

PYLJ: A TEACHING TOOL FOR CLASSICAL SIMULATION



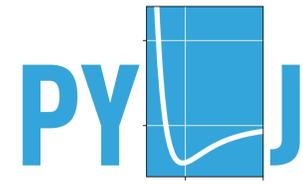
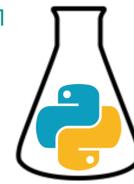
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BATH

Andrew R. McCluskey^{1,2}, Benjamin J. Morgan¹, Karen J. Edler¹, and Stephen C. Parker¹

¹ Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY

² Diamond Light Source, Diamond House, Rutherford Appleton Laboratory, Harwell Oxford, Oxon, OX11 0DE

e-mail: arm61@bath.ac.uk - twitter: [@an_drewmcc](https://twitter.com/an_drewmcc)



WHAT IS PYLJ?

- `pylj` is an open-source Python library to facilitate student interaction with classical simulation.
- Operating in a Jupyter notebook; it is easy to implement, and highly extensible.

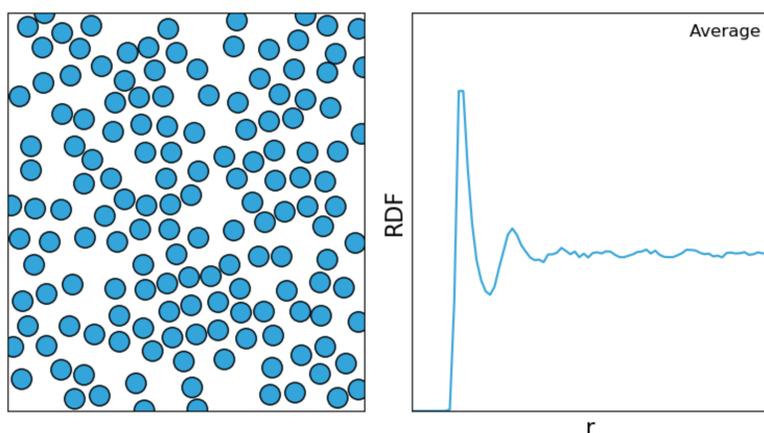


Figure 1. An example of the output available from `pylj`.

EXAMPLE EXERCISES

- Observing a deviation from the ideal gas law with increasing particle density; hence determining the value of a and b in the van der Waals' equation.
- The Scattering sampling class gives the scattering profile and the effect of particle density or temperature can be rationalised in terms of the "crystallinity". This exercise was developed for the ISIS Neutron Training Course.

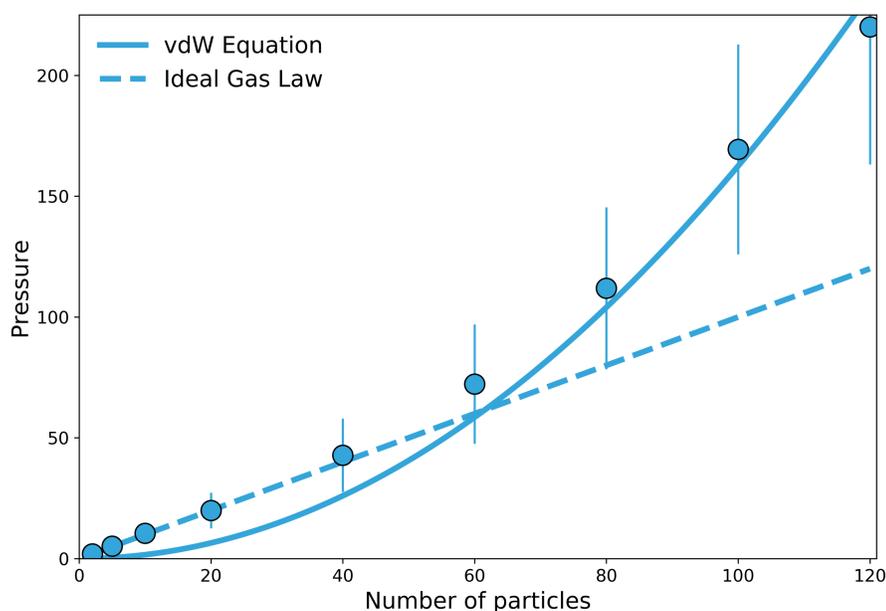


Figure 3. An ideal gas law plot showing the deviation from ideality at high particle density and the best fit of the van der Waals' equation.

ACKNOWLEDGEMENTS

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WHAT DOES PYLJ OFFER?

- Simulation of 2D Lennard-Jonesium; using both energy minimisation and molecular dynamics.
- NVE and NVT ensembles.
- A variety of sampling classes are provided including to produce scattering data; further custom sampling classes are easy to create.
- Can run on a typical university machine.

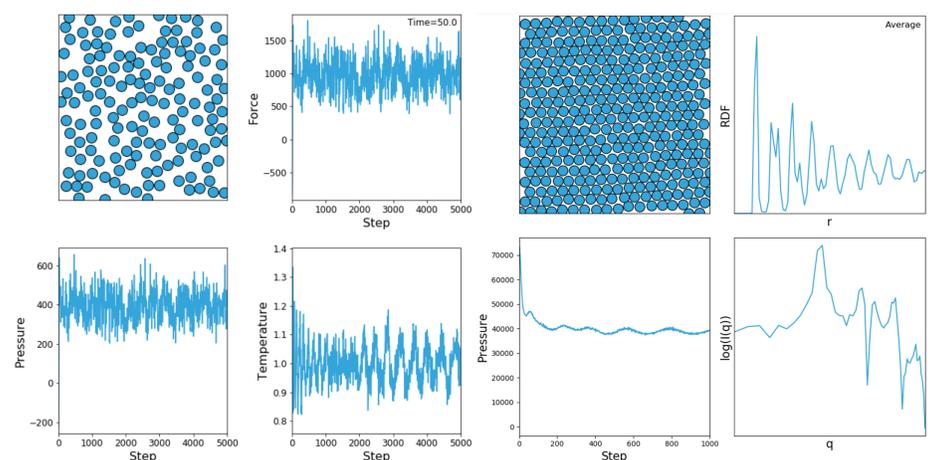


Figure 2. Examples of the Interactions and Scattering sampling classes packaged with `pylj`.

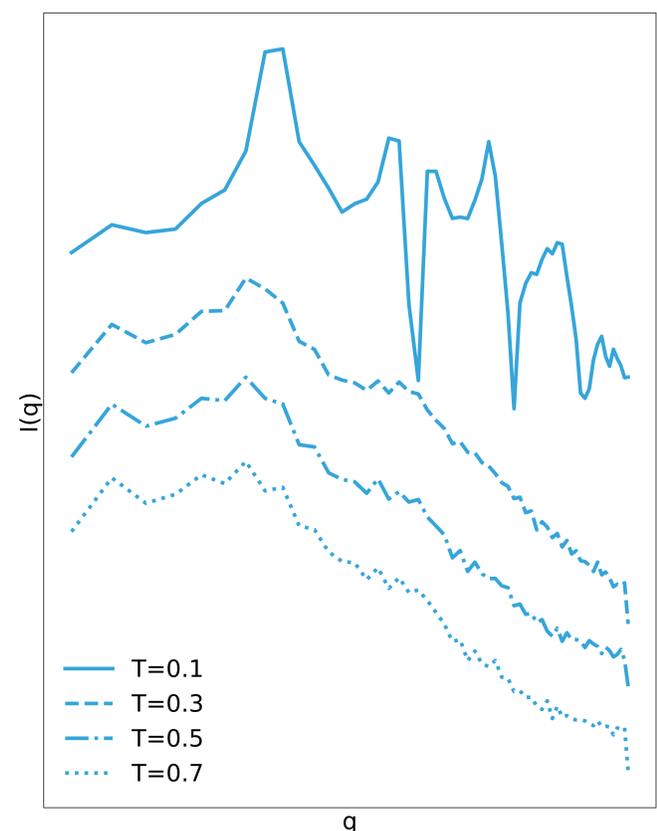


Figure 4. The scattering profiles obtained at different temperatures showing the increasing in crystallinity identifiable by the increasing peak intensity.

HOW DO I GET PYLJ?

If you are interested in using `pylj`, we are looking for alpha-testers. Speak to Andrew or check out pythoninchemistry.org/pylj