Computational Physics

Lecture 2

Organisation of the course - Team

Two teaching assistants here to help:

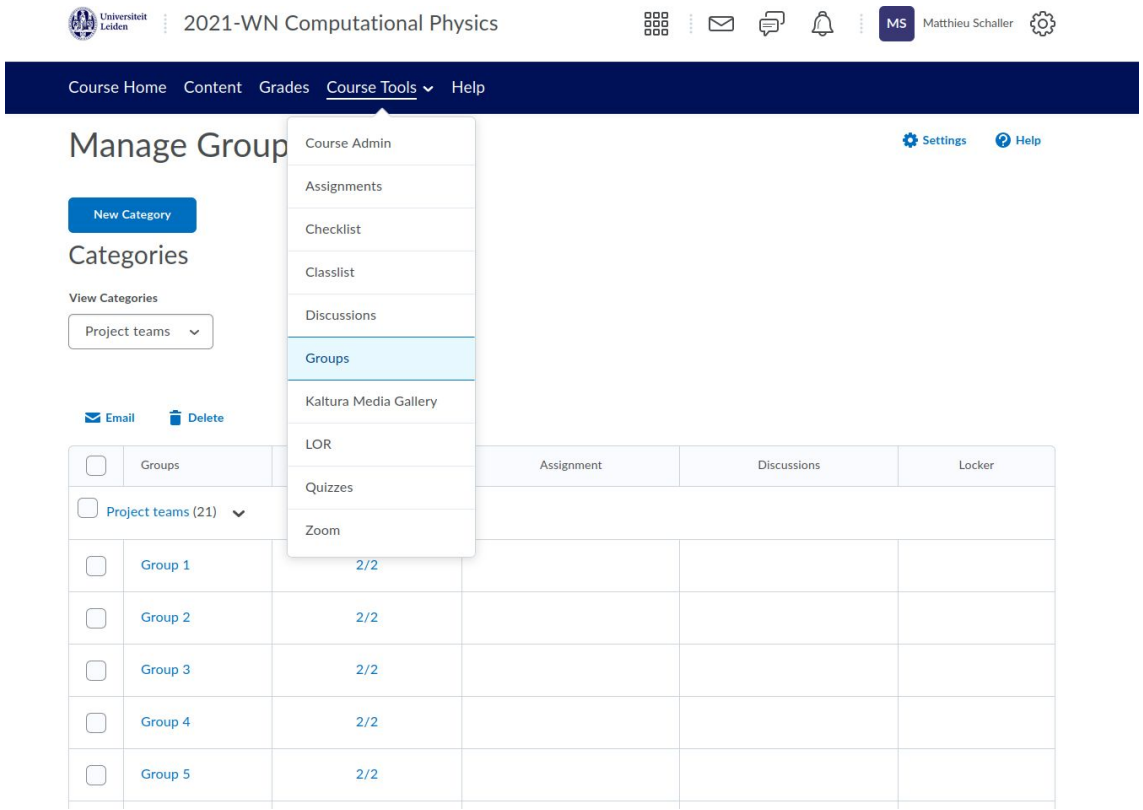
- Eloïc Vallée (vallee@lorentz.leidenuniv.nl)
- Orestis Karapiperis (karapiperis@lorentz.leidenuniv.nl)

TA hour: Wednesday 10am. Room 223 and room 258.

Organisation of the course - Teams

Please register your teams on *Brightspace*.

Pick any of the empty group.



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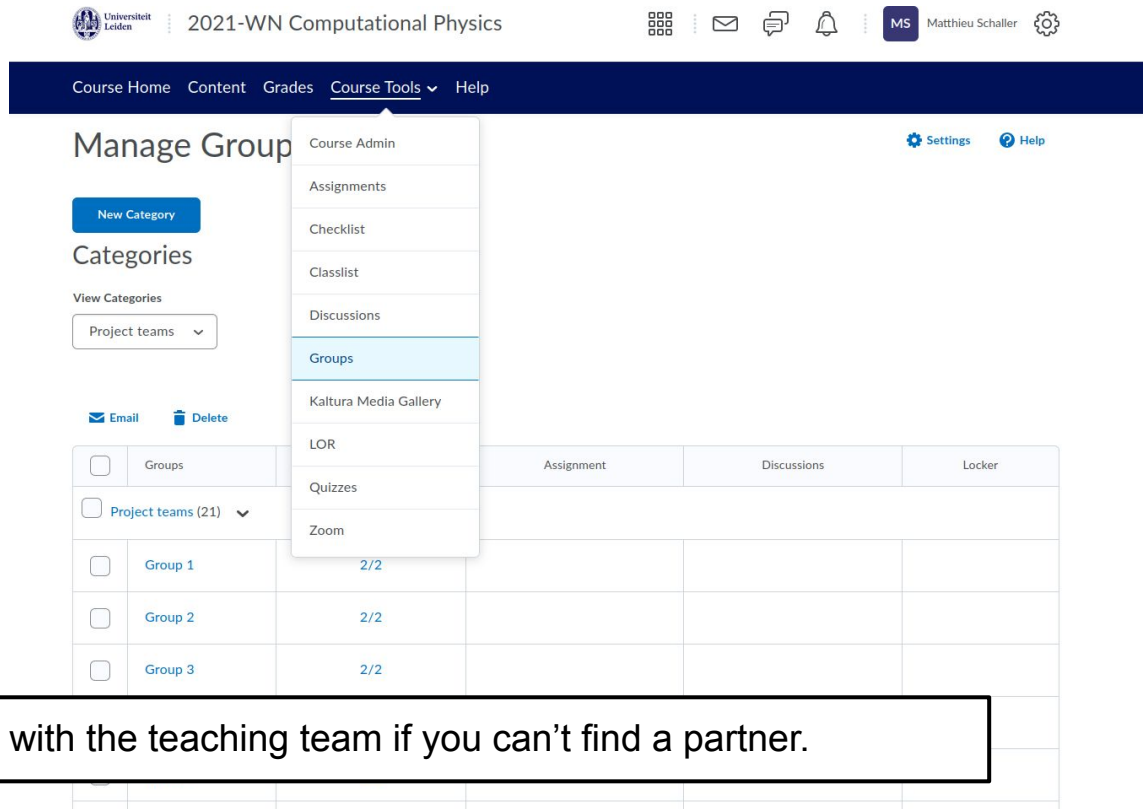
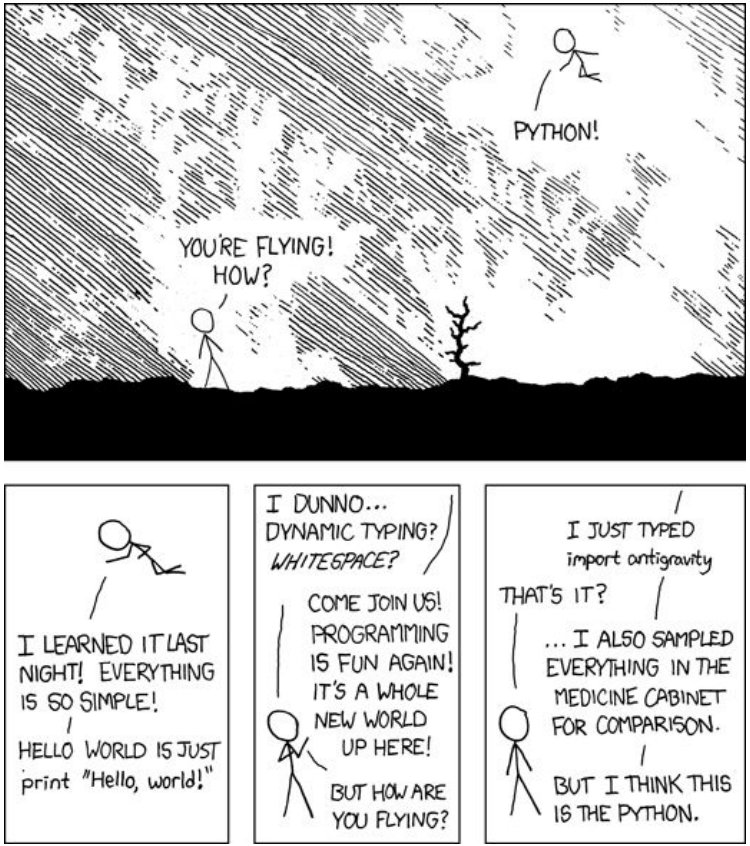


Get in touch with the teaching team if you can’t find a partner.

Organisation of the course - Marking

- Grading based on the simulation code (30%) and report (70%).
- Score sheet for the 1st project now on *Brightspace*:
  “General Information” → “Grading”.
- Also check the coding guidelines for recommendations.
  - See in particular the bit about *jupyter* notebooks.

Organisation of the course - Programming Language



https://xkcd.com/353/

Organisation of the course - Literature on MD

If you want to go beyond, this is an excellent article for MD practitioners:

- E. Braun et al., *Best Practices for Foundations in Molecular Simulations*, Living J.Comp.Mol.Sci, 2019 https://www.livecomsjournal.org/article/5957-best-practices-for-foundations-in-molecular-simulations-article-v1-0

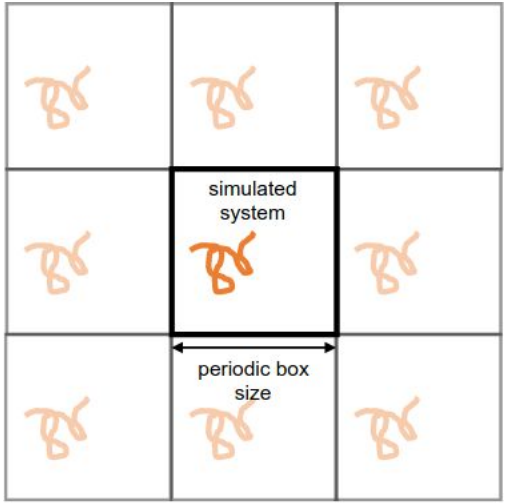


Figure 3. Periodic boundary conditions are shown for a simple 2D system. Note that the simulated system is a sub-ensemble within an infinite system of identical, small ensembles.

Organisation of the course - Program

Feb 09 – Introduction to MD, interactions, EoMs, boundary conditions

Feb 16 – Choice of units, energy of the system

Feb 23 – Verlet integration algorithm, minimum image convention

Mar 01 – Setting up initial conditions

Mar 08 – Observing the simulation: correlations & pressure

Mar 15 – Individual discussions

First project deadline: Thursday March 21 (midnight)

Questions?

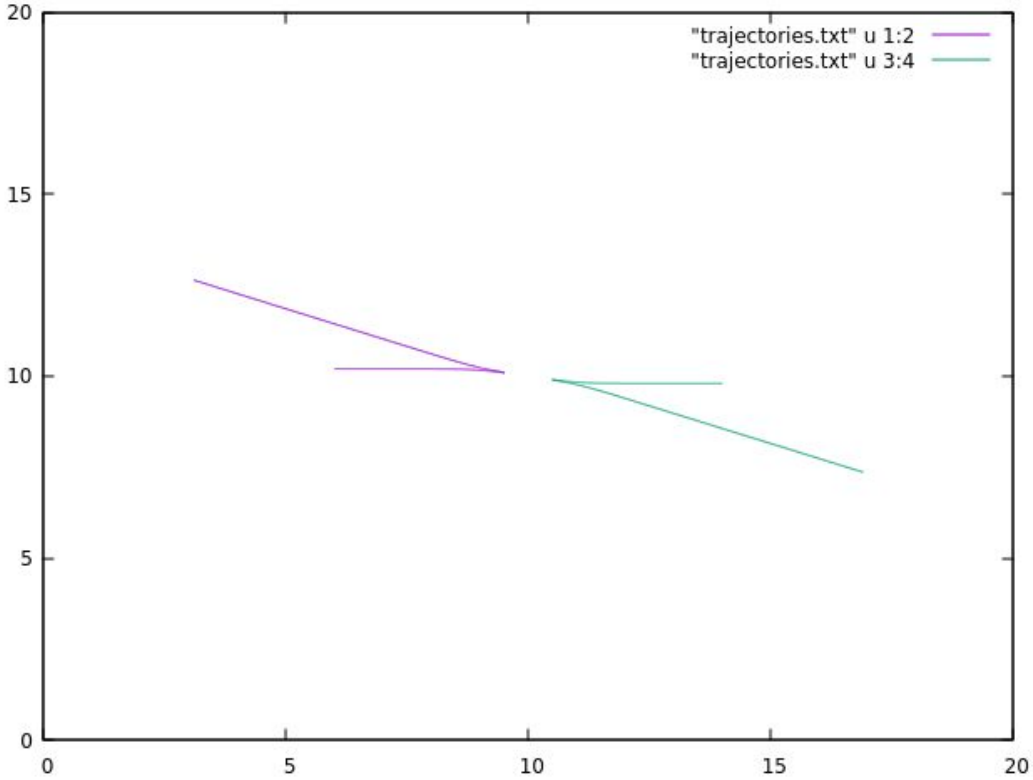
Project 1: Units and Energy

Last week's summary

- Considered the equations of motion (EoMs) for a set of atoms interacting via a *Lennard-Jones* potential; and specifically the case of some Argon atoms.
- Used a simple 1st order Taylor expansion to turn the 2nd order DEs (the EoMs) into a pair of *discretized* equations.
- Discussed a generic simulation step and looked at the time-step length h.
- Introduced *periodic boundary conditions* as a mean to simulate an infinite Universe. Used the *"minimal image convention"* to interact particles.

Question: How do we verify the validity of a simulation?

Last week’s summary: collisions



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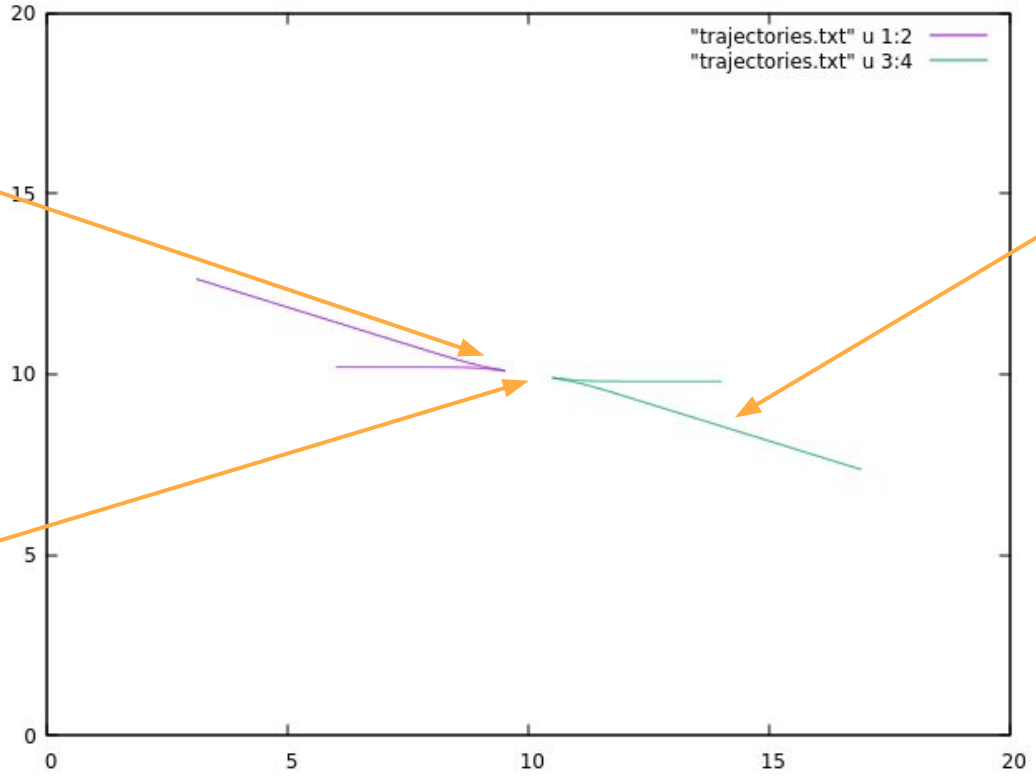
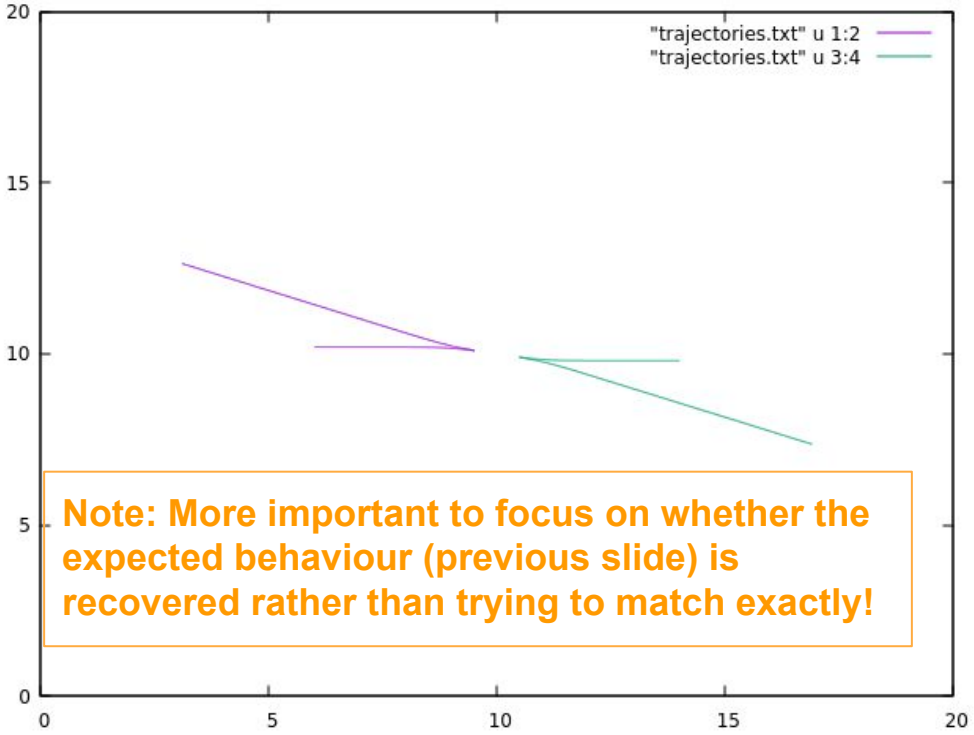


Attract each others first

Repel each others before contact

Move in straight lines before/after the collision.

Last week's summary: collisions



Note: More important to focus on whether the expected behaviour (previous slide) is recovered rather than trying to match exactly!

If you want to compare to your tests, I used a "fake" Argon model with:

$L = 20$ m

$\sigma = 1$ m

$\varepsilon = 1$ J

And starting points:

$x_1 = (0.3\ L, 0.51\ L)$ $v_1 = (0.09, 0)$

$x_2 = (0.7\ L, 0.49\ L)$ $v_2 = (-0.09, 0)$

Simulated to t = 100s, h = 0.1s

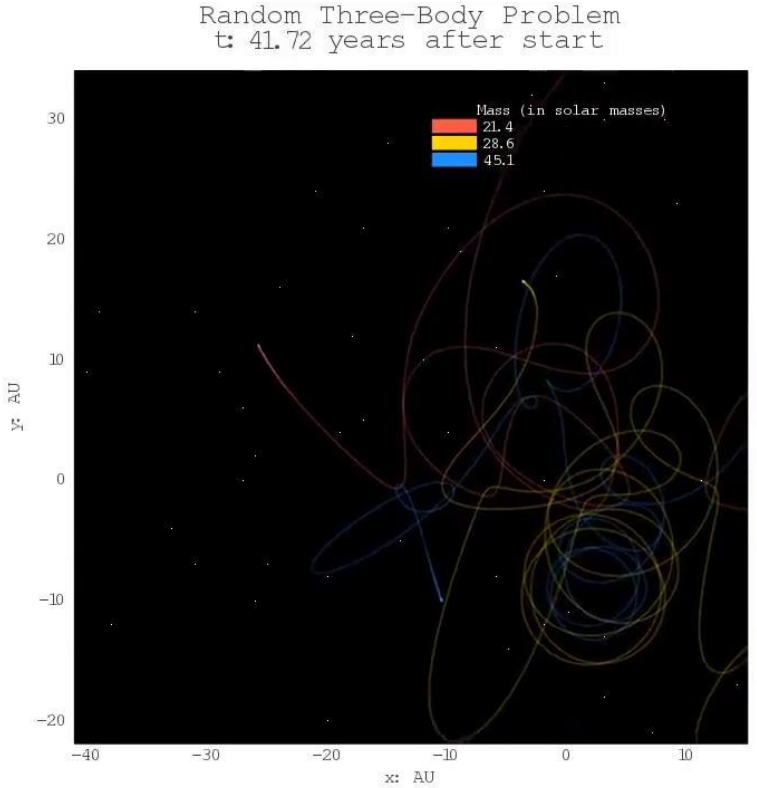
Last week's summary: collisions

For some fun, see:
https://twitter.com/threebodybot

They generate a random 3-body gravity problem everyday.

Not the same potential ($1/r^2$ vs. $1/r^{12} + 1/r^6$) but it is also impossible to solve analytically in the general case.

Leads to very complex and hard to predict trajectories.



Questions?

Units and dimensions

As *conscientious physicists*, we used **SI** units for our simulation. So:

- Argon atom mass: $m_{Ar} = 6.6 \times 10^{-26}$ kg
- Interaction length: $\sigma = 3.405 \times 10^{-10}$ m
- Interaction energy: $\varepsilon = 1.654 \times 10^{-21}$ J

Recall, the potential is:

$$U(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

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Not a great choice:

Prone to round-off errors.

Strange to manipulate.

These span a large of orders of magnitude and are a bit cumbersome to use.

Units and dimensions - One alternative

We could use a different set of units. For instance:

- Use $10^{-9}\ m$ for distances.
- Use $10^{-27}\ kg$ for masses.
- …

Question for you: What could we pick as a good unit of time?

This solves a lot of problems. This is used a lot in many simulation packages.

Units and dimensions - Better alternative

Instead, we can identify the characteristic scales of the problem.

Let's define:

$$\tilde{\mathbf{x}} = \mathbf{x}/\sigma$$
$$\tilde{U} = U(r)/\epsilon = 4\left(\tilde{r}^{-12} - \tilde{r}^{-6}\right)$$

And of course:

$$\tilde{r} = r/\sigma$$

These are the dimensionless positions and potential.

By construction, the tilde variables are all in a sensible range for the problem.

Dimensionless equations of motion

Pushing these definitions through the equations of motion, we get:

$$\frac{d^2\tilde{\mathbf{x}}}{dt^2} = \sigma^{-1}\frac{d^2\mathbf{x}}{dt^2} = -\sigma^{-1}\frac{1}{m}\nabla U\left(r\right) = -\frac{\epsilon}{m\sigma}\nabla\tilde{U}\left(\tilde{r}\right) = -\frac{\epsilon}{m\sigma^2}\tilde{\nabla}\tilde{U}\left(\tilde{r}\right)$$

At this point, we are only left with time as a dimension-full quantity.

Dimensionless equations of motion

We can finally define a dimensionless time unit:

$$\tilde{t} = t/\sqrt{\frac{m\sigma^2}{\epsilon}}$$

So we are now back to a very simple system: $$\boxed{\frac{d^2\tilde{\mathbf{x}}}{d\tilde{t}^2} = -\tilde{\nabla}\tilde{U}\left(\tilde{r}\right)}$$

We now measure distances in units of σ, energies in units of ϵ, and time in units of $\sqrt{m\sigma^2/\epsilon}$.

Dimensionless equations of motion

Questions for you:

- *What do the **discretized** equations look like in this framework?*
- *What are the expressions for the **kinetic** and **total energy**?*

But…. Why?

Why not use 10^{-9} m as a unit of distance and so on?

- Simpler equations to code (no need to carry units in the expressions).
- Proper insight into what the expected length- and time-scales are.
- Can easily rescale the output if we want to simulate a problem with a different distance scale (or others).

Questions?

Time-step length

Last week, we said we should pick the time-step length h to be *small enough*.

Now, that we identified the important scales of the system, we can come up with something better….

First, what is our time unit?

$$\sqrt{m\sigma^2/\epsilon} = 2.15 \times 10^{-12}\,\mathrm{s}.$$

Recall, for Argon:

$$\epsilon/k_B = 119.8\,\mathrm{K}$$
$$\sigma = 3.405\,\text{Å}$$

Natural velocities

Applying the same procedure, we get for the velocities:

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Recall, for Argon: $\epsilon/k_B = 119.8\,\mathrm{K}$

If we now pick $T \sim 100\ \mathrm{K}$,

we get: $\tilde{v} \approx 1$!!

Natural units - Conclusion

What did we learn from all this:

At a temperature of order $T = 100\ \mathrm{K}$, the particles move a typical distance of order σ (our natural length unit) in a time $\sqrt{m\sigma^2/\epsilon}$ (our natural time unit).

Natural units - Time-step length

What did we learn from all this:

At a temperature of order $T = 100\ \mathrm{K}$, the particles move a typical distance of order σ (our natural length unit) in a time $\sqrt{m\sigma^2/\epsilon}$ (our natural time unit).

Coming back to the original question: What is a small enough time-step length?

We can now estimate this. **Small compared to our natural unit !!**

So let's take $h = 0.01$ **or** 0.001 (in our natural units).

Coding aspects

A few things to think about before typing:

- What do we now do with constants and units?
- Are there new functions to consider?
- Any new data structures?

Second Milestone

- Derive the expression for the kinetic energy in dimensionless units.
- Update your MD code from last time to use dimensionless variables and simulate ***a few*** atoms in 3D.
- Plot the evolution of the kinetic, potential, and total energy of the system. Play with the time-step length h and see what happens if it is too large.