Scientific Programming with Python
Assignment: The Interaction Between Two Atoms

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Goal The goal of this assignment is to make use of the knowledge about scientific computing learned so far. Specifically, you will build upon your previous work involving the Lennard-Jones equation [1], learn and encode an alternative equation for modeling nonbonded interactions [2], and explore the Pandas library [3, 4].

Problem and Input Data As learned previously, the simplest classical-physics model simulating how atoms interact is the Lennard-Jones equation [1] with the following form:

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

Recently, a more robust model was derived by Yang et al. that is an exponential equation [2] with the following form:

$$V_{Exp}(r) = \varepsilon \left[e^{\alpha\left(1-\frac{r}{\sigma}\right)} - \left(\left(\frac{r}{\sigma}\right)^{4} - 2\left(\frac{r}{\sigma}\right)^{2} + 3 \right) e^{\left(\frac{\alpha}{2}\right)\left(1-\frac{r}{\sigma}\right)} \right] \tag{2}$$

In both equations, $V(r)$ is the potential energy (in eV) of the interaction, ϵ (well depth in eV) and σ (the ideal distance at the energy minimum in Å) terms are atom-pair dependent parameters, and r (Å) is the actual distance between the atoms. In Eq. 2, the α (no units) parameter is a weighting factor that controls the influence of the exponential terms and is also atom-pair dependent.

Yang et al. also published, in supplementary information, the following suggestions for ϵ, σ and α parameters for Ar_2, which are given in Table 1 [2].

Table 1. Argon dimer parameters for use in Lennard-Jones (Eq., 1) and exponential (Eq., 2) equations.

Species	ϵ (kJ/mol)	σ (Å)	α
Ar_2	1.178	3.75	13.18

Finally, Cybulski and Toczyłowski used very accurate quantum mechanics (QM) calculations to determined $V(r)$ (in Hartree) at different r distances for several rare gas dimers – including Ar_2 – which can be used as benchmark target data [5]. The data from these calculations can be found in the CSV-formatted file CybulskiT1999_Ar2.csv.

Assignment Tasks

Task 1 QM target data

- Load the QM target data for Ar_2.
- Clean the input data by removing rows with
  - duplicated data, and
  - missing data
- Convert the potential energies from Hartree to kJ/mol units, including them into their dataframes.

Hint: Pandas has built in functions that help you clean the data.

Task 2 Compute the following using the distances within the QM target data:

- the Lennard-Jones potential energy (Eq. 1),
- the exponential potential energy (Eq. 2)

Task 3 Plot the following data using lines:

- the QM target energies
- the Lennard-Jones energies (Eq. 1),
- the exponential energies (Eq. 2)

Hint: The x-axis should be the distances (i.e., R (Å)).

Task 4 Save the following data to a CSV-formatted file:

- the distances
- the QM target energies (Hartree),
- the QM target energies (kJ/mol),
- the Lennard-Jones energies (kJ/mol),
- the exponential energies (kJ/mol)

Allowed Python3 [6, 7] functions & libraries/modules

- All built-in functions
- Pandas library [3, 4]
- math library
- typing library (if needed)

Assignment Due Turn in your solution as a **Jupyter-notebook** [8] to **LEA** by **Monday, November 27$^{\text{th}}$, 2023 at 09:00**.

Note 1 : Please include your **SciPro_ID** at the **top** of your notebook.

Note 2 : **Do not** consider **significant figures** in this solution.

References

[1] Wikipedia contributors, "Lennard-Jones potential." Wikimedia Foundation. Last modified July 24, 2022. https://en.wikipedia.org/wiki/Lennard-Jones_potential. Accessed on September 12, 2023.

[2] Yang, L.; Sun, L. & Deng, W.-Q. (2020) van der Waals Function for Molecular Mechanics. J. Phys. Chem. A, 124, 2102–2107

[3] The Pandas Development Team pandas-dev/pandas: Pandas Zenodo, 2020 (https://pandas.pydata.org)

[4] Pandas user guide. Available at https://pandas.pydata.org/docs/user_guide/index.html. Accessed on November 7, 2023.

[5] Cybulski, S.M. & Toczyłowski, R.R. (1999) Ground state potential energy curves for He_2, Ne_2, Ar_2, He–Ne, He–Ar, and Ne–Ar: A Coupled-Cluster Study J. Chem. Phys., 111, 10520–10528

[6] Python Software Foundation. Python Language Reference, version 3.11. Available at http://www.python.org. Accessed on October 22, 2023.

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

[8] 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.

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