

PYLJ: A TEACHING TOOL FOR CLASSICAL SIMULATION



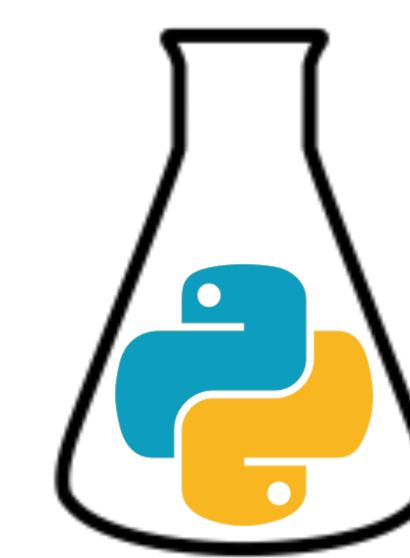
UNIVERSITY OF
BATH

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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.

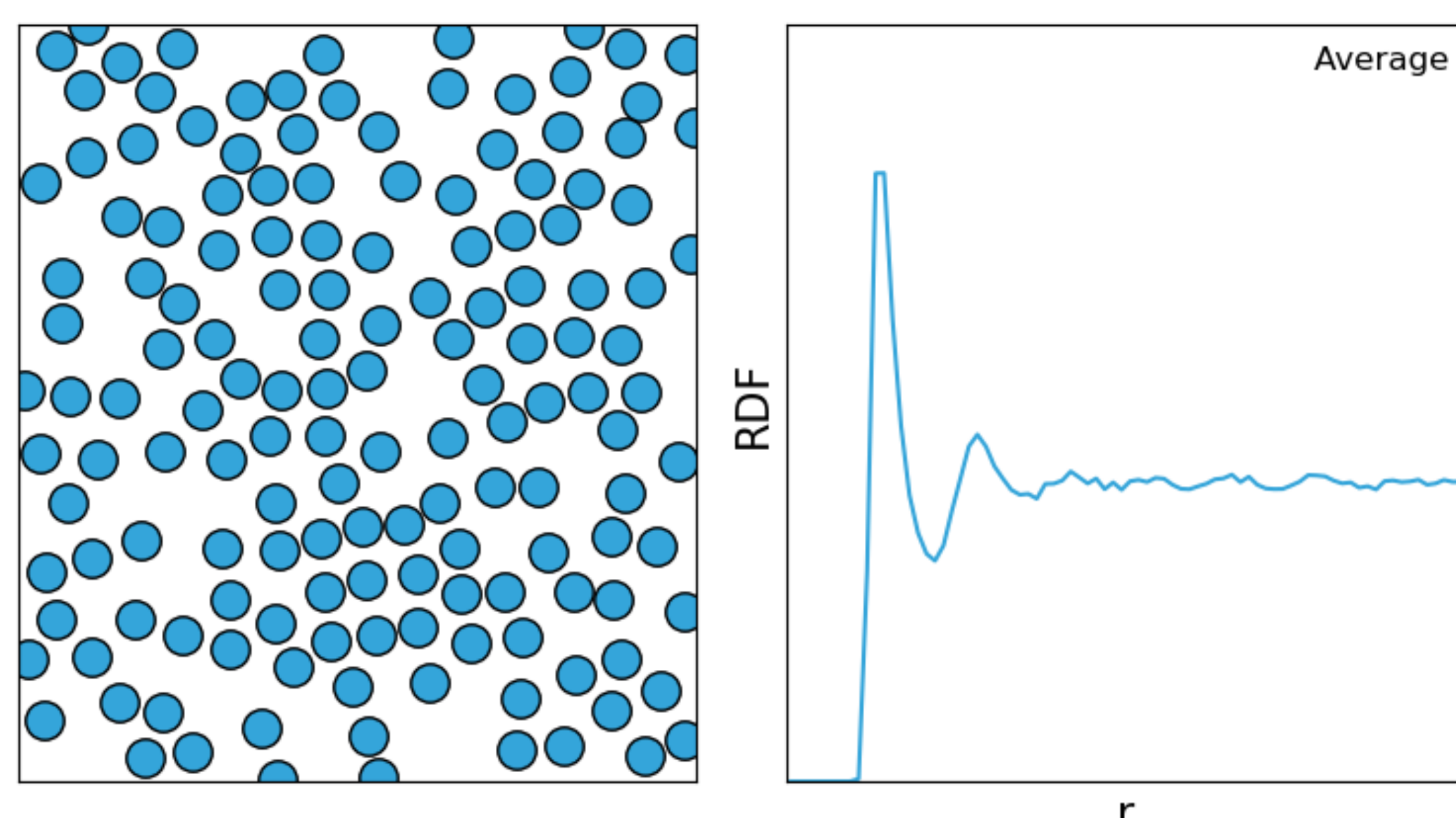


Figure 1. An example of the output available from pylj.

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.

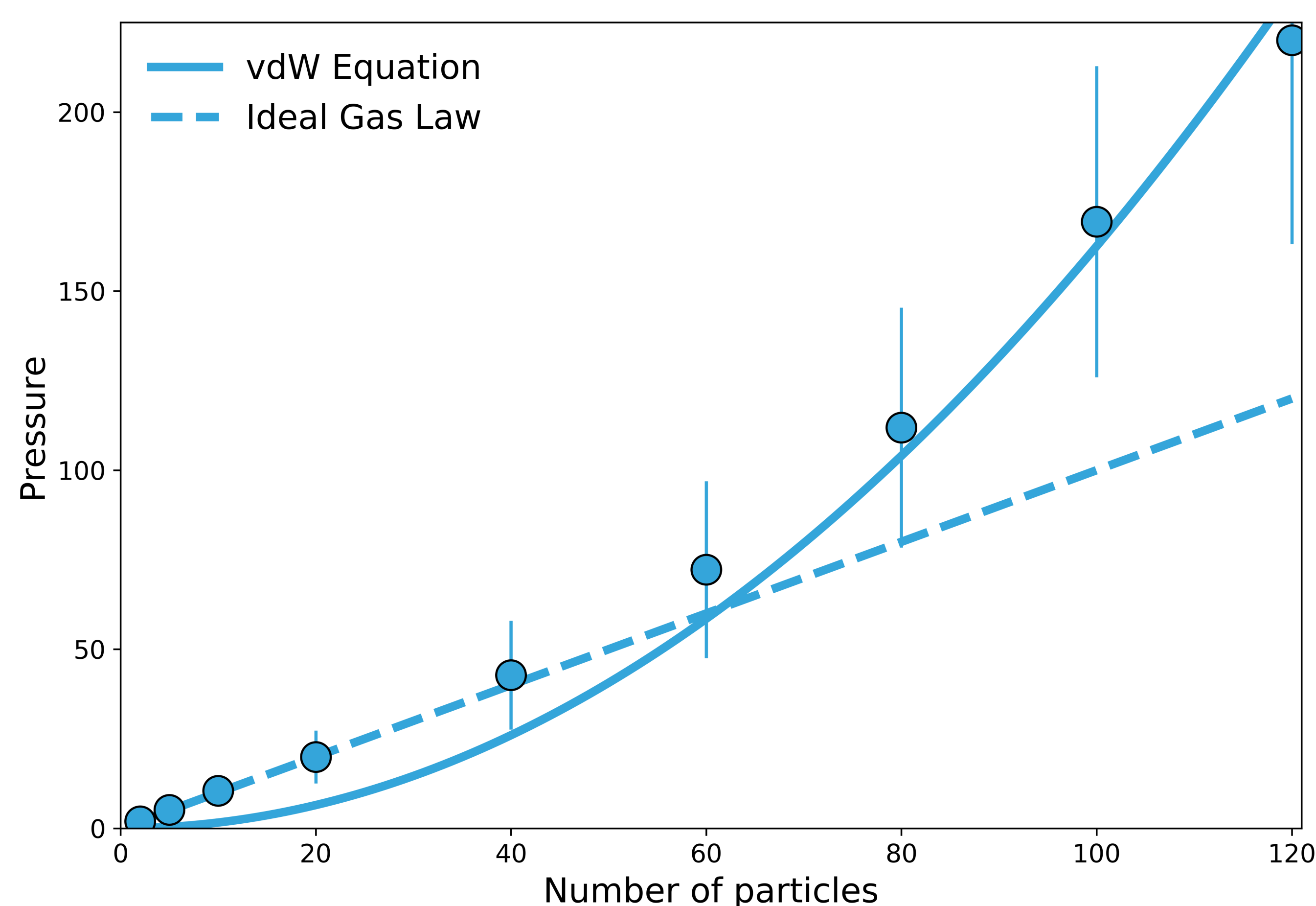


Figure 3. An ideal gas law plot showing the deviation from ideality at high particle density and the best fit of the van der Waals' equation.

ACKNOWLEDGEMENTS

ARM is grateful to Diamond Light Source and the University of Bath Faculty of Science for co-funding a PhD Studentship.

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.

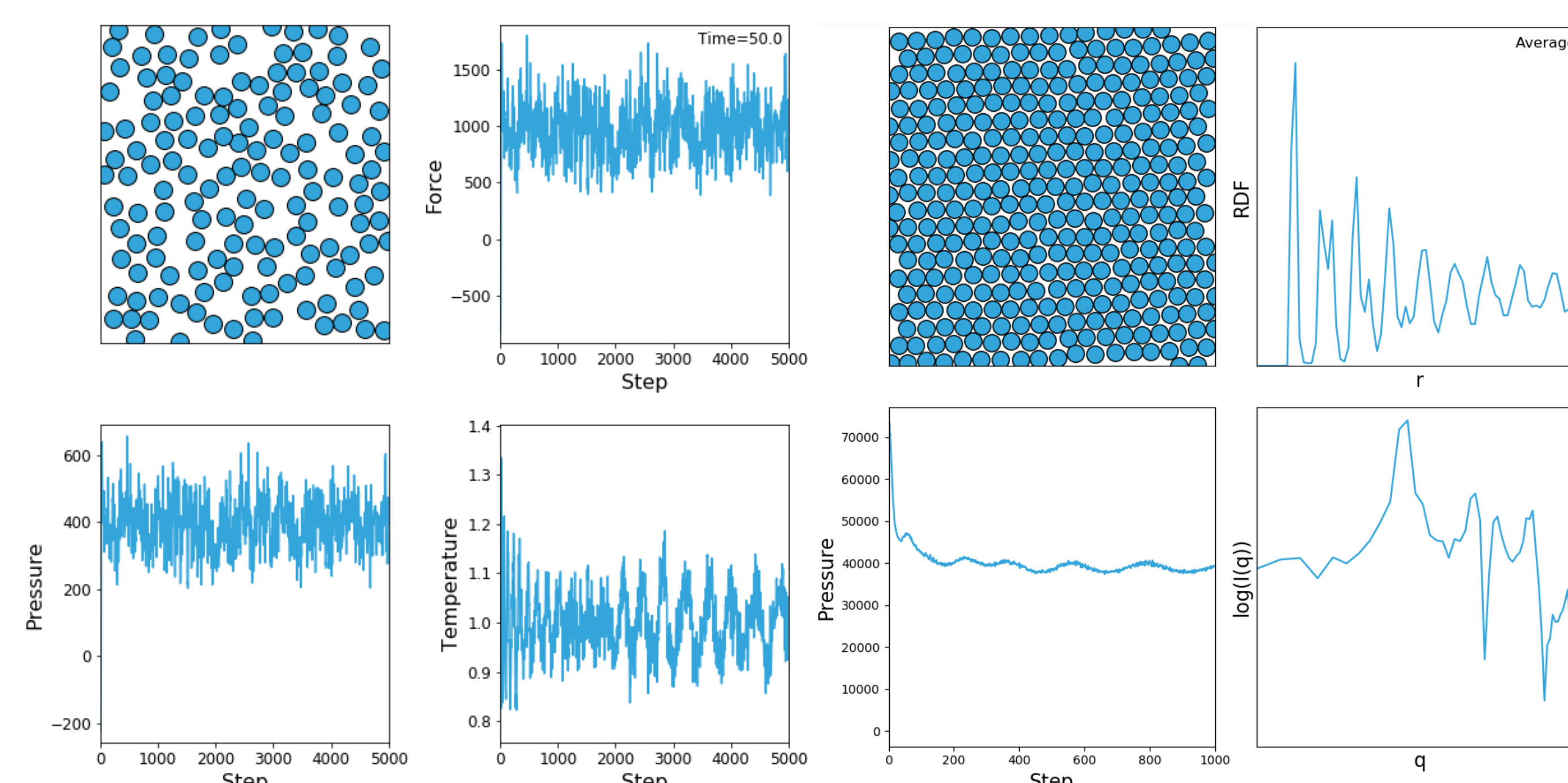


Figure 2. Examples of the Interactions and Scattering sampling classes packaged with pylj.

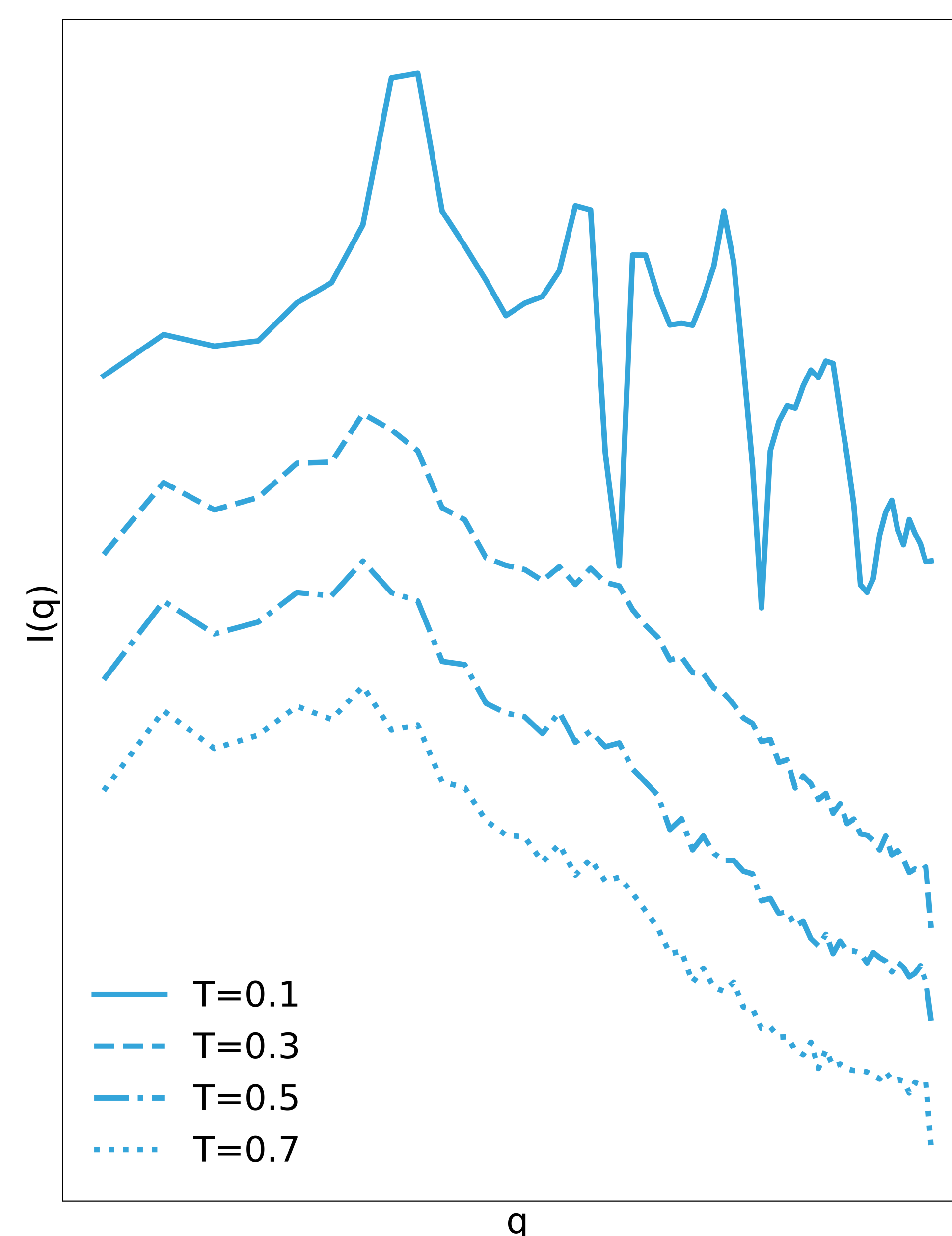


Figure 4. The scattering profiles obtained at different temperatures showing the increasing in crystallinity identifiable by the increasing peak intensity.

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