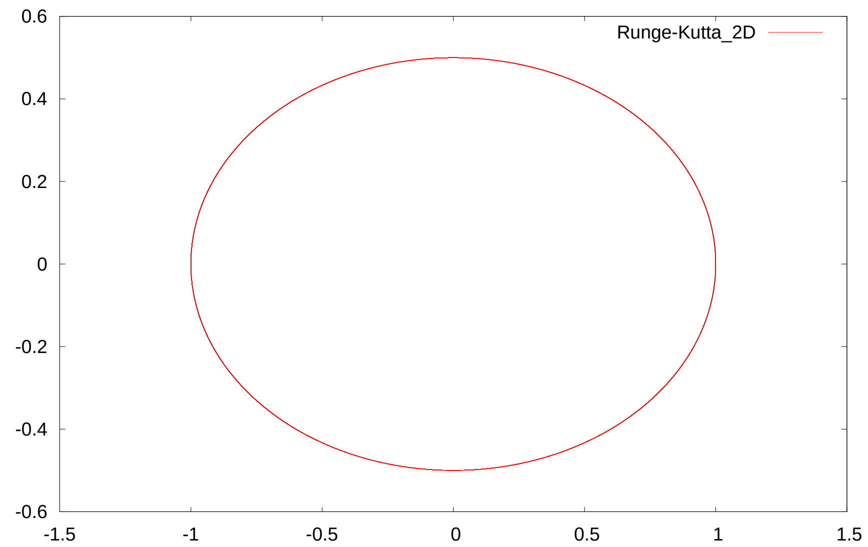
0.2
0
-0.2
-0.4
-1
-0.5
0
0.5
1


Runge-Kutta_2D
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-1.5
-1
-0.5
0
0.5
1
1.5

2D

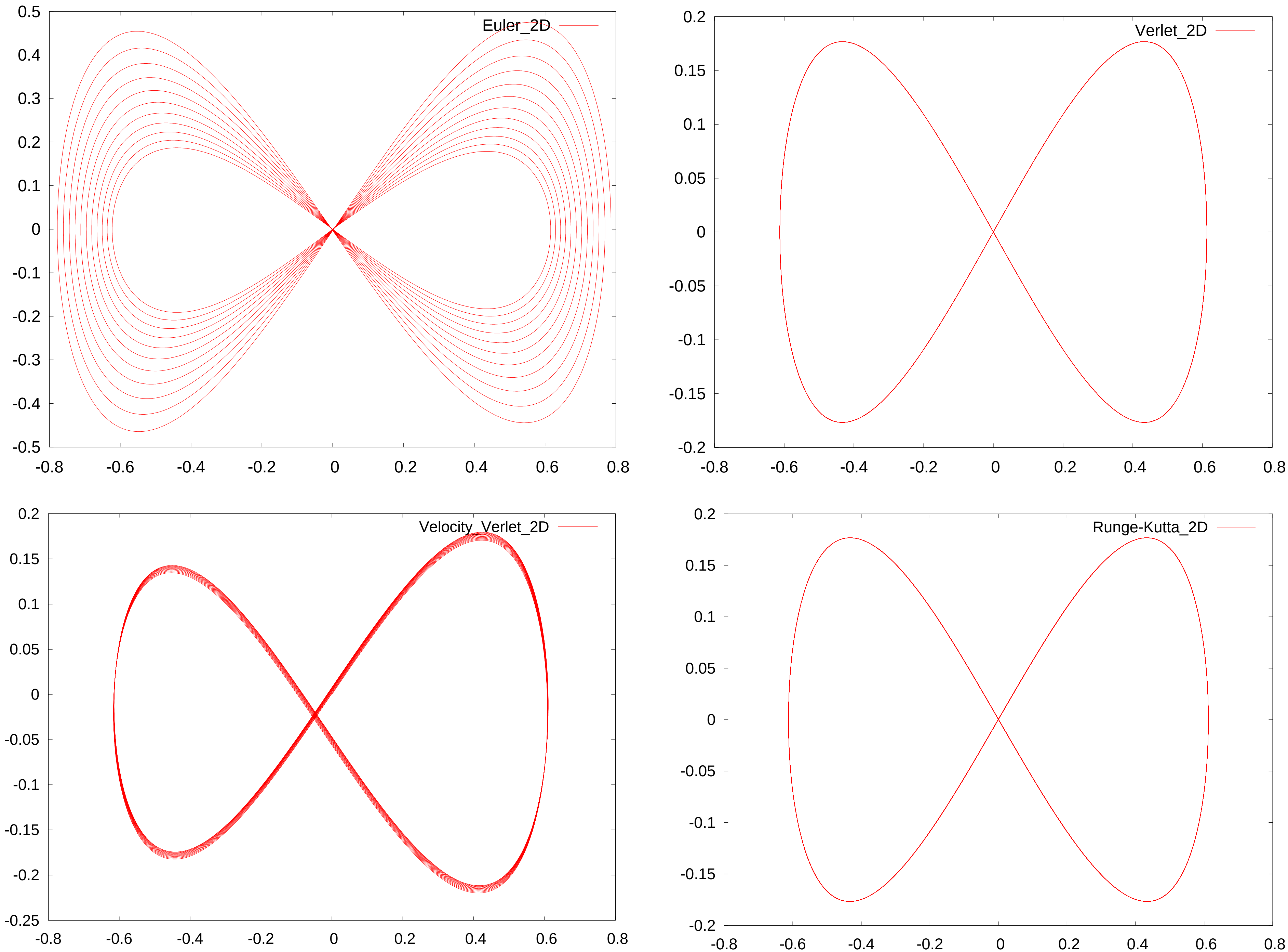
$$\boxed{\begin{aligned} f_x &= -0.5x \\ f_y &= -2.0y \end{aligned}}$$

$$m = 1$$

$$\begin{cases} x(t=0) = 0.0 \\ y(t=0) = 0.0 \end{cases}$$

$$\begin{cases} v_0 = 0.5 \\ \theta = 30^\circ \end{cases}$$

$$\begin{cases} v_x = v_0 Cos\theta \\ v_y = v_0 Sin\theta \end{cases}$$


Euler_2D
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8
Verlet_2D
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8
Velocity_Verlet_2D
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
-0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8
Runge-Kutta_2D
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8

Boundary-value and eigenvalue problems

$$\varphi'' = f(\varphi, \varphi', x)$$

The solution of the Poisson equation with a given charge distribution and known boundary values of the electrostatic potential.

$$\nabla^2 \varphi = -\frac{\rho}{\varepsilon_\circ}$$

The stationary Schrodinger equation with a given potential and boundary conditions.

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi$$

Boundary-value problems

$$\varphi'' = f(\varphi, \varphi', x) \xrightarrow{\text{For example}}$$

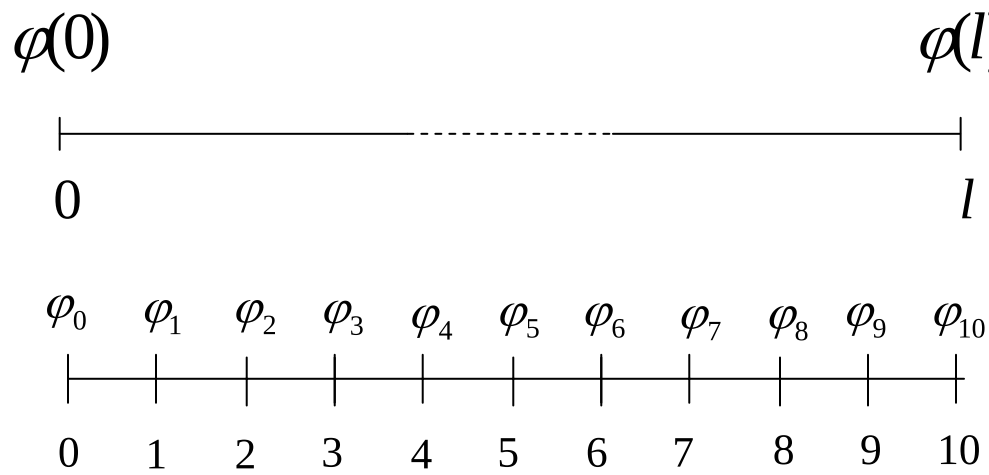
$$\frac{d^2\varphi}{dx^2} = 0 \quad , \quad \varphi(0) = 0 \quad , \quad \varphi(l) = \varphi_0$$

Analytical solution :

$$\frac{d^2\varphi}{dx^2} = 0 \Rightarrow \varphi(x) = ax + b$$

$$\varphi(0) = 0 \quad , \quad \varphi(l) = \varphi_0 \Rightarrow \begin{cases} 0 = b \\ \varphi_0 = al + b \end{cases} \Rightarrow \varphi(x) = \varphi_0 \frac{x}{l}$$

Boundary-value problems

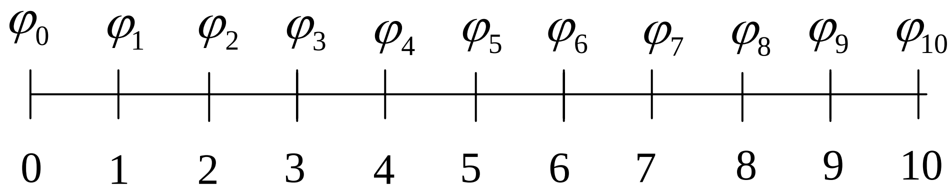


$$\Delta x = \frac{l}{10}$$

$$\frac{\varphi_{i-1} - 2\varphi_i + \varphi_{i+1}}{\Delta x^2} = 0 \Rightarrow \varphi_{i-1} - 2\varphi_i + \varphi_{i+1} = 0$$

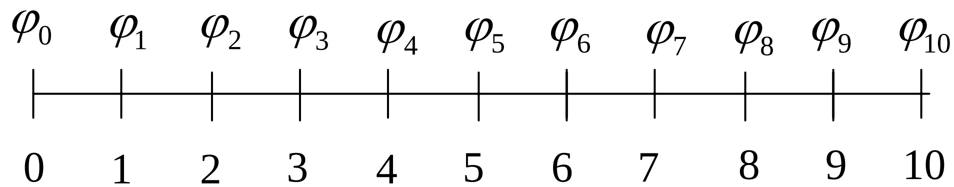
$$\varphi_0 = 0 \quad , \quad \varphi_{10} = \varphi_0$$

Matrix Method



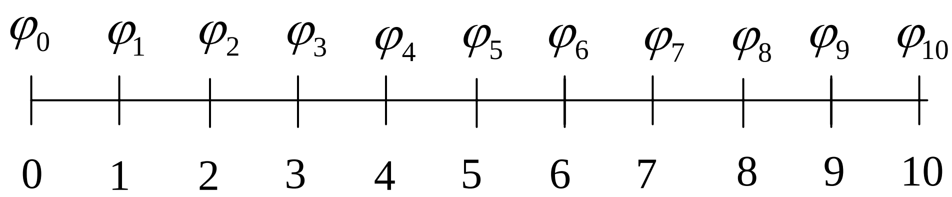
$$
\begin{cases}
\varphi_0 - 2\varphi_1 + \varphi_2 = 0 \\
\varphi_1 - 2\varphi_2 + \varphi_3 = 0 \\
\vdots \\
\varphi_{i-1} - 2\varphi_i + \varphi_{i+1} = 0 \\
\vdots \\
\varphi_7 - 2\varphi_8 + \varphi_9 = 0 \\
\varphi_8 - 2\varphi_9 + \varphi_{10} = 0
\end{cases}
\qquad
\begin{cases}
-2\varphi_1 + \varphi_2 = -\varphi_0 \\
\varphi_1 - 2\varphi_2 + \varphi_3 = 0 \\
\vdots \\
\varphi_{i-1} - 2\varphi_i + \varphi_{i+1} = 0 \\
\vdots \\
\varphi_7 - 2\varphi_8 + \varphi_9 = 0 \\
\varphi_8 - 2\varphi_9 = -\varphi_{10}
\end{cases}
$$

Matrix Method



$$
\begin{bmatrix}
-2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2
\end{bmatrix}
\begin{bmatrix}
\varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \\ \varphi_5 \\ \varphi_6 \\ \varphi_7 \\ \varphi_8 \\ \varphi_9
\end{bmatrix}
=
\begin{bmatrix}
\varphi_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \varphi_{10}
\end{bmatrix}
$$

Iterative Method



$$\begin{cases} \varphi_0 - 2\varphi_1 + \varphi_2 = 0 \\ \varphi_1 - 2\varphi_2 + \varphi_3 = 0 \\ \vdots \\ \varphi_{i-1} - 2\varphi_i + \varphi_{i+1} = 0 \\ \vdots \\ \varphi_7 - 2\varphi_8 + \varphi_9 = 0 \\ \varphi_8 - 2\varphi_9 + \varphi_{10} = 0 \end{cases}$$

$$\begin{cases} \varphi_1 = \frac{1}{2}(\varphi_0 + \varphi_2) \\ \varphi_2 = \frac{1}{2}(\varphi_1 + \varphi_3) \\ \vdots \\ \varphi_i = \frac{1}{2}(\varphi_{i-1} + \varphi_{i+1}) \\ \vdots \\ \varphi_8 = \frac{1}{2}(\varphi_7 + \varphi_9) \\ \varphi_9 = \frac{1}{2}(\varphi_8 + \varphi_{10}) \end{cases}$$

Iterative Method

start

$$\left\{\varphi_1^{old}, \varphi_2^{old}, \ldots, \varphi_8^{old}, \varphi_8^{old}\right\}$$

$$\begin{cases}
\varphi_1^{new} = \frac{1}{2}(\varphi_0^{old} + \varphi_2^{old}) \\
\varphi_2^{new} = \frac{1}{2}(\varphi_1^{old} + \varphi_3^{old}) \\
\vdots \\
\varphi_i^{new} = \frac{1}{2}(\varphi_{i-1}^{old} + \varphi_{i+1}^{old}) \\
\vdots \\
\varphi_8^{new} = \frac{1}{2}(\varphi_7^{old} + \varphi_9^{old}) \\
\varphi_9^{new} = \frac{1}{2}(\varphi_8^{old} + \varphi_{10}^{old})
\end{cases}$$

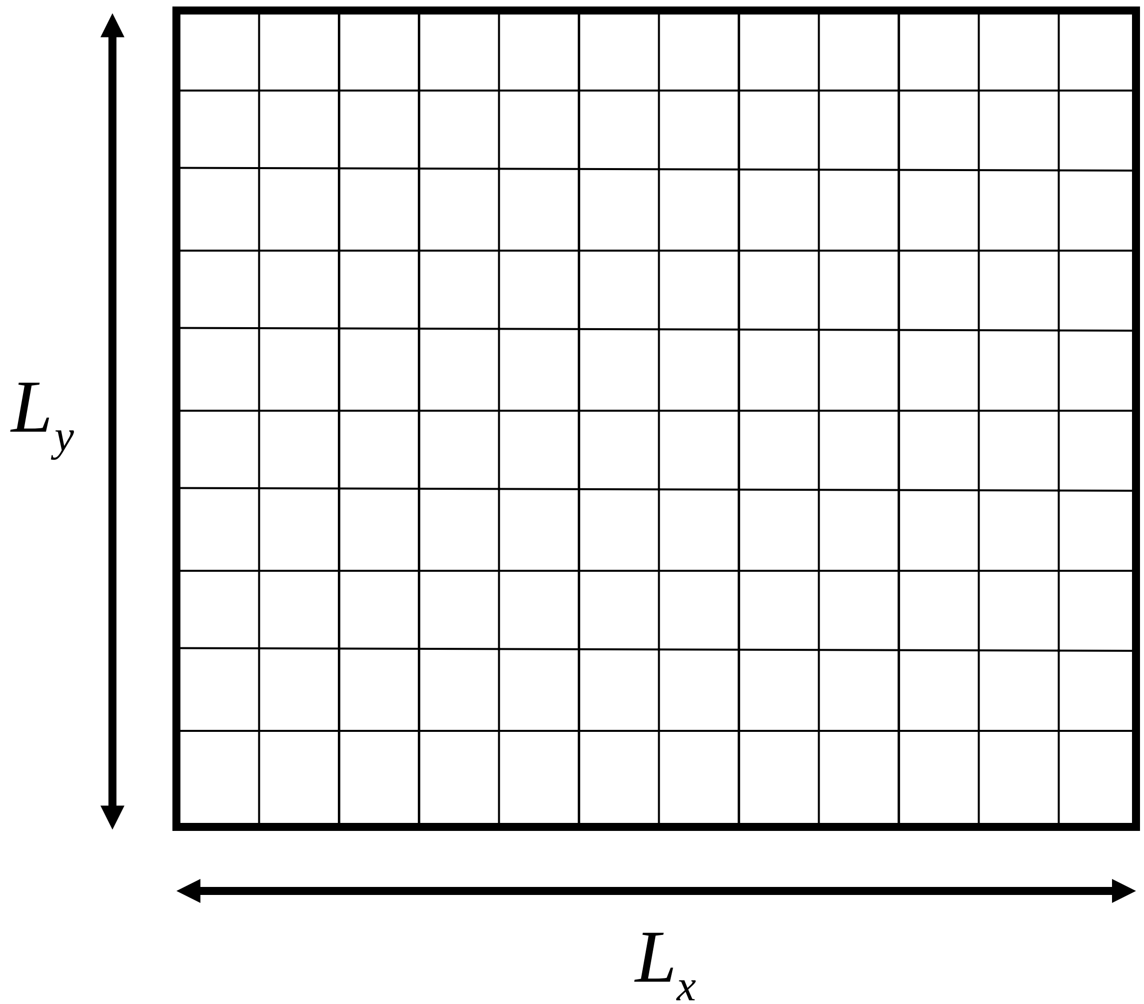
$$R = \sqrt{\sum_{i=1}^{9} (\varphi_i^{new} - \varphi_i^{old})^2}$$

$$\left\{\varphi_1^{new}, \varphi_2^{new}, \ldots, \varphi_8^{new}, \varphi_8^{new}\right\}$$

R<Tol

2D

$$\nabla^2\varphi = 0 \Rightarrow \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} = 0$$



$$\Delta x = \frac{L_x}{m}$$

$$\Delta y = \frac{L_y}{n}$$

2D

$$
\begin{array}{ccccccccc}
\varphi_{0,0} & \varphi_{0,1} & \varphi_{0,2} & & & & \varphi_{0,m-2} & \varphi_{0,m-1} & \varphi_{0,m} \\
\varphi_{1,0} & \varphi_{1,1} & \varphi_{1,2} & \cdots & \cdots & \cdots & \varphi_{1,m-2} & \varphi_{1,m-1} & \varphi_{1,m} \\
\varphi_{2,0} & \varphi_{2,1} & \varphi_{2,2} & & & & \varphi_{2,m-2} & \varphi_{2,m-1} & \varphi_{2,m} \\
 & \vdots & & \ddots & & & & \vdots & \\
 & \vdots & & & \ddots & & & \vdots & \\
 & \vdots & & & & \ddots & & \vdots & \\
\varphi_{n-2,0} & \varphi_{n-2,1} & \varphi_{n-2,2} & & & & \varphi_{n-2,m-2} & \varphi_{n-2,m-1} & \varphi_{n-2,m} \\
\varphi_{n-1,0} & \varphi_{n-1,1} & \varphi_{n-1,2} & \cdots & \cdots & \cdots & \varphi_{n-1,m-2} & \varphi_{n-1,m-1} & \varphi_{n-1,m} \\
\varphi_{n,0} & \varphi_{n,1} & \varphi_{n,2} & & & & \varphi_{n,m-2} & \varphi_{n,m-1} & \varphi_{n,m}
\end{array}
$$

2D

$$
\begin{array}{c|cccccc|c}
\varphi_{0,0} & \varphi_{0,1} & \varphi_{0,2} & & & \varphi_{0,m-2} & \varphi_{0,m-1} & \varphi_{0,m} \\
\hline
\varphi_{1,0} & \varphi_{1,1} & \varphi_{1,2} & \cdots & \cdots\ \cdots & \varphi_{1,m-2} & \varphi_{1,m-1} & \varphi_{1,m} \\
\varphi_{2,0} & \varphi_{2,1} & \varphi_{2,2} & & & \varphi_{2,m-2} & \varphi_{2,m-1} & \varphi_{2,m} \\
 & \vdots & & \ddots & & & \vdots & \\
 & \vdots & & & \ddots & & \vdots & \\
 & \vdots & & & & \ddots & \vdots & \\
\varphi_{n-2,0} & \varphi_{n-2,1} & \varphi_{n-2,2} & & & \varphi_{n-2,m-2} & \varphi_{n-2,m-1} & \varphi_{n-2,m} \\
\varphi_{n-1,0} & \varphi_{n-1,1} & \varphi_{n-1,2} & \cdots & \cdots\ \cdots & \varphi_{n-1,m-2} & \varphi_{n-1,m-1} & \varphi_{n-1,m} \\
\hline
\varphi_{n,0} & \varphi_{n,1} & \varphi_{n,2} & & & \varphi_{n,m-2} & \varphi_{n,m-1} & \varphi_{n,m}
\end{array}
$$

2D

$$\nabla^2\varphi = 0 \Rightarrow \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} = 0$$

$$\nabla^2\varphi = 0 \Rightarrow \frac{\varphi_{i-1,j} - 2\varphi_{i,j} + \varphi_{i+1,j}}{\Delta x^2} + \frac{\varphi_{i,j-1} - 2\varphi_{i,j} + \varphi_{i,j+1}}{\Delta y^2} = 0$$

$$\frac{\varphi_{i-1,j} + \varphi_{i+1,j}}{\Delta x^2} - 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)\varphi_{i,j} + \frac{\varphi_{i,j-1} + \varphi_{i,j+1}}{\Delta y^2} = 0$$

Iterative Method

$$\frac{\varphi_{i-1,j} + \varphi_{i+1,j}}{\Delta x^2} - 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)\varphi_{i,j} + \frac{\varphi_{i,j-1} + \varphi_{i,j+1}}{\Delta y^2} = 0$$

$$2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)\varphi_{i,j} = \frac{\varphi_{i-1,j} + \varphi_{i+1,j}}{\Delta x^2} + \frac{\varphi_{i,j-1} + \varphi_{i,j+1}}{\Delta y^2}$$

$$\varphi_{i,j} = \frac{1}{2}\left(\frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2}\right)\left(\frac{\varphi_{i-1,j} + \varphi_{i+1,j}}{\Delta x^2} + \frac{\varphi_{i,j-1} + \varphi_{i,j+1}}{\Delta y^2}\right)$$

Iterative Method

$$\left\{\varphi_{1,1}^{old}, \varphi_{1,2}^{old}, \ldots, \varphi_{1,n-1}^{old}, \varphi_{2,1}^{old}, \varphi_{2,2}^{old}, \ldots, \varphi_{2,n-1}^{old}, \ldots\ldots, \varphi_{m-1,1}^{old}, \varphi_{m-1,2}^{old}, \ldots, \varphi_{m-1,n-1}^{old}\right\}$$

$R < Tol$

$$\varphi_{i,j}^{new} = \frac{1}{2}\left(\frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2}\right)\left(\frac{\varphi_{i-1,j}^{old} + \varphi_{i+1,j}^{old}}{\Delta x^2} + \frac{\varphi_{i,j-1}^{old} + \varphi_{i,j+1}^{old}}{\Delta y^2}\right)$$

$$\left\{\varphi_{1,1}^{new}, \varphi_{1,2}^{new}, \ldots, \varphi_{1,n-1}^{new}, \varphi_{2,1}^{new}, \varphi_{2,2}^{new}, \ldots, \varphi_{2,n-1}^{new}, \ldots\ldots, \varphi_{m-1,1}^{new}, \varphi_{m-1,2}^{new}, \ldots, \varphi_{m-1,n-1}^{new}\right\}$$

Iterative Method

$$\left\{\varphi_{1,1}^{old},\varphi_{1,2}^{old},\ldots,\varphi_{1,n-1}^{old},\varphi_{2,1}^{old},\varphi_{2,2}^{old},\ldots,\varphi_{2,n-1}^{old},\ldots\ldots,\varphi_{m-1,1}^{old},\varphi_{m-1,2}^{old},\ldots,\varphi_{m-1,n-1}^{old}\right\}$$

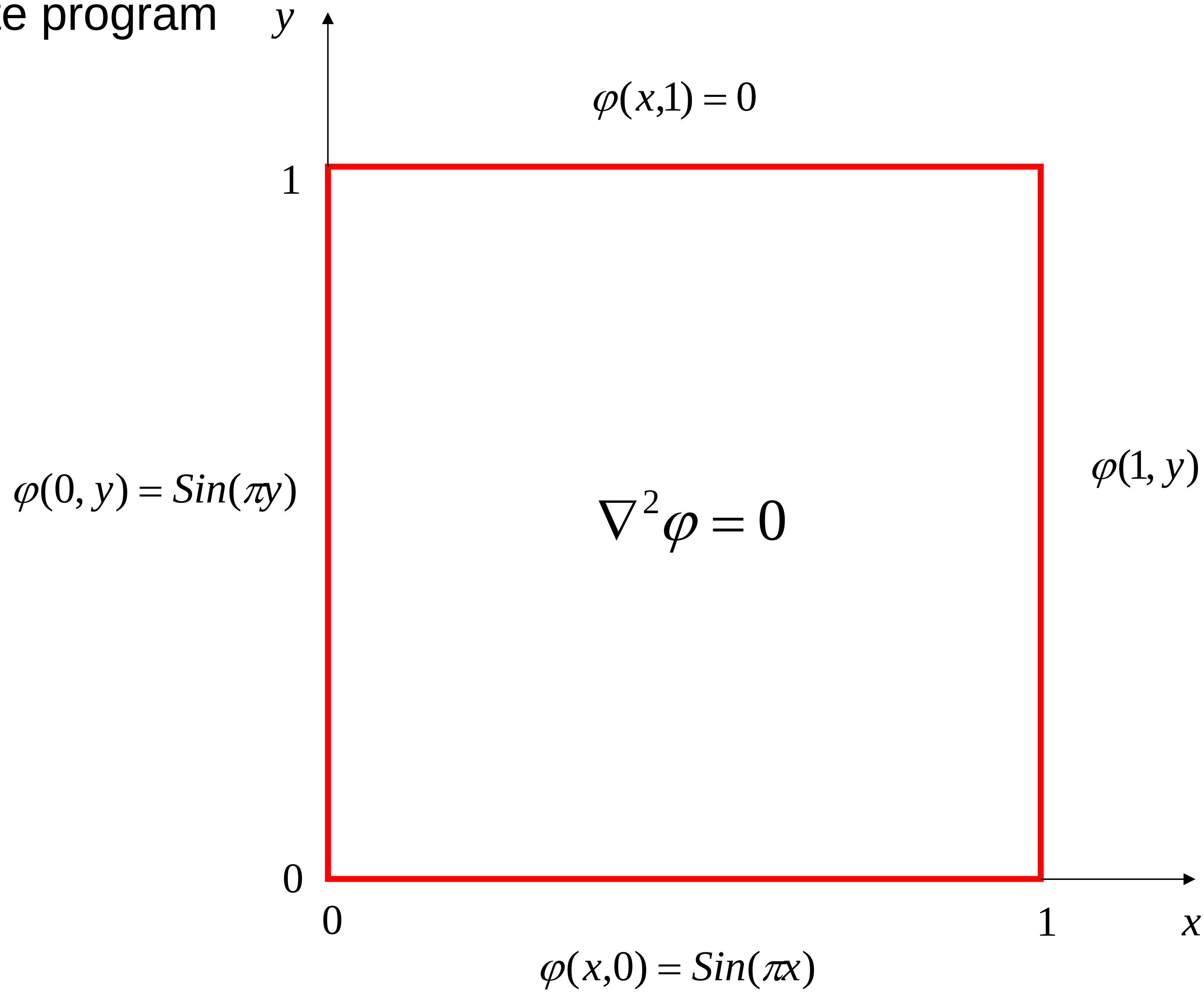
$$\varphi_{i,j}^{new}=\frac{1}{2}\left(\frac{\Delta x^2\Delta y^2}{\Delta x^2+\Delta y^2}\right)\left(\frac{\varphi_{i-1,j}^{old}+\varphi_{i+1,j}^{old}}{\Delta x^2}+\frac{\varphi_{i,j-1}^{old}+\varphi_{i,j+1}^{old}}{\Delta y^2}\right)$$

$$R=\sqrt{\sum_{i=1}^{m-1}\sum_{j=1}^{n-1}(\varphi_{i,j}^{new}-\varphi_{i,j}^{old})^2}$$

$$\left\{\varphi_{1,1}^{new},\varphi_{1,2}^{new},\ldots,\varphi_{1,n-1}^{new},\varphi_{2,1}^{new},\varphi_{2,2}^{new},\ldots,\varphi_{2,n-1}^{new},\ldots\ldots,\varphi_{m-1,1}^{new},\varphi_{m-1,2}^{new},\ldots,\varphi_{m-1,n-1}^{new}\right\}$$

$$R<Tol$$

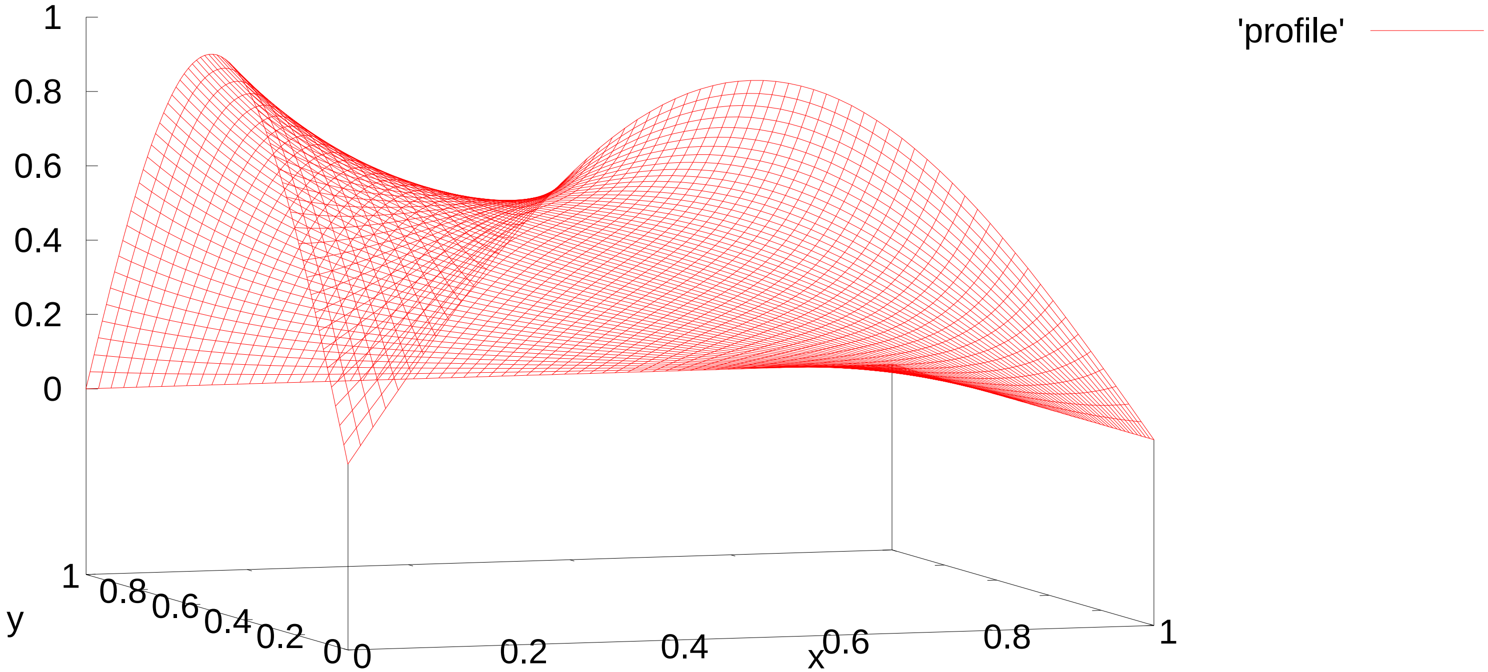
Write program



$$m = 64 \quad , \quad n = 64$$

$$Tol = 1.0d-4$$

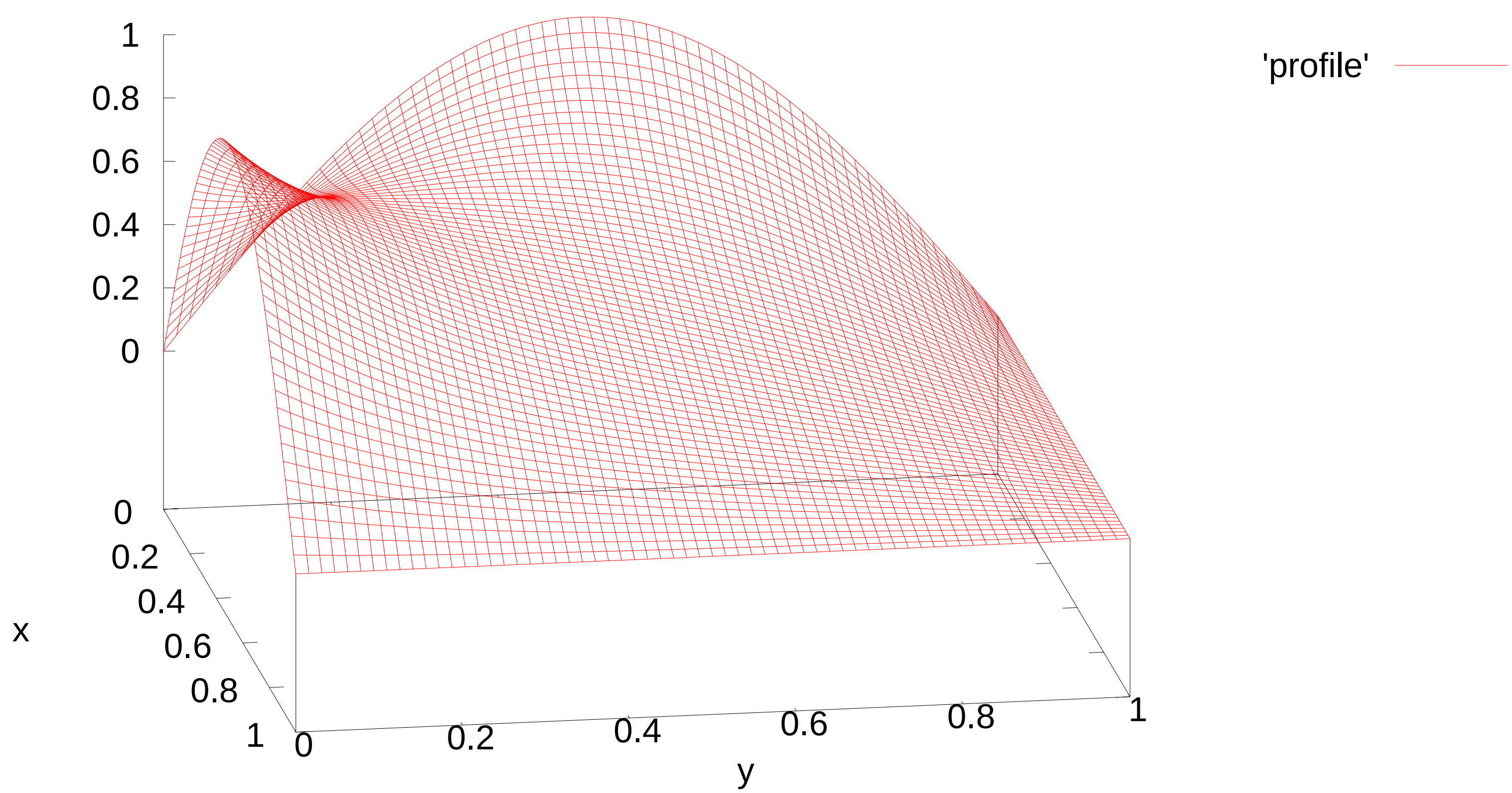
$$\varphi(i, j) = 1.0 \quad i = 1, \ldots, m-1 \quad \& \quad j = 1, \ldots, n-1$$



$$m = 64 \quad , \quad n = 64$$

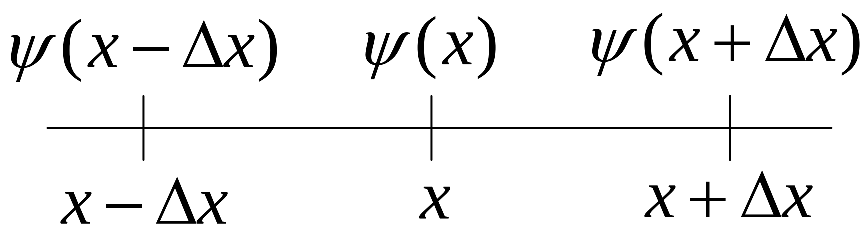
$$Tol = 1.0d - 4$$

$$\varphi(i, j) = 1.0 \quad i = 1, \ldots, m-1 \quad \& \quad j = 1, \ldots, n-1$$

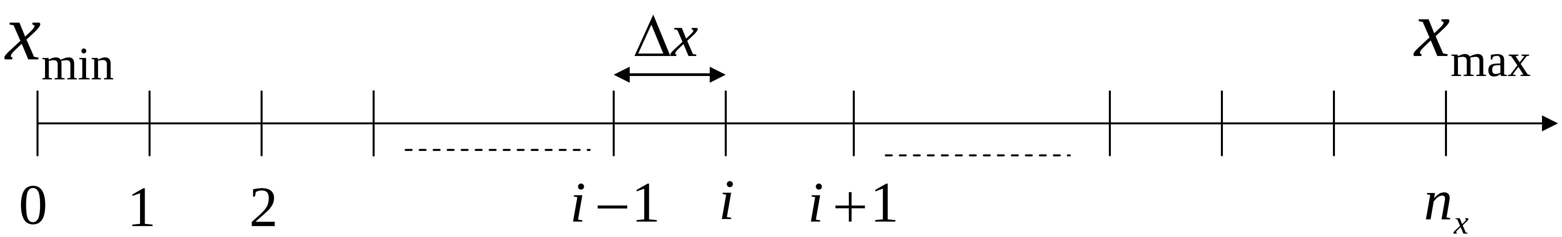


Eigenvalue problems

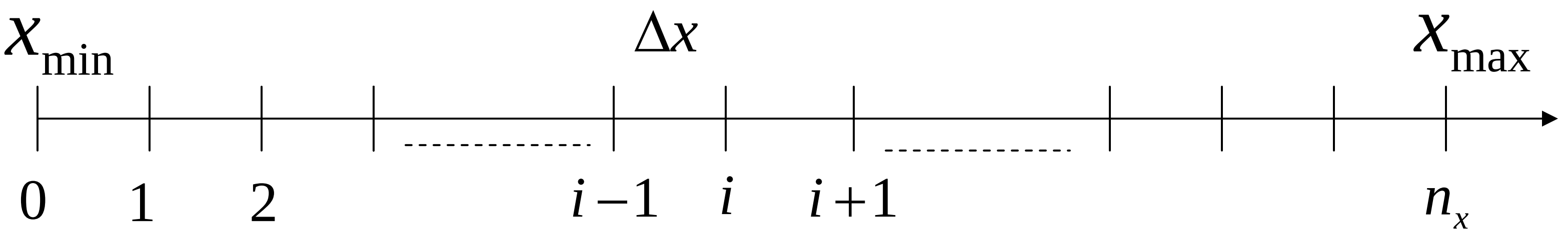
$$\frac{-1}{2}\frac{d^2\psi}{dx^2}+V(x)\psi = E\psi \qquad \hbar = m = 1, \qquad V(x)=\frac{1}{2}x^2, \qquad k=1$$



$$\boxed{\frac{d^2\psi}{dx^2}=\frac{\psi(x+\Delta x)-2\psi(x)+\psi(x-\Delta x)}{\Delta x^2}}$$



$$i \quad : \quad \frac{-1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\Delta x^2}\right)+V_i\psi_i = E\psi_i \ , \qquad V_i = V(x_{\mathrm{min}}+i\Delta x)$$



$$\psi_0 = \psi_{n_x} = 0$$

$$\begin{cases} i=1 \quad : \quad \dfrac{-1}{2}\left(\dfrac{\psi_0 - 2\psi_1 + \psi_2}{\Delta x^2}\right) + V_1\psi_1 = E\psi_1 \\ i=2 \quad : \quad \dfrac{-1}{2}\left(\dfrac{\psi_1 - 2\psi_2 + \psi_3}{\Delta x^2}\right) + V_2\psi_2 = E\psi_2 \\ \vdots \\ i=n_x\text{-}1 \ : \quad \dfrac{-1}{2}\left(\dfrac{\psi_{n_x-2} - 2\psi_{n_x-1} + \psi_{n_x}}{\Delta x^2}\right) + V_{n_x-1}\psi_{n_x-1} = E\psi_{n_x-1} \end{cases}$$

$$i \quad : \quad \frac{-1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\Delta x^2}\right)+V_i\psi_i=E\,\psi_i$$

$$\begin{pmatrix} \frac{1}{\Delta x^2}+V_1 & \frac{-1}{2\Delta x^2} & & & & \\ \frac{-1}{2\Delta x^2} & \frac{1}{\Delta x^2}+V_2 & \frac{-1}{2\Delta x^2} & & \phi & \\ & & \ddots & & & \\ & & \frac{-1}{2\Delta x^2} & \frac{1}{\Delta x^2}+V_i & \frac{-1}{2\Delta x^2} & \\ & \phi & & & \ddots & \\ & & & & \frac{-1}{2\Delta x^2} & \frac{1}{\Delta x^2}+V_{n_x-1} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_i \\ \vdots \\ \psi_{n_x-1} \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_i \\ \vdots \\ \psi_{n_x-1} \end{pmatrix}$$

Use library IMSL

Iterative method and Numerov Algorithm

- For one specific energy value "E"
- We know $\psi_{\min} = 0$ and also assume that $\left(\frac{d\psi}{dx}\right)_{\min}$ is specific
- Don't forget $\psi_{\max} = 0$

$$\frac{-1}{2}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \qquad \hbar = m = 1, \qquad V(x) = \frac{1}{2}x^2, \qquad k = 1$$

$$i \quad : \quad \frac{-1}{2}\left(\frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{\Delta x^2}\right) + V_i\psi_i = E\psi_i \ , \qquad V_i = V(x_{\min} + i\Delta x)$$

$$i = 1 \quad : \quad \frac{-1}{2}\left(\frac{\psi_0 - 2\psi_1 + \psi_2}{\Delta x^2}\right) + V_1\psi_1 = E\psi_1, \qquad \psi_0 = 0$$

$$\boxed{\psi_2 = 2\left(1 - \Delta x^2 (E - V_1)\right)\psi_1}$$

$$i = 2 \quad : \quad \frac{-1}{2}\left(\frac{\psi_1 - 2\psi_2 + \psi_3}{\Delta x^2}\right) + V_2\psi_2 = E\psi_2$$

$$\boxed{\psi_3 = -\psi_1 + 2\left(1 - \Delta x^2 (E - V_1)\right)\psi_2}$$

•
•
•

$$i = n_x \text{ -1} \quad : \quad \frac{-1}{2}\left(\frac{\psi_{n_x-2} - 2\psi_{n_x-1} + \psi_{n_x}}{\Delta x^2}\right) + V_{n_x-1}\psi_{n_x-1} = E\psi_{n_x-1}$$

$$\boxed{\psi_{n_x} = -\psi_{n_x-2} + 2\left(1 - \Delta x^2 (E - V_{n_x-1})\right)\psi_{n_x-1}}$$

If $\psi_{n_x} \rightarrow 0$ then the energy “E” is eigen value and $\{\psi_i\}$ is corresponding eigen function.