Program-M6

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Write and execute a FORTRAN program for computing motion of a particle trapped in a 1-dimensional box.

1 Theory

1.1 Particle in a 1D box

The particle moves freely on the x axis for $0 < x < L$, when it reaches the boundries $x = 0$ and $x = L$, it bounces and its velocity instantly reverses. The potential energy is given by (1).

$$V(x) = \begin{cases} 0 & 0 < x < L \\ +\infty & \text{elsewhere} \end{cases} \tag{1}$$

Initially, we know that the particle's initial position x_0 with initial velocity v_0 at time t_0. Equation of motions are:

$$x(t + dt) = x(t) + v(t)dt \tag{2}$$

When the particle bounces of the boundary $v(t) \to -v(t)$.

2 Numerical Solution

Assuming,

$$\begin{gathered} x_0 = 0.0 \\ v_x = 1.0 \text{ m/s} \\ t_0 = 0.0;\ t_f = 30.0;\ dt = 0.1 \\ L_0 = 0.0\ m \\ L_1 = 10.0\ m \\ \text{We expect } v(t) \to -v(t) \text{ at } x = 10,\ 20,\ 30,\ 40\ \ldots \end{gathered} \tag{3}$$

3 Program Algorithm

NOTE: Blue-colored text represents variables in the algorithm, eg. variable.

1. Program open.
2. Define variables (x0, t0, tf, dt, t, x, vx, l0, l1, fmt1).
3. Open a writable data file.
4. Get input from user for initial position (x0), inital velocity(v0), bounds (l0, l1) and time period(t0, tf, dt).
5. Print parameters to stdout for the user.
6. Write appropiate comments in the data file and initialize other parameters.
7. Define a do while loop with index t which runs from t0 to tf.
8. Compute the parameter x.
9. Write the parameters to stdout and data file.
10. If x reaches l0 or l1, v0 = - v0.
11. Increment the index according to t = t + dt
12. End do-while loop.
13. Close data file.
14. Program close.

4 Program

4.1 Fortran program:

For computing the parameters

```
!=========================================
! particle1d.f90
! Author: Devansh Shukla
!-----------------------------------------
program particle_1D
    ! Program to compute motion of a particle trapped in a one dimension box.

    implicit none
    real*8 :: x0=0.0, t0=0.0, tf=0.0, dt=0.0, t=0.0
    real*8 :: x=0.0, vx=0.0, l0=0.0, l1=0.0
    character(len=*), parameter :: fmt1 = "(F10.4, x, F10.4, x, F10.4)"

    open(unit=8, file="Particle1D.dat")

    print *, "---------------------------------------"
    print *, "Enter initial position x0"
    read *, x0

    print *, "Enter velocity vx"
    read *, vx

    print *, "Enter bounds l0, l1"
    read *, l0, l1

    print *, "Enter t0, tf, dt"
    read *, t0, tf, dt
    print *, "---------------------------------------"

    print "(x,A,F10.4)", "x0=", x0
    print "(x,A,F10.4,F10.4)", "l0, l1=", l0, l1
    print "(x,A,F10.4,F10.4,F10.4)", "t0, tf, dt=", t0, tf, dt
    print *, "---------------------------------------"

    print "(A10,A10,A10)", "time", "x(t)", "vx"

    ! Formatting l0, l1 to our standards for fortran floating point arithmatic
    l0 = l0
    l1 = l1 - dt
    t = t0
    x = x0
    do while (t .le. tf)
        write (*, fmt1) t, x, vx
        write (8, fmt1) t, x, vx
        x = x + vx * dt
        t = t + dt
        if (x .lt. l0 .or. x .gt. l1) vx = -vx
    enddo
    print *, "---------------------------------------"
    close(8)
end program particle_1D
```

4.2 Python program: Plots

```
#!/usr/bin/env python
"""
Author: Devansh Shukla
"""
# In[0]
import pandas as pd
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec

custom_rcparams = {
    "axes.labelsize": 8,
    "axes.titlesize": 10,
    "axes.grid": True,
    # Figure
    "figure.figsize": (8, 8),
    "figure.autolayout": True,
    "figure.titlesize": 10,
    "savefig.format": "pdf",
    "lines.linewidth": 1,
    # Legend
    "legend.fontsize": 8,
    "legend.frameon": True,
    # Ticks
```

```
    "xtick.labelsize": 7,
    "ytick.labelsize": 7,
    "xtick.minor.visible": True,
    "xtick.direction": "in",
    "ytick.direction": "in",
    "ytick.minor.visible": True,
    # TeX
    "pgf.texsystem": "lualatex",
}
mpl.rcParams.update(custom_rcparams)
mpl.use("pgf")
plt.ioff()

# t, x, y, vx, vy
df = pd.read_csv("Particle1D.dat", engine="python", delimiter=" ", header=None, skipinitialspace=True, comment="#")

gs = gridspec.GridSpec(2, 2)

ax = plt.subplot(gs[0, 0])
ax.plot(df[0], df[1], "o-", markersize=1.5, color="C0", label=r"$x(t)$")
ax.set_xlim(left=0, right=34)
ax.set_ylim(-0.5, 11)
ax.set_xlabel(r"$Time(s)$")
ax.set_ylabel(r"$Position(m)$")
ax.legend(loc="upper right")
plt.title("Position")

ax = plt.subplot(gs[0, 1])
ax.plot(df[0], df[2], "o-", markersize=1.5, color="C0", label=r"$v_{x}(t)$")
ax.set_xlim(left=0)
ax.set_ylim(-1.5, 1.5)
ax.set_xlabel(r"$Time(s)$")
ax.set_ylabel(r"$Velocity(m/s)$")
ax.legend(loc="upper right")
plt.title("Velocity")

ax = plt.subplot(gs[1, :])
ax.plot(df[1], [0]*len(df[1]), "o-", markersize=1.5, color="C0", label=r"$trace$")
ax.vlines(df[1].values.max(), -2, 2, "red", label=rf"$x={df[1].values.max()}$")
ax.vlines(df[1].values.min(), -2, 2, "red", label=rf"$x={np.abs(df[1].values.min())}$")
ax.set_xlim(left=df[1].values.min()-1, right=df[1].values.max()+1)
ax.set_ylim(-2, 2)
ax.set_xlabel(r"$X$")
ax.set_ylabel(r"$Y$")
ax.legend(loc="upper right")
plt.title("Trajectory")

# plt.show()
plt.savefig("plots/1d.pdf")
```

4.3 Python program: Animation

```
#!/usr/bin/env python
"""
Author: Devansh Shukla
"""
import pandas as pd
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
from matplotlib.animation import FuncAnimation, FFMpegWriter
import matplotlib.gridspec as gridspec

custom_rcparams = {
    "axes.labelsize": 7,
    "axes.titlesize": 8,
    "axes.grid": True,
    # Figure
    "figure.autolayout": True,
    "figure.titlesize": 9,
    "figure.figsize": (10, 3),
    # "figure.dpi": 150,
    "savefig.format": "pdf",
    "lines.linewidth": 1,
    # Legend
    "legend.fontsize": 8,
    "legend.frameon": True,
    # Ticks
    "xtick.labelsize": 8,
    "ytick.labelsize": 8,
```

```
    "xtick.minor.visible": True,
    "xtick.direction": "in",
    "ytick.direction": "in",
    "ytick.minor.visible": True,
}
mpl.rcParams.update(custom_rcparams)

# t, x, y, vx, vy
df = pd.read_csv("Particle1D.dat", engine="python", delimiter=" ", header=None, skipinitialspace=True, comment="#")
print(df)

time = df[0].values
pos_x = df[1].values
vel_x = df[2].values

gs = gridspec.GridSpec(1, 2, width_ratios=[2, 1], hspace=0)

fig = plt.figure()
ax1 = plt.subplot(gs[0, 0])
ax2 = plt.subplot(gs[0, 1])
plt.tight_layout()

line1, = ax1.plot([], [], 'o', lw=2, label="particle")
trace, = ax1.plot([], [], '-', lw=1, label="trace")
time_template = "time = %.2fs"
time_text = ax1.text(0.05, 0.8, '', transform=ax1.transAxes)

line_arrow = ax1.plot([], [], "-", color="C4", label=r"$v_x$")
patch = plt.Arrow(pos_x[0], 0, vel_x[0], 0, width=0.15, color="C4")
ax1.add_patch(patch)

line_vx, = ax2.plot([], [], '-', lw=2, label=r"$v_{x}(t)$")
ax2.legend()

line = [line1, line_vx, ]
ax1.set_xlim(left=pos_x.min()-1, right=pos_x.max()+1)
ax1.set_ylim(-2, 2)
ax1.vlines(pos_x.max(), -2, 2, "red", label=rf"$x={pos_x.max()}$")
ax1.vlines(pos_x.min(), -2, 2, "red", label=rf"$x={pos_x.min()}$")
ax1.set_xlabel(r"$X$", labelpad=-0.5)
ax1.set_ylabel(r"$Y$", labelpad=-0.5)
ax1.legend()

ax2.set_xlim(0, time[-1]+1)
ax2.set_ylim(-1.5, 1.5)
ax2.set_xlabel(r"$Time(s)$", labelpad=0)
ax2.set_ylabel(r"$v(m/s)$", labelpad=0)

def init():
    line[0].set_data([], [])
    line[1].set_data([], [])
    trace.set_data([], [])
    return line, trace

def animate(i):
    global time, pos_x, vel_x

    line[0].set_data(pos_x[i], 0)
    trace.set_data(pos_x[:i], 0)
    time_text.set_text(time_template % (time[i]))

    line[1].set_data(time[:i], vel_x[:i])

    global ax1, patch
    ax1.patches.remove(patch)
    patch = plt.Arrow(pos_x[i], 0, vel_x[i], 0, width=0.15, color="C4")
    ax1.add_patch(patch)
    return line, trace, time_text

def toggle_capture(*args, **kwargs):
    global ani, capture_no
    ani.pause()
    plt.gcf().savefig(f"plots/1d_{capture_no}.pdf")
    capture_no += 1
    ani.resume()

capture_no = 0
ani = FuncAnimation(fig, animate, frames=len(time), interval=10, init_func=init, blit=False, repeat=False)
fig.canvas.mpl_connect('button_press_event', toggle_capture)
```

```
writer = FFMpegWriter(fps=10)
ani.save('animation.mp4', writer=writer)
plt.show()
```

5 Results

5.1 Terminal Output

```
 ---------------------------------------
 Enter initial position x0
0.0
 Enter velocity vx
1.0
 Enter bounds l0, l1
0.0 10.0
 Enter t0, tf, dt
0.0 30.0 0.1
 ---------------------------------------
 x0=    0.0000
 l0, l1=    0.0000   10.0000
 t0, tf, dt=    0.0000   30.0000    0.1000
 ---------------------------------------
      time      x(t)      vx
    0.0000    0.0000    1.0000
    0.1000    0.1000    1.0000
    0.2000    0.2000    1.0000
    0.3000    0.3000    1.0000
    0.4000    0.4000    1.0000
    0.5000    0.5000    1.0000
    0.6000    0.6000    1.0000
    0.7000    0.7000    1.0000
    0.8000    0.8000    1.0000
    0.9000    0.9000    1.0000
    1.0000    1.0000    1.0000
    1.1000    1.1000    1.0000
    1.2000    1.2000    1.0000
    1.3000    1.3000    1.0000
    1.4000    1.4000    1.0000
    1.5000    1.5000    1.0000
    1.6000    1.6000    1.0000
    1.7000    1.7000    1.0000
    1.8000    1.8000    1.0000
    1.9000    1.9000    1.0000
    2.0000    2.0000    1.0000
    2.1000    2.1000    1.0000
    2.2000    2.2000    1.0000
    2.3000    2.3000    1.0000
    2.4000    2.4000    1.0000
    2.5000    2.5000    1.0000
    2.6000    2.6000    1.0000
    2.7000    2.7000    1.0000
    2.8000    2.8000    1.0000
    2.9000    2.9000    1.0000
    3.0000    3.0000    1.0000
    3.1000    3.1000    1.0000
    3.2000    3.2000    1.0000
    3.3000    3.3000    1.0000
    3.4000    3.4000    1.0000
    3.5000    3.5000    1.0000
    3.6000    3.6000    1.0000
    3.7000    3.7000    1.0000
    3.8000    3.8000    1.0000
    3.9000    3.9000    1.0000
    4.0000    4.0000    1.0000
    4.1000    4.1000    1.0000
    4.2000    4.2000    1.0000
    4.3000    4.3000    1.0000
    4.4000    4.4000    1.0000
    4.5000    4.5000    1.0000
    4.6000    4.6000    1.0000
    4.7000    4.7000    1.0000
    4.8000    4.8000    1.0000
    4.9000    4.9000    1.0000
    5.0000    5.0000    1.0000
    5.1000    5.1000    1.0000
    5.2000    5.2000    1.0000
    5.3000    5.3000    1.0000
    5.4000    5.4000    1.0000
    5.5000    5.5000    1.0000
```

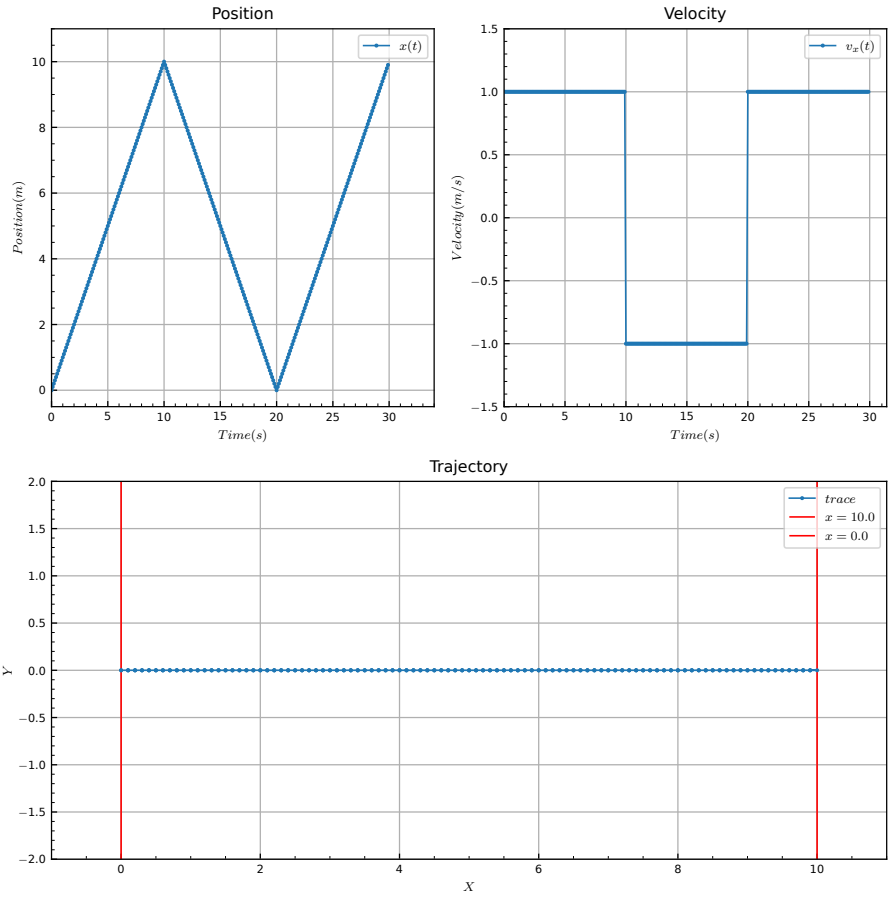
```
   5.6000    5.6000    1.0000
   5.7000    5.7000    1.0000
   5.8000    5.8000    1.0000
   5.9000    5.9000    1.0000
   6.0000    6.0000    1.0000
   6.1000    6.1000    1.0000
   6.2000    6.2000    1.0000
   6.3000    6.3000    1.0000
   6.4000    6.4000    1.0000
   6.5000    6.5000    1.0000
   6.6000    6.6000    1.0000
   6.7000    6.7000    1.0000
   6.8000    6.8000    1.0000
   6.9000    6.9000    1.0000
   7.0000    7.0000    1.0000
   7.1000    7.1000    1.0000
   7.2000    7.2000    1.0000
   7.3000    7.3000    1.0000
   7.4000    7.4000    1.0000
   7.5000    7.5000    1.0000
   7.6000    7.6000    1.0000
   7.7000    7.7000    1.0000
   7.8000    7.8000    1.0000
   7.9000    7.9000    1.0000
   8.0000    8.0000    1.0000
   8.1000    8.1000    1.0000
   8.2000    8.2000    1.0000
   8.3000    8.3000    1.0000
   8.4000    8.4000    1.0000
   8.5000    8.5000    1.0000
   8.6000    8.6000    1.0000
   8.7000    8.7000    1.0000
   8.8000    8.8000    1.0000
   8.9000    8.9000    1.0000
   9.0000    9.0000    1.0000
   9.1000    9.1000    1.0000
   9.2000    9.2000    1.0000
   9.3000    9.3000    1.0000
   9.4000    9.4000    1.0000
   9.5000    9.5000    1.0000
   9.6000    9.6000    1.0000
   9.7000    9.7000    1.0000
   9.8000    9.8000    1.0000
   9.9000    9.9000    1.0000
  10.0000   10.0000   -1.0000
  10.1000    9.9000   -1.0000
  10.2000    9.8000   -1.0000
  10.3000    9.7000   -1.0000
  10.4000    9.6000   -1.0000
  10.5000    9.5000   -1.0000
  10.6000    9.4000   -1.0000
  10.7000    9.3000   -1.0000
  10.8000    9.2000   -1.0000
  10.9000    9.1000   -1.0000
  11.0000    9.0000   -1.0000
  11.1000    8.9000   -1.0000
  11.2000    8.8000   -1.0000
  11.3000    8.7000   -1.0000
  11.4000    8.6000   -1.0000
  11.5000    8.5000   -1.0000
  11.6000    8.4000   -1.0000
  11.7000    8.3000   -1.0000
  11.8000    8.2000   -1.0000
  11.9000    8.1000   -1.0000
  12.0000    8.0000   -1.0000
  12.1000    7.9000   -1.0000
  12.2000    7.8000   -1.0000
  12.3000    7.7000   -1.0000
  12.4000    7.6000   -1.0000
  12.5000    7.5000   -1.0000
  12.6000    7.4000   -1.0000
  12.7000    7.3000   -1.0000
  12.8000    7.2000   -1.0000
  12.9000    7.1000   -1.0000
  13.0000    7.0000   -1.0000
  13.1000    6.9000   -1.0000
  13.2000    6.8000   -1.0000
  13.3000    6.7000   -1.0000
  13.4000    6.6000   -1.0000
```

```
  13.5000    6.5000   -1.0000
  13.6000    6.4000   -1.0000
  13.7000    6.3000   -1.0000
  13.8000    6.2000   -1.0000
  13.9000    6.1000   -1.0000
  14.0000    6.0000   -1.0000
  14.1000    5.9000   -1.0000
  14.2000    5.8000   -1.0000
  14.3000    5.7000   -1.0000
  14.4000    5.6000   -1.0000
  14.5000    5.5000   -1.0000
  14.6000    5.4000   -1.0000
  14.7000    5.3000   -1.0000
  14.8000    5.2000   -1.0000
  14.9000    5.1000   -1.0000
  15.0000    5.0000   -1.0000
  15.1000    4.9000   -1.0000
  15.2000    4.8000   -1.0000
  15.3000    4.7000   -1.0000
  15.4000    4.6000   -1.0000
  15.5000    4.5000   -1.0000
  15.6000    4.4000   -1.0000
  15.7000    4.3000   -1.0000
  15.8000    4.2000   -1.0000
  15.9000    4.1000   -1.0000
  16.0000    4.0000   -1.0000
  16.1000    3.9000   -1.0000
  16.2000    3.8000   -1.0000
  16.3000    3.7000   -1.0000
  16.4000    3.6000   -1.0000
  16.5000    3.5000   -1.0000
  16.6000    3.4000   -1.0000
  16.7000    3.3000   -1.0000
  16.8000    3.2000   -1.0000
  16.9000    3.1000   -1.0000
  17.0000    3.0000   -1.0000
  17.1000    2.9000   -1.0000
  17.2000    2.8000   -1.0000
  17.3000    2.7000   -1.0000
  17.4000    2.6000   -1.0000
  17.5000    2.5000   -1.0000
  17.6000    2.4000   -1.0000
  17.7000    2.3000   -1.0000
  17.8000    2.2000   -1.0000
  17.9000    2.1000   -1.0000
  18.0000    2.0000   -1.0000
  18.1000    1.9000   -1.0000
  18.2000    1.8000   -1.0000
  18.3000    1.7000   -1.0000
  18.4000    1.6000   -1.0000
  18.5000    1.5000   -1.0000
  18.6000    1.4000   -1.0000
  18.7000    1.3000   -1.0000
  18.8000    1.2000   -1.0000
  18.9000    1.1000   -1.0000
  19.0000    1.0000   -1.0000
  19.1000    0.9000   -1.0000
  19.2000    0.8000   -1.0000
  19.3000    0.7000   -1.0000
  19.4000    0.6000   -1.0000
  19.5000    0.5000   -1.0000
  19.6000    0.4000   -1.0000
  19.7000    0.3000   -1.0000
  19.8000    0.2000   -1.0000
  19.9000    0.1000   -1.0000
  20.0000   -0.0000    1.0000
  20.1000    0.1000    1.0000
  20.2000    0.2000    1.0000
  20.3000    0.3000    1.0000
  20.4000    0.4000    1.0000
  20.5000    0.5000    1.0000
  20.6000    0.6000    1.0000
  20.7000    0.7000    1.0000
  20.8000    0.8000    1.0000
  20.9000    0.9000    1.0000
  21.0000    1.0000    1.0000
  21.1000    1.1000    1.0000
  21.2000    1.2000    1.0000
  21.3000    1.3000    1.0000
```

```
  21.4000     1.4000     1.0000
  21.5000     1.5000     1.0000
  21.6000     1.6000     1.0000
  21.7000     1.7000     1.0000
  21.8000     1.8000     1.0000
  21.9000     1.9000     1.0000
  22.0000     2.0000     1.0000
  22.1000     2.1000     1.0000
  22.2000     2.2000     1.0000
  22.3000     2.3000     1.0000
  22.4000     2.4000     1.0000
  22.5000     2.5000     1.0000
  22.6000     2.6000     1.0000
  22.7000     2.7000     1.0000
  22.8000     2.8000     1.0000
  22.9000     2.9000     1.0000
  23.0000     3.0000     1.0000
  23.1000     3.1000     1.0000
  23.2000     3.2000     1.0000
  23.3000     3.3000     1.0000
  23.4000     3.4000     1.0000
  23.5000     3.5000     1.0000
  23.6000     3.6000     1.0000
  23.7000     3.7000     1.0000
  23.8000     3.8000     1.0000
  23.9000     3.9000     1.0000
  24.0000     4.0000     1.0000
  24.1000     4.1000     1.0000
  24.2000     4.2000     1.0000
  24.3000     4.3000     1.0000
  24.4000     4.4000     1.0000
  24.5000     4.5000     1.0000
  24.6000     4.6000     1.0000
  24.7000     4.7000     1.0000
  24.8000     4.8000     1.0000
  24.9000     4.9000     1.0000
  25.0000     5.0000     1.0000
  25.1000     5.1000     1.0000
  25.2000     5.2000     1.0000
  25.3000     5.3000     1.0000
  25.4000     5.4000     1.0000
  25.5000     5.5000     1.0000
  25.6000     5.6000     1.0000
  25.7000     5.7000     1.0000
  25.8000     5.8000     1.0000
  25.9000     5.9000     1.0000
  26.0000     6.0000     1.0000
  26.1000     6.1000     1.0000
  26.2000     6.2000     1.0000
  26.3000     6.3000     1.0000
  26.4000     6.4000     1.0000
  26.5000     6.5000     1.0000
  26.6000     6.6000     1.0000
  26.7000     6.7000     1.0000
  26.8000     6.8000     1.0000
  26.9000     6.9000     1.0000
  27.0000     7.0000     1.0000
  27.1000     7.1000     1.0000
  27.2000     7.2000     1.0000
  27.3000     7.3000     1.0000
  27.4000     7.4000     1.0000
  27.5000     7.5000     1.0000
  27.6000     7.6000     1.0000
  27.7000     7.7000     1.0000
  27.8000     7.8000     1.0000
  27.9000     7.9000     1.0000
  28.0000     8.0000     1.0000
  28.1000     8.1000     1.0000
  28.2000     8.2000     1.0000
  28.3000     8.3000     1.0000
  28.4000     8.4000     1.0000
  28.5000     8.5000     1.0000
  28.6000     8.6000     1.0000
  28.7000     8.7000     1.0000
  28.8000     8.8000     1.0000
  28.9000     8.9000     1.0000
  29.0000     9.0000     1.0000
  29.1000     9.1000     1.0000
  29.2000     9.2000     1.0000
```

```
  29.3000     9.3000     1.0000
  29.4000     9.4000     1.0000
  29.5000     9.5000     1.0000
  29.6000     9.6000     1.0000
  29.7000     9.7000     1.0000
  29.8000     9.8000     1.0000
  29.9000     9.9000     1.0000
-------------------------------------
```

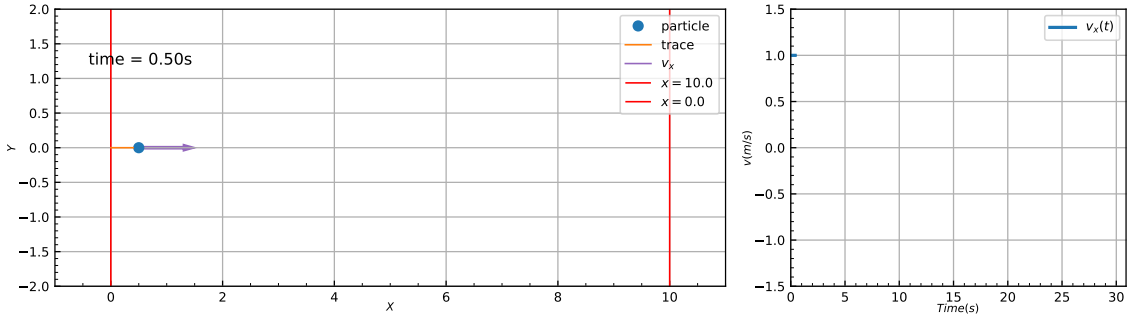
5.1.1 Plots

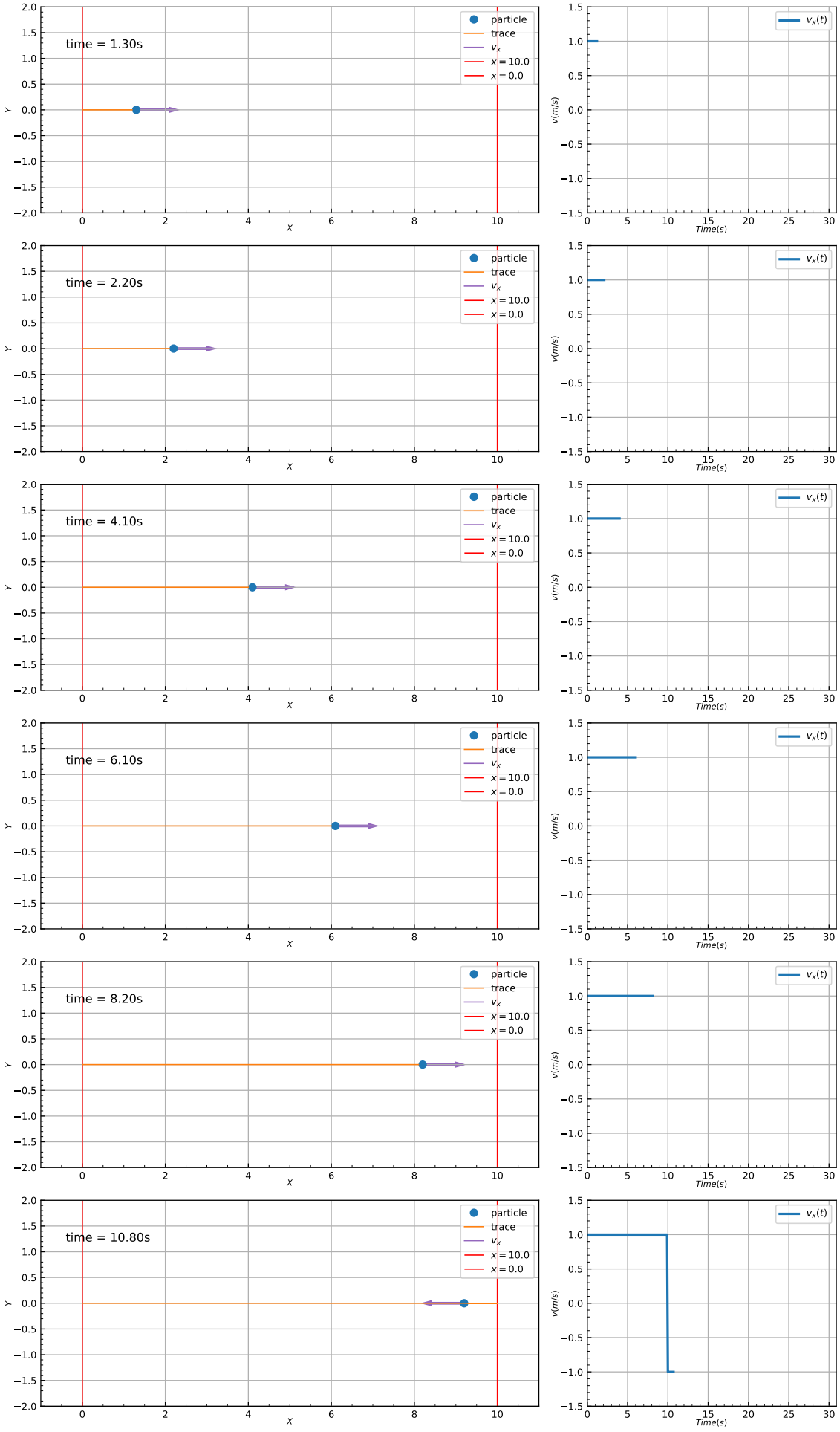


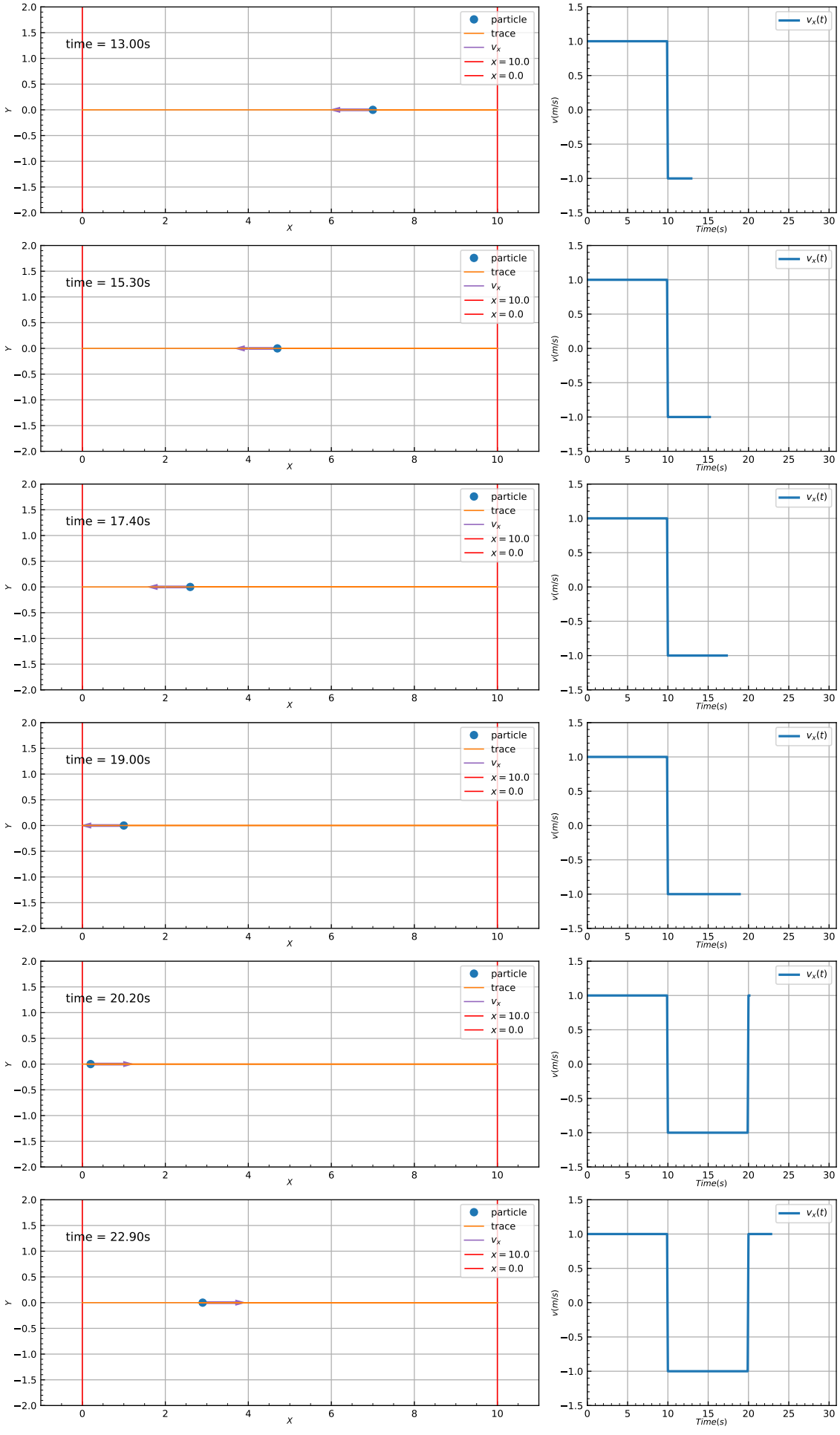
5.1.2 Animation

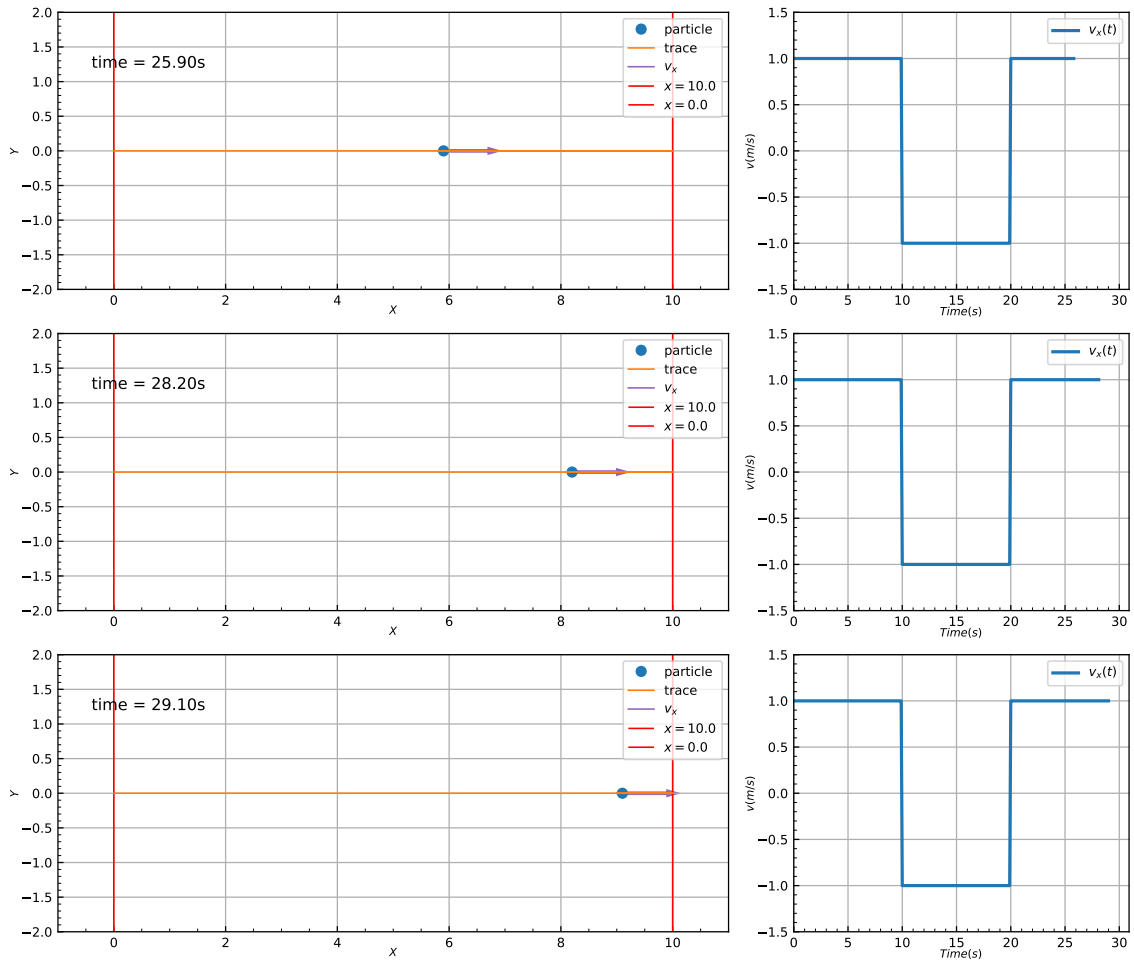
Note: Input parameters,

$$
\begin{aligned}
&x_0 = 0.0 \\
&v_x = 1.0 \text{ m/s} \\
&t_0 = 0.0;\ t_f = 30.0,\ dt = 0.1 \\
&L_0 = 0.0\ m \\
&L_1 = 10.0\ m
\end{aligned}
\tag{4}
$$




time = 1.30s
time = 2.20s
time = 4.10s
time = 6.10s
time = 8.20s
time = 10.80s
particle
trace
v_x
$x = 10.0$
$x = 0.0$
$v_x(t)$
X
Y
Time(s)
v(m/s)


time = 13.00s
time = 15.30s
time = 17.40s
time = 19.00s
time = 20.20s
time = 22.90s
particle
trace
v_x
$x = 10.0$
$x = 0.0$
$v_x(t)$
X
Y
Time(s)
v(m/s)



6 Remarks

The program can be used to numerically trace and simulate the motion of a particle trapped in a box, provided the required parameters are defined.

The parameters computed numerically and via the programs are in agreement.