Scientific Programming with Python
Assignment: Lennard-Jones Equation

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Goal The goal of this assignment is familiarize yourself with Jupyter-notebooks [1] and/or Google Collaboratory [2], to demonstrate your level of Python3 [3, 4] knowledge, and to learn a bit about the Lennard-Jones potential for modeling molecular interactions and unit conversion.

Problem and Input Data Computer simulations of molecular systems are often done in scientific research. The simplest atomistic model uses the Lennard-Jones potential equation to approximate how atoms are attracted and repulsed from one another [5]. The Lennard-Jones equation has the following form:

$$V_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{1}$$

where $V_{LJ}(r)$ is the potential energy (in eV) of the interaction, ϵ (eV) and σ (Å) terms are atom-dependent parameters, and r (Å) is the distance between the atoms. The 6^{th} and 12^{th} powers terms model the attractive and repulsive forces, respectively.

Assignment Tasks

Task 1 Calculate the nonbonded potential energy between two argon atoms that are 3.5 Å apart using the Lennard-Jones equation. For argon atoms, $\varepsilon = 0.0103$ eV and $\sigma = 3.40$ Å [6].

Provide the final $V_{LJ}(r)$ energy in the "International Unit for Energy" [7]

Allowed Python3 [3, 4] functions & libraries/modules

- All built-in functions

Assignment Due Turn in your solution as a **Jupyter-notebook** to **LEA** by **Monday, October 9th, 2023 at 09:00**.

Note: Please include your **SciPro_ID** at the **top** of your notebook.

References

[1] Kluyver, T. et al., (2016) Jupyter Notebooks – a publishing format for reproducible computational workflows. In F. Loizides & B. Schmidt, eds. Positioning and Power in Academic Publishing: Players, Agents and Agendas. pp. 87–90.

[2] Bisong, E. (2019). Google Colaboratory. In: Building Machine Learning and Deep Learning Models on Google Cloud Platform. Apress, Berkeley, CA. https://doi.org/10.1007/978-1-4842-4470-8_7

[3] Python Software Foundation. Python Language Reference, version 3.11. Available at http://www.python.org.

[4] van Rossum, G. Python tutorial, Technical Report CS-R9526, Centrum voor Wiskunde en Informatica (CWI), Amsterdam, 1995.

[5] Wikipedia contributors, "Lennard-Jones potential." Wikimedia Foundation. Last modified August 30, 2023. https://en.wikipedia.org/wiki/Lennard-Jones_potential. Accessed on September 12, 2023.

[6] Rahman A. (1964) Correlations in the motion of atoms in liquid argon. Physical Review. 136(2A), A405–A411. https://doi.org/10.1103/PhysRev.136.A405.

[7] Wikipedia contributors, "International System of Units." Wikimedia Foundation. Last modified September 4, 2023. https://en.wikipedia.org/wiki/International_System_of_Units. Accessed on September 12, 2023.

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