Computational Physics – Exercise 5: Molecular dynamics simulations

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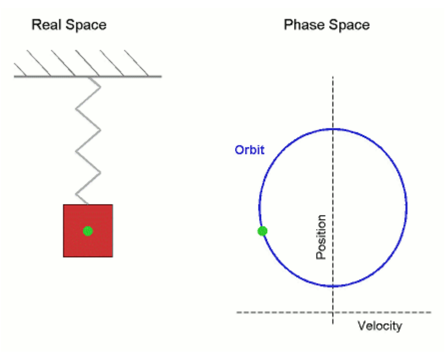
Molecular dynamics

Exercise 1

- Equation of motion $m_n \mathbf{a}_n = \mathbf{F}_n$
  - Mass of particle n : m_n
  - Acceleration of particle n : $\mathbf{a}_n = \dfrac{d^2 \mathbf{r}_n}{dt^2}$
  - Force acting on particle n : $\mathbf{F}_n$
- Harmonic oscillator

$$m \frac{d^2 x}{dt^2} = m\ddot{x} = -kx$$

http://en.wikipedia.org/wiki/Simple_harmonic_motion



Molecular dynamics
Exercise 1

- Implement the Euler algorithm for the harmonic oscillator ($V'(x) = kx$)
- Choice of units: $m = 1 \quad , \quad k = 1$
- Initial position and velocity: $x(0) = 0$ and $v(0) = 1$
- Solve using $\Delta t = 0.1, 0.01, 0.001$ for $j = 1, \ldots, [10000 / \Delta t]$
- Plot $x(j\Delta t)$ and compare with $\sin(j\Delta t)$
- Argue whether this algorithm is useful or not
  - It is not!

Molecular dynamics
Exercise 2

- Implement the two variants (a) and (b) of the Euler-Cromer algorithm for the harmonic oscillator ($V'(x) = x$) and repeat the calculations of exercise 1
- Implementation:

$$(a) = \begin{cases} p((j+1)\Delta t) = p(j\Delta t) - \Delta t V'(x(j\Delta t)) \\ x((j+1)\Delta t) = x(j\Delta t) + \Delta t p((j+1)\Delta t) \end{cases}$$

$$(b) = \begin{cases} x((j+1)\Delta t) = x(j\Delta t) + \Delta t p(j\Delta t) \\ p((j+1)\Delta t) = p(j\Delta t) - \Delta t V'(x((j+1)\Delta t)) \end{cases}$$

Argue whether these algorithms are useful or not

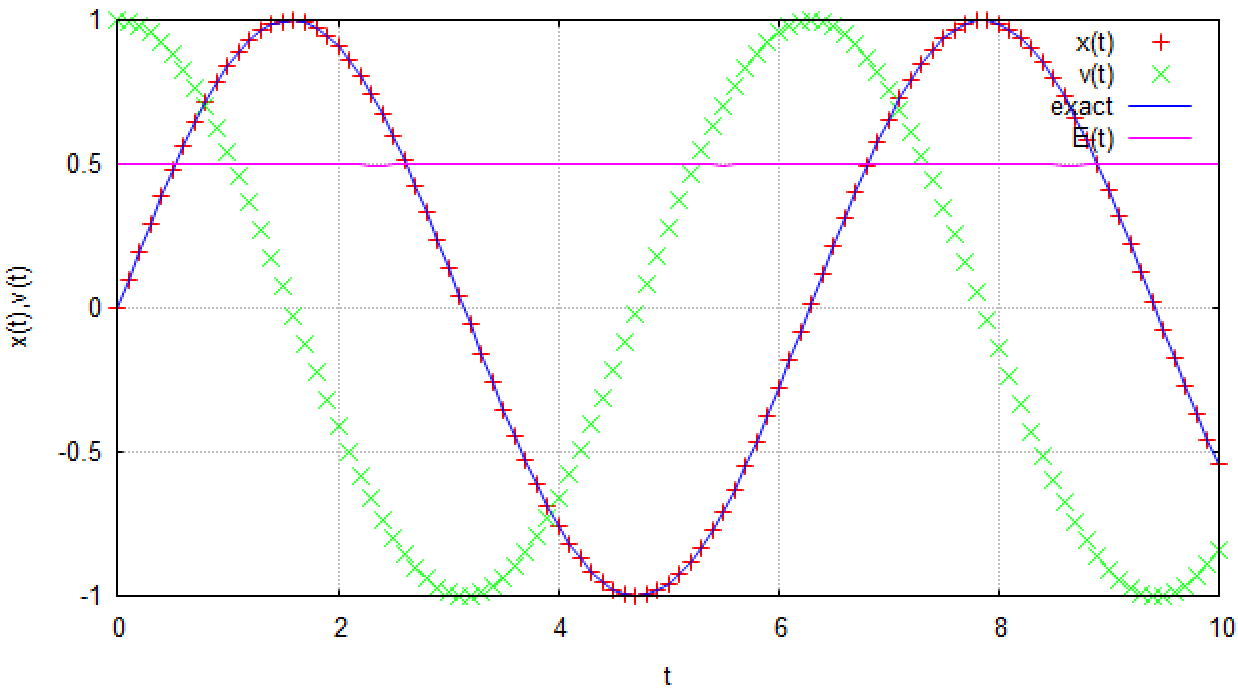
Molecular dynamics

Exercise 2

- Plot $x(t)$, $v(t)$, and the energy $E(t)=v^2(t)/2+V(x(t))$ and also plot the analytical solution $x(t)=\sin t$ and $E=1/2$ for comparison. Explain why the energy $E(t)$ is not exactly constant, as it should be according to classical mechanics
  - Use e.g $\Delta t=0.01$ for $j=1,\ldots,1000$ for plotting purposes

Molecular dynamics
Exercise 2

- Example of such a plot



Molecular dynamics
Exercise 3

- Use the velocity Verlet algorithm and repeat the simulations of exercise 2
- Use $\Delta t = 0.1, \quad 0.01$
- Plot $x(t), v(t)$ and the energy $E(t) = v^2(t)/2 + V(x(t))$ and also plot the analytical solution $x(t) = \sin t$ and $E = 1/2$ for comparison.
- Discuss the differences with the results of the Verlet and Euler-Cromer algorithms

Molecular dynamics
Exercise 4

- Use the velocity Verlet algorithm to solve the equation of motion of many coupled oscillators:

$$H = K + V = \frac{1}{2}\sum_{n=1}^{N} v_n^2 + \frac{1}{2}\sum_{n=1}^{N-1} (x_n - x_{n+1})^2$$

$$\frac{\partial V}{\partial x_k} = 2x_k - x_{k-1} - x_{k+1} \quad , \quad 1 < k < N$$

$$\frac{\partial V}{\partial x_1} = x_1 - x_2 \quad , \quad \frac{\partial V}{\partial x_N} = x_N - x_{N-1}$$

Molecular dynamics

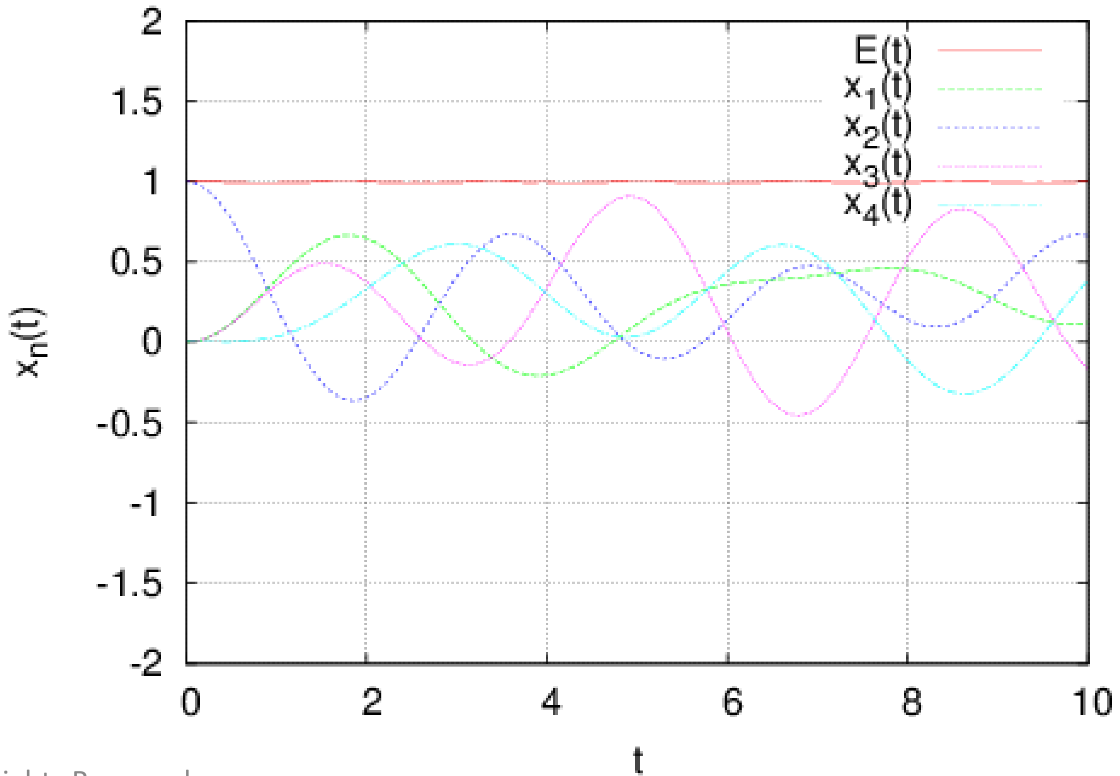
Exercise 4

- For $N = 4, 16, 128$ and $\Delta\mathrm{t} = 0.1, \quad 0.01$
- Initial configurations
  1. $v_1(0), \ldots, v_N(0) = 0$
     $x_1(0), \ldots, x_N(0) = 0$ except $x_{N/2}(0) = 1$
  2. $v_1(0), \ldots, v_N(0) = 0$
     $x_k(0) = \sin\frac{\pi jk}{N+1}$ for $k = 1, \ldots, N$ and $j = 1, N/2$
- Plot the results for several $x_k(t)$ and interpret!

Molecular dynamics

Exercise 4

- Example for $N = 4, \Delta t = 0.1$ and initial configuration (1)



Report

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- Filename: Follow the instructions by the tutors
- Content of the report:
  - Names + matricle numbers + e-mail addresses + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 10 AM, June 4, 2024