

BMB 173 – Winter 2017

Homework Set 9.1 (120 points) – Assigned 3/7/17. Due 3/14/17

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Office Hours:

Friday 3/10/17 from 2-3pm in Spalding B123 or by appointment

Monday 3/13/17 from 3-4pm in Spalding B123 or by appointment

1. Methods of Integration (55 points)

Several methods exist to numerically integrate Newton's equations of motion and solve molecular dynamics problems. Two of the most commonly used are Euler integration and Velocity Verlet integration.

Please refer to the following resources to understand and compare these methods:

https://en.wikipedia.org/wiki/Verlet_integration

https://en.wikipedia.org/wiki/Euler_method

<http://gafferongames.com/game-physics/integration-basics/>

Note: There are three common flavors of Verlet integration schemes: the Basic Verlet algorithm, the Verlet Leapfrog algorithm, and the Velocity Verlet algorithm. This problem set asks about the Velocity Verlet algorithm.

- a. (15 points) The Euler and Velocity Verlet integration methods follow different algorithms to numerically integrate. The Velocity Verlet algorithm has 4 steps, listed below. Referring to the above sources, fill in the missing components (denoted by light gray boxes) for the Velocity Verlet integration algorithm:

1. Calculate: $\vec{v}\left(t + \frac{1}{2}\Delta t\right) = \vec{v}(t) + \boxed{}$

2. Calculate: $\boxed{} = \vec{x}(t) + \vec{v}\left(t + \frac{1}{2}\Delta t\right)\Delta t$

3. Derive $\vec{a}(t + \Delta t)$ from the interaction potential using $\vec{x}(t + \Delta t)$ where $\vec{a} = \frac{\vec{F}(x)}{m}$

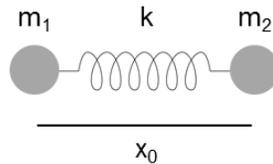
4. Calculate: $\vec{v}(t + \Delta t) = \vec{v}(t) + \boxed{}$

- b. (5 points) Which of these two integration methods is simpler?
- c. (10 points) Under what condition will Euler integration yield a correct result?
- d. (10 points) How can one adjust Euler Integration to get a more accurate result? What is the tradeoff in doing this?
- e. (15 points) As you can see, MD simulation is constrained by the choice of the numerical integration algorithm used. What are three other limits of MD simulation?

2. Harmonic Potential (65 points)

Next, we will use molecular dynamics to solve a classic two-body problem: simulation of the positions of two masses connected by a spring.

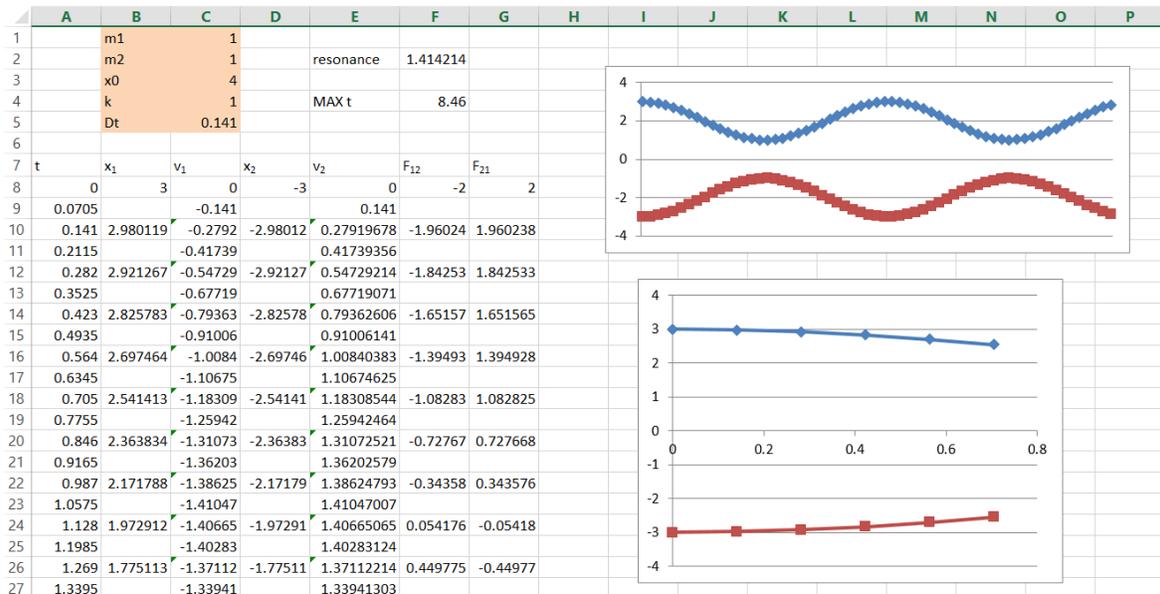
Consider m_1 and m_2 , shown below, on a spring with a force constant k describing the stiffness of the spring. The initial distance between the two masses is x_0 .



The potential energy can be modeled as the following harmonic potential:

$$U(x) = \left(\frac{k}{2}\right)(x - x_0)^2$$

In the spreadsheet associated with this homework, the Velocity Verlet algorithm can be used to simulate the positions of the two masses. An example of the filled in spreadsheet is below. The orange box denotes the input parameters.



- a. (10 points) Note that in the table, all of the values in rows 8 and 10 are filled in, while values are missing in row 9. This is on purpose. Explain the reason for this choice in terms of Velocity Verlet integration algorithm. What is the computational benefit of this choice?

- b. (15 points) Now, let's use Velocity Verlet integration to simulate this system.
- i. (5 points) First, derive the force, $F(x)$, for this harmonic oscillator.
 - ii. (10 points) Next, write equations to update the velocity and position as well. Use these equations to fill in the missing rows of the spreadsheet. Take the time out to cell A128. You will know you have the correct solution when your values match those in the screenshot above.
- c. (10 points) The equation for the resonance frequency, ω , is found in cell F2.

By the way, the resonance frequency is found by solving the equations of motion analytically:

$$F(x) = ma = m \frac{d^2x}{dt^2}$$

Substituting in what we know about our system, we can arrive at the following second order linear differential equation:

$$\frac{d^2x}{dt^2} = -\omega^2 x$$

where $\omega = \sqrt{\frac{k(m_1+m_2)}{m_1m_2}} = \sqrt{\frac{k}{\mu}}$.

You can derive this yourself, if you would like.

The solution to this differential equation is of the form:

$$x(t) = A \cos \omega t + B \sin \omega t$$

Why is the resonance frequency important for this system? What constraint does it place on an important MD parameter?

- d. (10 points) Reproduce the graph for each of the following time steps:
- i. 10% of the resonance frequency
 - ii. 1
 - iii. The resonance frequency
 - iv. 1.415

- e. (20 points) Let's further analyze the results in part d:
- i. What time step best simulates the actual event?
 - ii. What time step shows the positions of the masses diverging over the simulation?
 - iii. Why does this time step lead to divergence of the mass positions?
 - iv. Now compare graphs for $\Delta t = 1$ and $\Delta t = 10\%$ of the resonance frequency. Does the $\Delta t = 1$ time step give more or less detail about positions of the masses during one oscillation? Does the $\Delta t = 1$ time step give more or less detail about positions of the masses over time (i.e. multiple oscillations)?
 - v. How might this compromise play out in modeling a protein dynamic system?