PYLJ: A TEACHING TOOL FOR CLASSICAL SIMULATION

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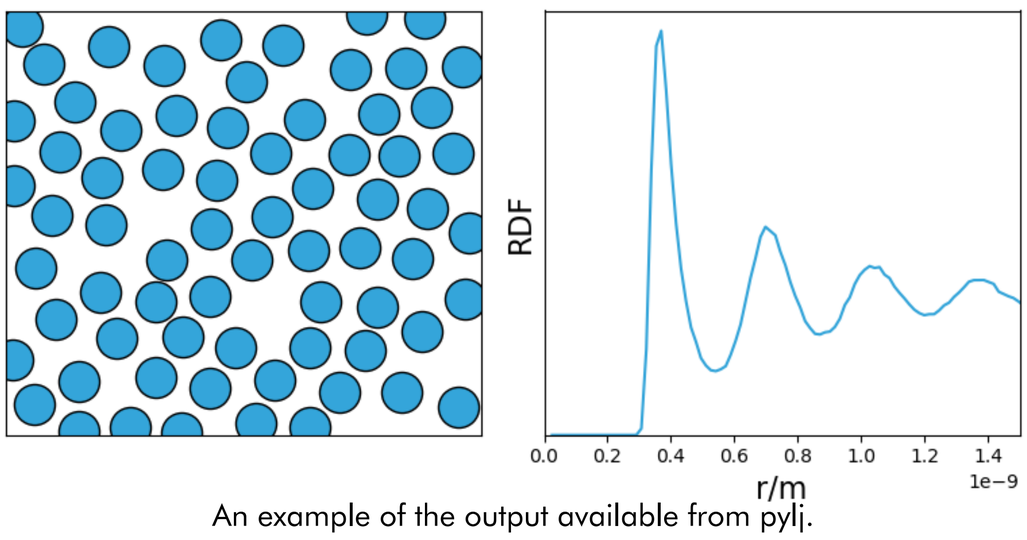
WHAT IS PYLJ?

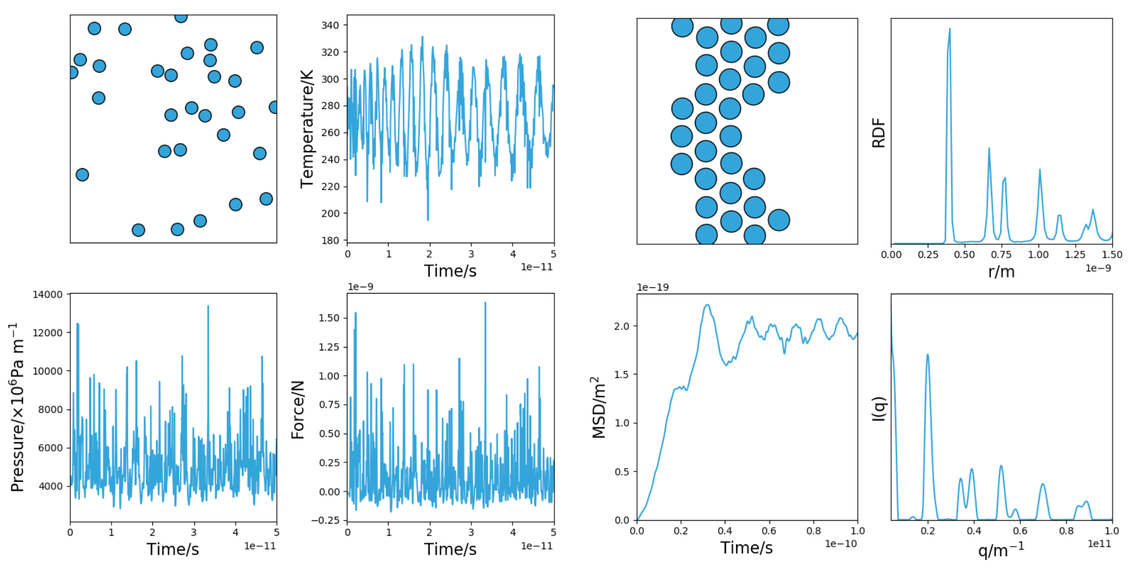
- pylj is an open-source Python library to facilitate student interaction with classical simulation
- Operating in a Jupyter notebook; it is easy to implement and highly extensible
- Can run easily on a typical university machine



An example of the output available from pylj.

WHAT DOES PYLJ OFFER?

- Simulation of 2D argon; using molecular dynamics and Monte-Carlo
- NVE and NVT ensembles
- Packaged with a variety of sampling classes and custom sampling classes are easy to create



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

EXAMPLE EXERCISES

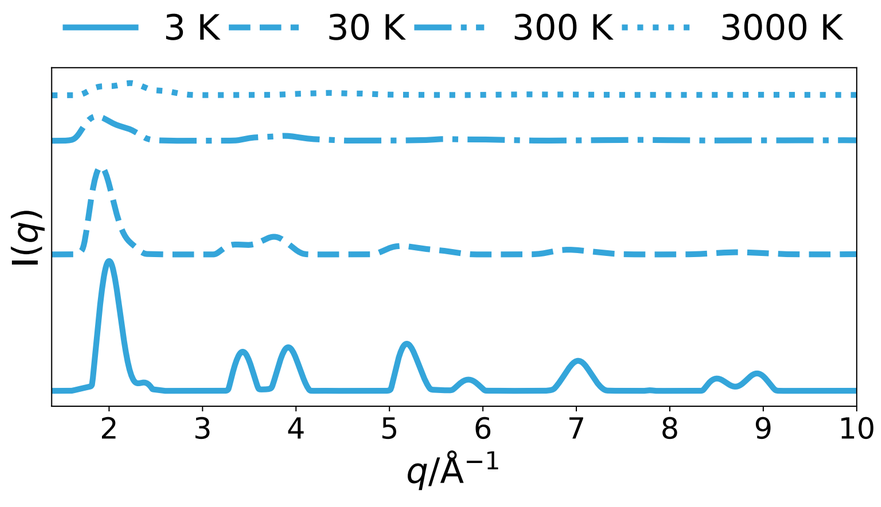
- Introducing molecular dynamics, or Monte Carlo algorithms

```python
from pylj import md, sample

def md_simulation(n, t, cell):
    %matplotlib notebook
    simulation = md.initialise(n, t, cell, 'square')
    sampler = sample.JustCell(simulation)
    simulation.time = 0
    for i in range(10000):
        simulation.integrate(md.velocity_verlet)
        simulation.md_sample()
        simulation.heat_bath(t)
        simulation.time += simulation.timestep_length
        simulation.step += 1
        if simulation.step % 25 == 0:
            sampler.update(system)
    return simulation
```

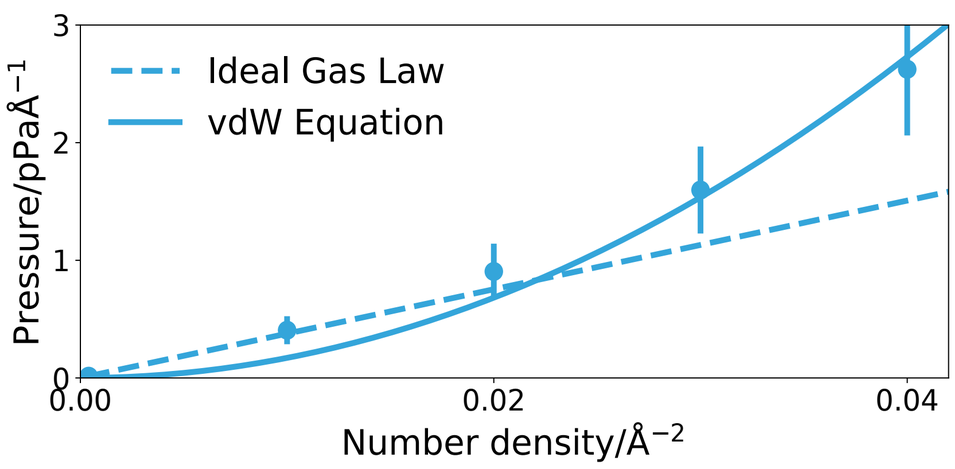
An example of the implementation of a molecular dynamics algorithm in pylj.

- The effect of temperature on the scattering profile, to rationalise "crystallinity"



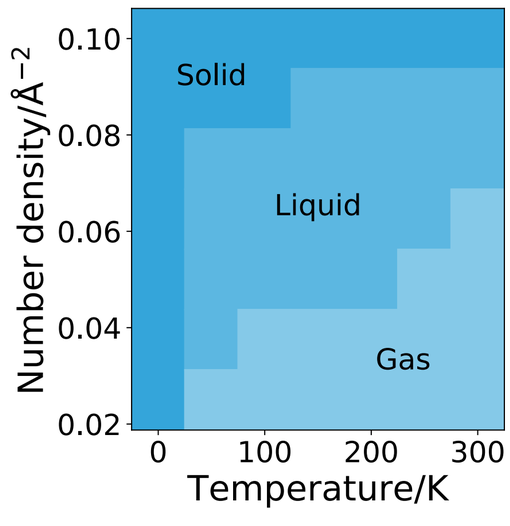
Scattering profiles at different temperatures, the data have been offset by an arbitrary amount in the *y*-axis.

- Observing the deviation from the ideal gas law with increasing particle density



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

- Investigation of the phase diagram for a 2D argon system



The phase diagram for 2D argon as determined using pylj.

ACKNOWLEDGEMENTS

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HOW DO I GET PYLJ?

If you are interested in using pylj, speak to Andrew, check out pythoninchemistry.org/pylj or read the paper (DOI: 10.21105/jose.00019).