arm61.github.io/talks/vicephec18

Introducing programming to undergraduate chemists: and the tools we've developed to help them

VICEPHEC18 &emdash 2018/08/24

the python_in_chemistry project.

PRESENTED BY

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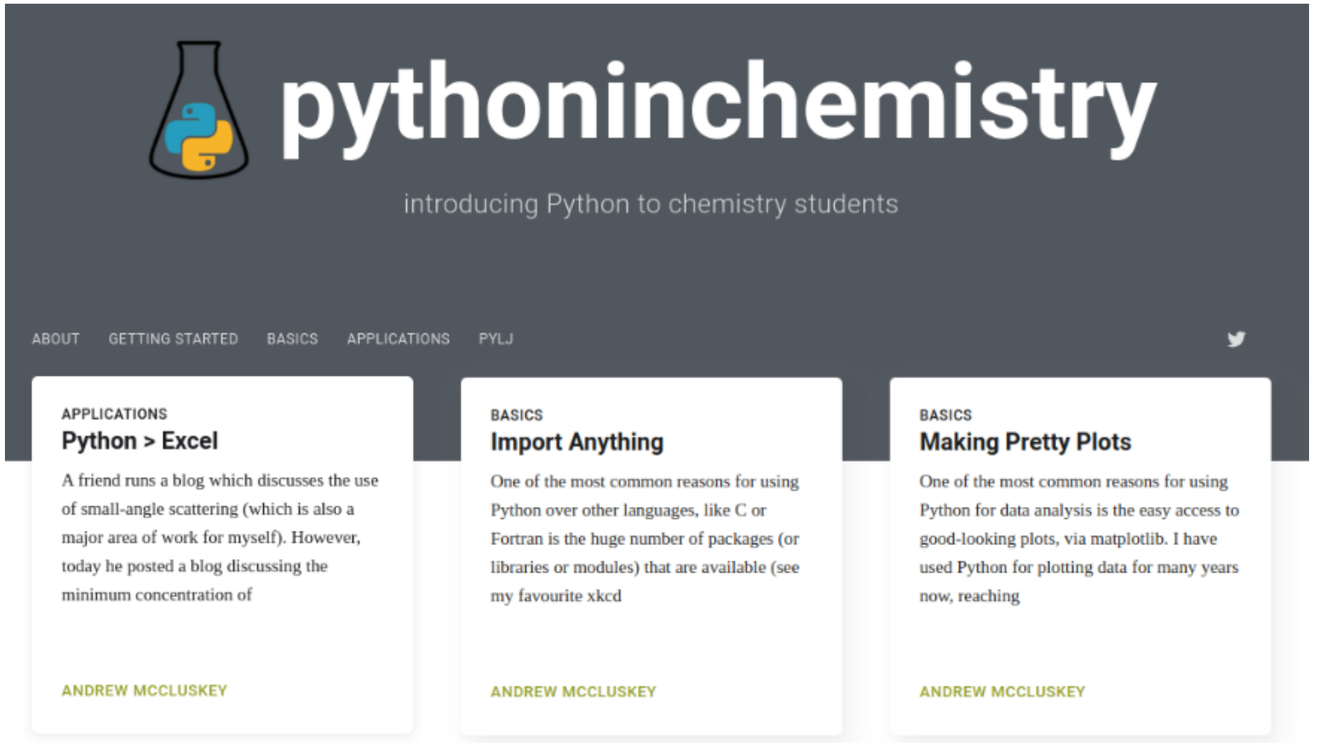
pythoninchemistry project



A talk of two halves:

1. Python in UG chemistry tutorials
2. Open-source teaching tools; pylj and pysing

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python_in_tutorials

Using **programming** as a chemistry teaching tool

who?

- First year natural science students
- Mixture of chem/phys and bio/chem

how?

- Jupyter notebooks provides a user-friendly environment
- Students can access the notebooks online via MyBinder
- Even possible to write presentations in a notebook

why?

- Programming forces the educator to be detail oriented
- Requires the mathematics to be **broken down**
- Can provide instantenous feedback in problem based learning

example

but is it worthwhile?

- Does it improve engagement?
- Will it foster transferable skills?
- Do the students like it?

informal feedback

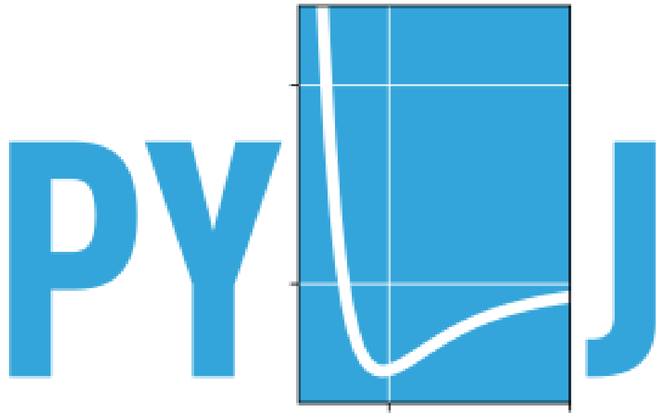
- Students appear anecdotally engaged during tutorials
- Tutorial students attached modified notebooks to **help** emails

tools we've developed

- Bath has dedicated computational chemistry labs
- Needed a tool to introduce molecular dynamics/Monte-Carlo

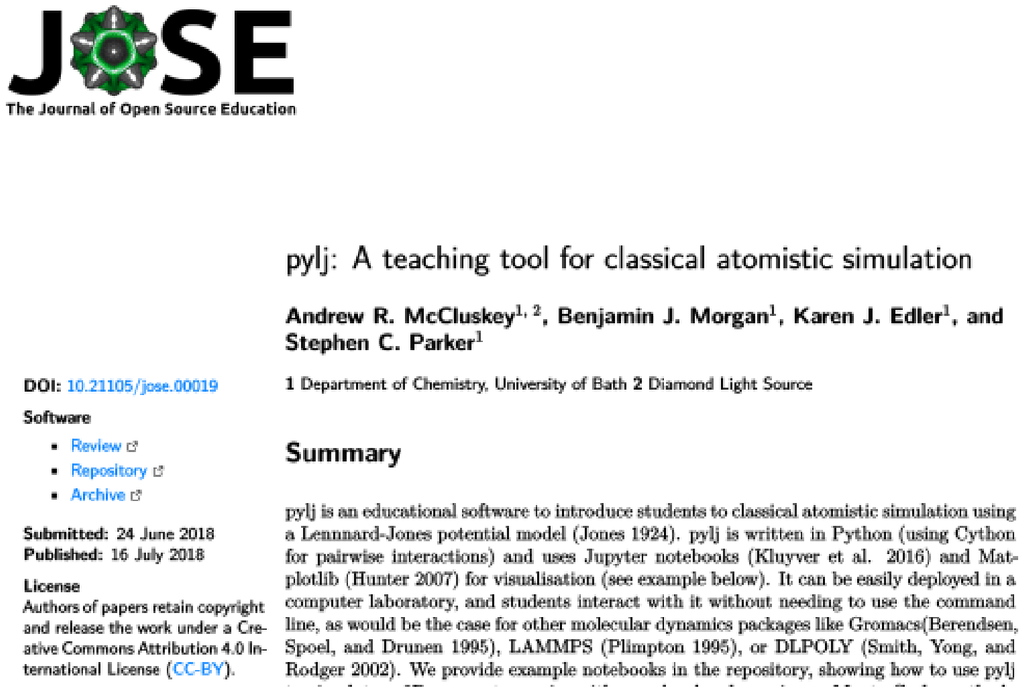
pylj

- Open-source, Python library to engage students in classical atomistic simulation
- Can be used to introduce molecular dynamics or Monte-Carlo simulation
- Or used to show how simulation can describe physical systems



pylj

- Paper in Journal of Open-Source Education, 1(2), 19. DOI: 10.21105/jose.00019
- MIT Licence; do almost anything you want with it
- Source code available on GitHub



JOSE
The Journal of Open Source Education

pylj: A teaching tool for classical atomistic simulation

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Software

- Review
- Repository
- Archive

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Summary

pylj is an educational software to introduce students to classical atomistic simulation using a Lennard-Jones potential model (Jones 1924). pylj is written in Python (using Cython for pairwise interactions) and uses Jupyter notebooks (Kluyver et al. 2016) and Matplotlib (Hunter 2007) for visualisation (see example below). It can be easily deployed in a computer laboratory, and students interact with it without needing to use the command line, as would be the case for other molecular dynamics packages like Gromacs(Berendsen, Spoel, and Drunen 1995), LAMMPS (Plimpton 1995), or DLPOLY (Smith, Yong, and Rodger 2002). We provide example notebooks in the repository, showing how to use pylj

example

Try pylj out for yourself

- Molecular dynamics - pythoninchemistry.org/pylj/md
- Monte Carlo - pythoninchemistry.org/pylj/mc

pysing

- Ian Thompson (Physics PDRA) used the pylj code to create pysing
- Simple Ising model Monte-Carlo

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how to find out more

- Check out pythoninchemistry.org
- Utilise tools like Jupyter notebooks, pylj, and pysing
- Engage students to analyse data programmatically
- Come have a chat!

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thanks for listening!

Sadie, my dog