Hello,

My name is Nathaniel Smith and I am a Python Engineer based in Berlin. I am currently finishing my thesis in computational Chemistry at the Freie Universität and working as a student lab and admin assistant at EU Openscreen.

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Projects I've Worked On

Work Projects

The below projects are a collection of scripts that I wrote as part of my position as a working student. Generally these projects are optimisations to improve workflow where desired, instead of performing a task manually.

Twitter CSV Parser

Converts the exported .csv data from twitter into an excel file, as the Tweet text included in the file breaks the format from a standard .csv file with newline breaks.

Chemistry Projects

These projects are scripts I wrote as part of my MSc in Chemistry at the Freie Universität. Scripts are improvements to streamline the creation of files for a QM/MM calculation using a GROMACS grofile obtained from a .pdb file, or mathematical calculations of some kind.

B Matrix

This Program accepts atoms via a Cartesian coordinate system, and calculates the B matrix from said coordinates.

create_start_file

Written during my MSc. thesis, this script is designed to create a start.sh file commonly used in job schedulers (in this case slurm) for the purposes of using the gmx2qmmm program.
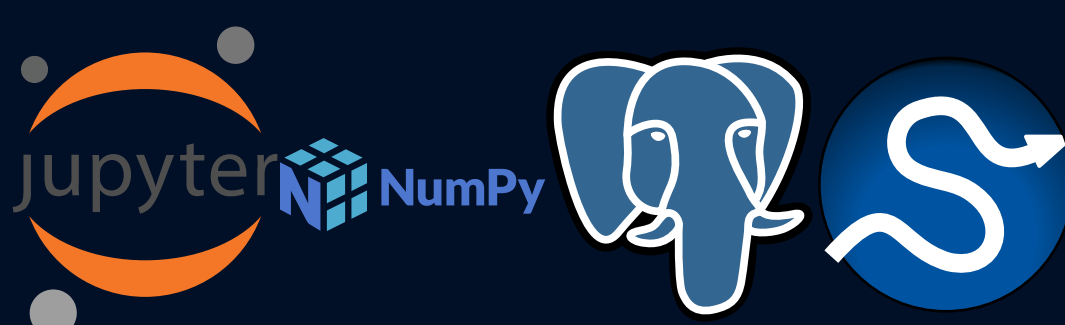
setup_calculations

setup_calculations uses the create_start_file program entirely, alongside other functions designed to select a QM and MM region of atoms with a VMD script.

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Tools

Languages

Python Tools