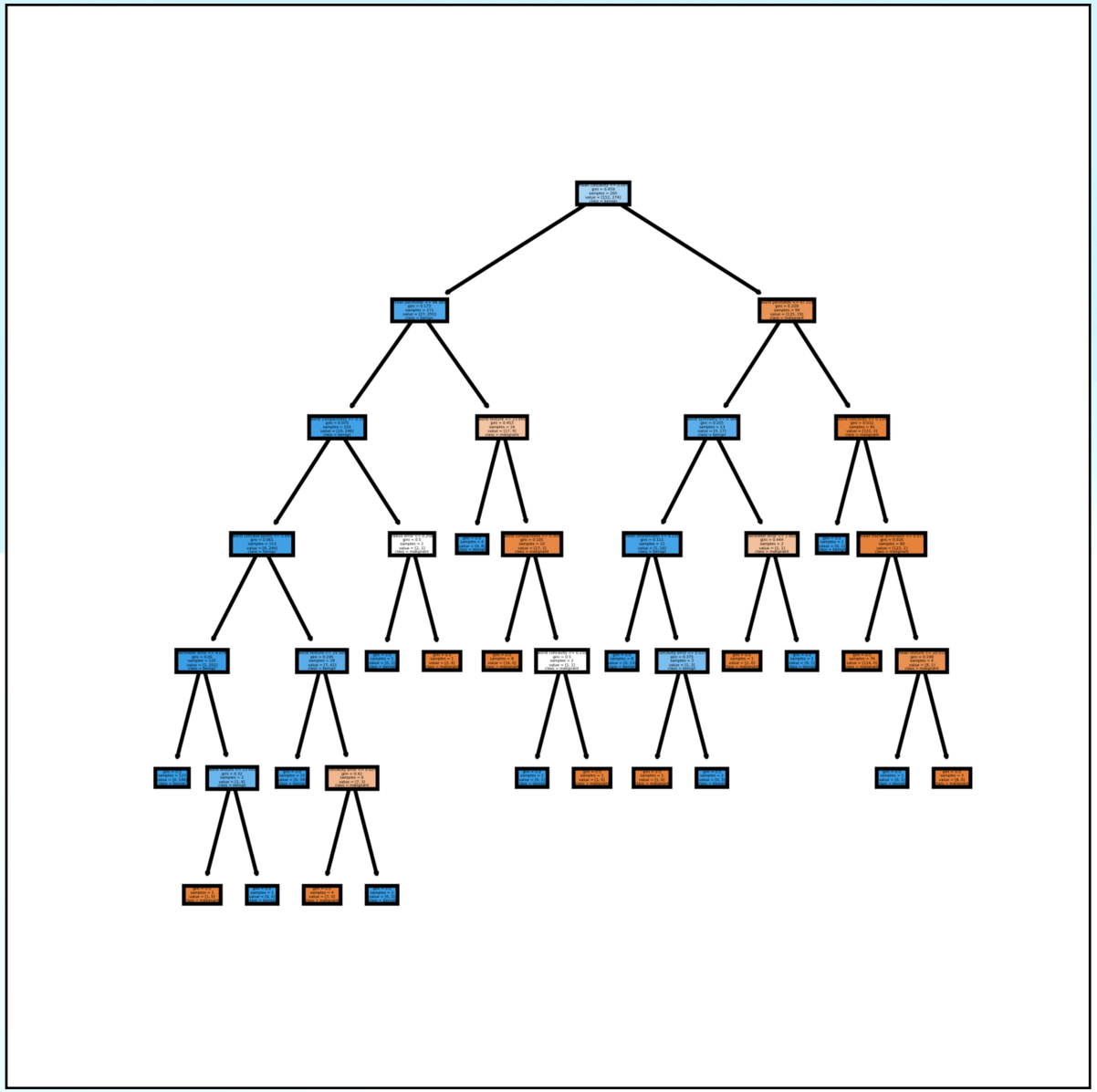
pyiron developer meeting

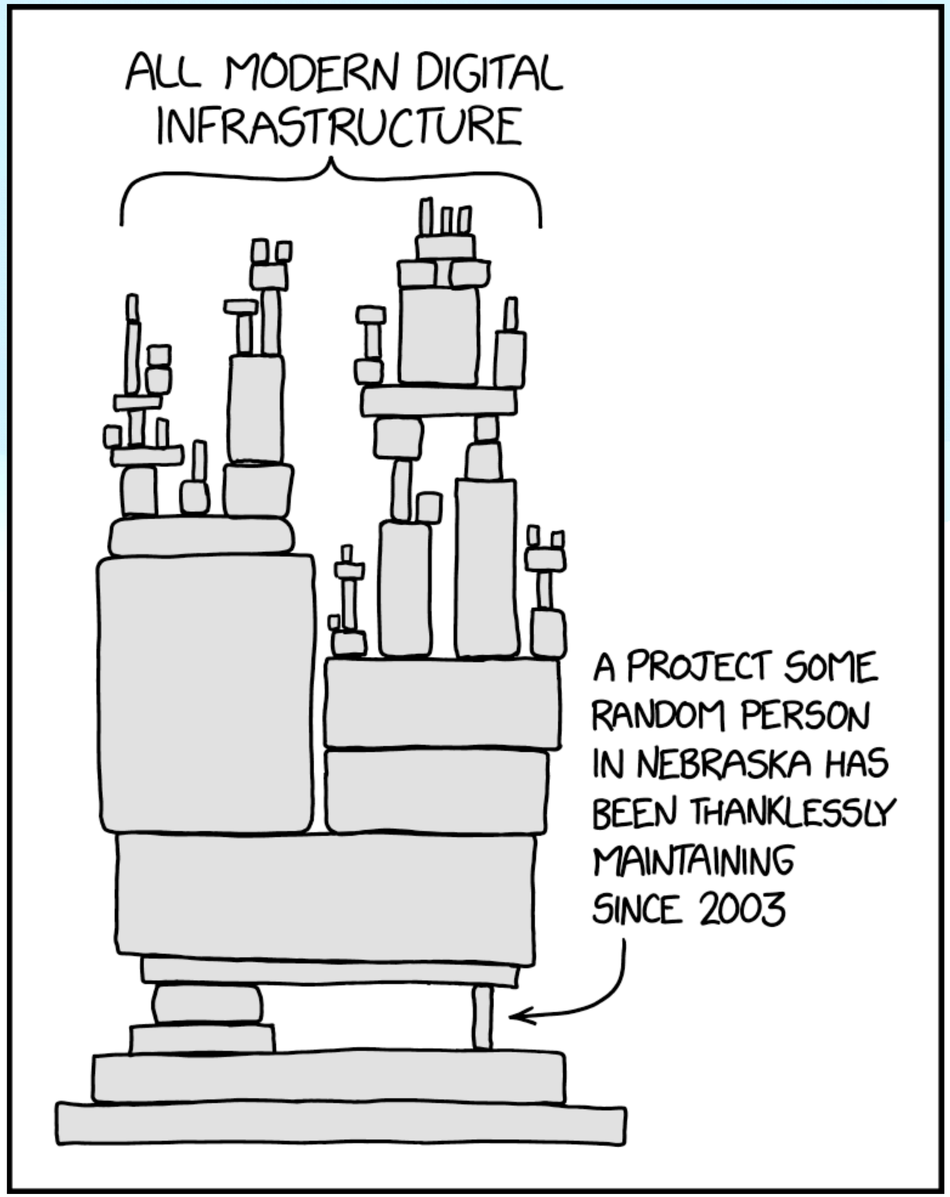
July 26-27 2022

Sam and his friends

What outsiders think pyiron is like



What pyiron actually is like



https://xkcd.com/2347/

How we became developers (without being required)

- Jan
  - Motivated by the idea to no longer use bash scripts, but to use combined python framework
- Sam: The draftee
  - Used pyiron as a basis for an interactive class → Jörg & Jan wanted to see it inside pyiron
- Liam: The reluctant convert
  - Re-invented many wheels for his GB calculations for two years, then realized spending a couple months learning the pyiron codebase would save years of time going forward. Now a pyiron zealot
- Marvin: The Padawan (now a Master) ;)
  - I think DataContainer/InputList was my first contribution. Iirc there was some amount of nudging from Liam's side though for me to get involved.

Developer success stories

Today's schedule

- Introduction to pycharm (code editor) @Liam
- Presentation of `pyiron_base` (i.e. general architecture of pyiron) @Jan
- Presentation of different classes in `pyiron_atomistics` (LAMMPS, SPHInX, VASP, Murnaghan etc.) @Sam
- Writing workflows

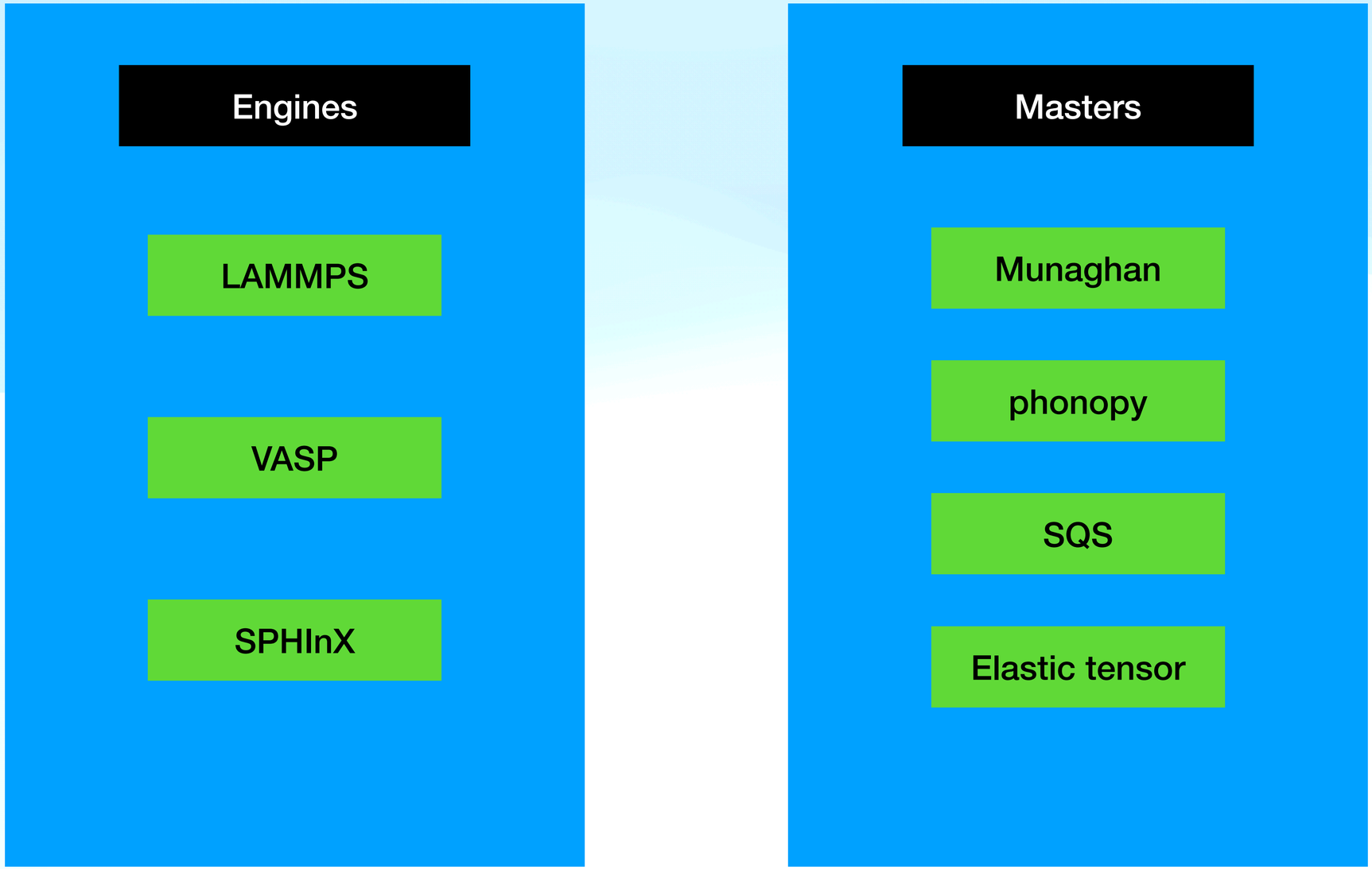
Tomorrow's schedule

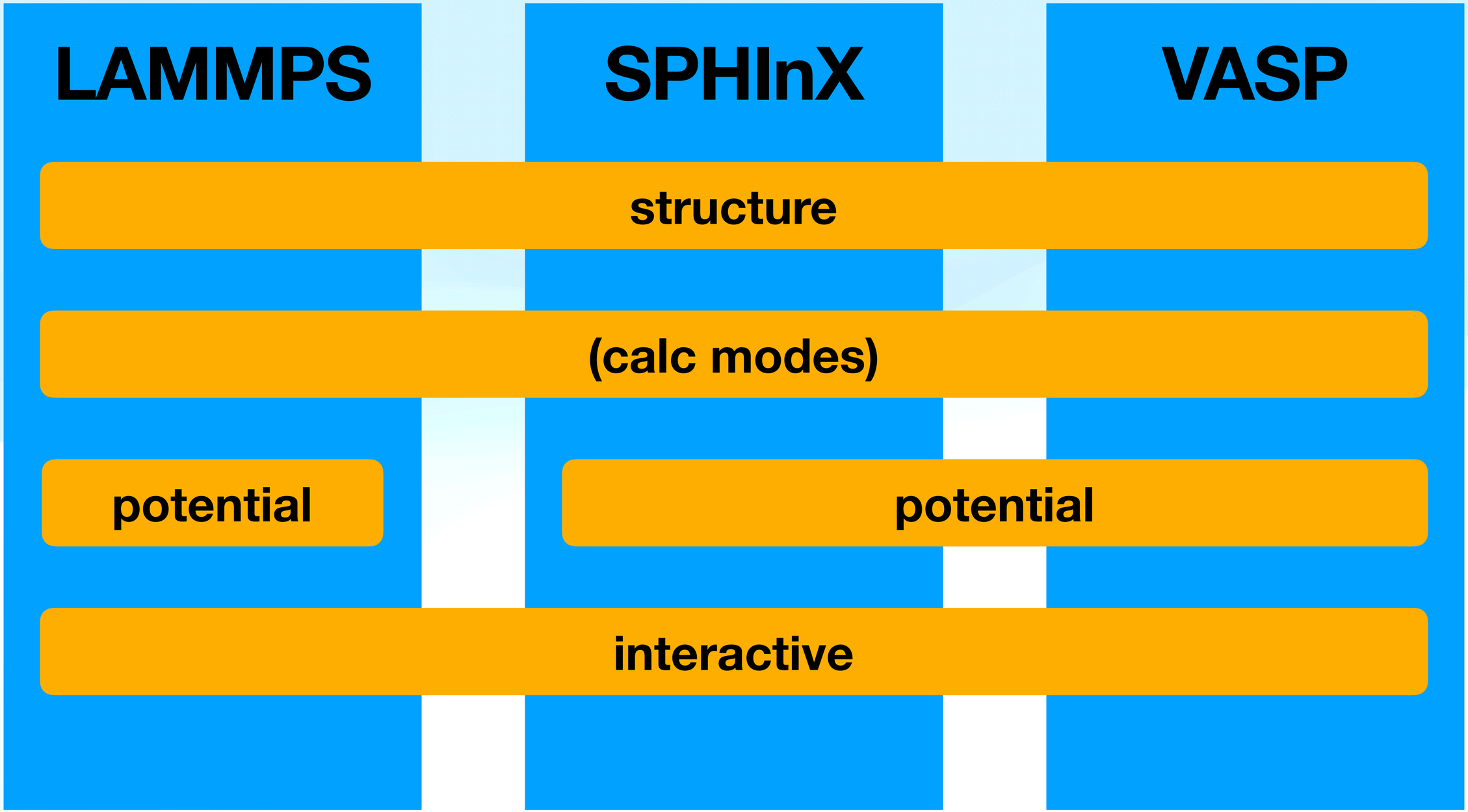
- Workflow on GitHub @Sarath
- Getting a dev environment setup on the cluster @Marvin
- Refactoring, i.e. how to write beautiful python codes @Niklas
- Unit tests & Docstring @Marvin
- Peer-review of pull requests from the previous day
- Introduction to easy issues
- Discussion

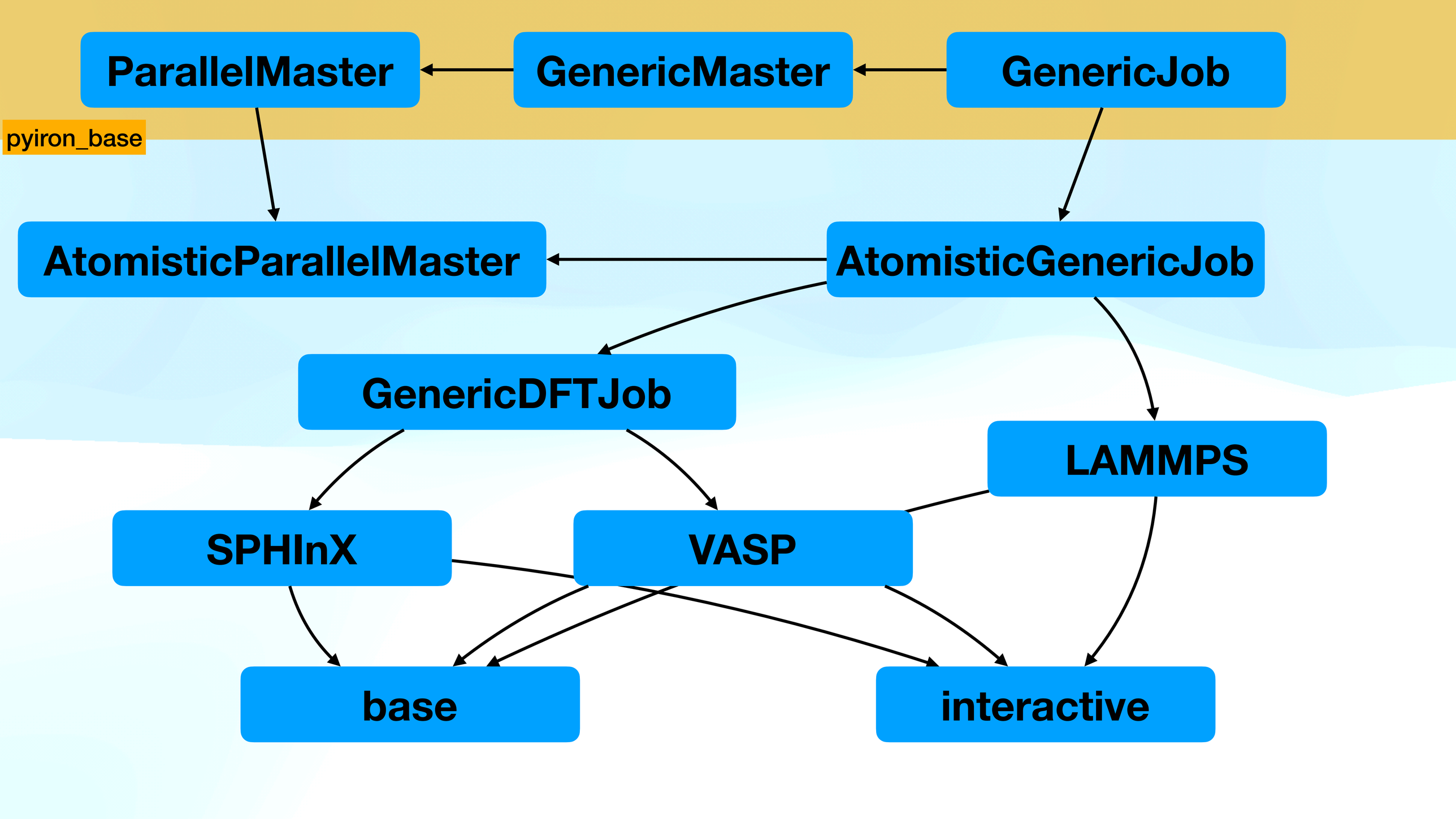
History of `pyiron_atomistics`

- ~2015
  - pyCMW (prehistoric pyiron)
- 2016
  - Database and job table
- 2017
  - Mostly known as “pyiron”
  - VASP (Sudarsan) & LAMMPS for simulation engines
  - Murnaghan for benchmarking
- 2018
  - SPHInX (Sam)
  - Interactive mode
- 2019
  - Liam’s protocol
- 2020
  - `DataContainer` → Coexistence with `GenericParameters`
  - pyiron structure becomes ASE based

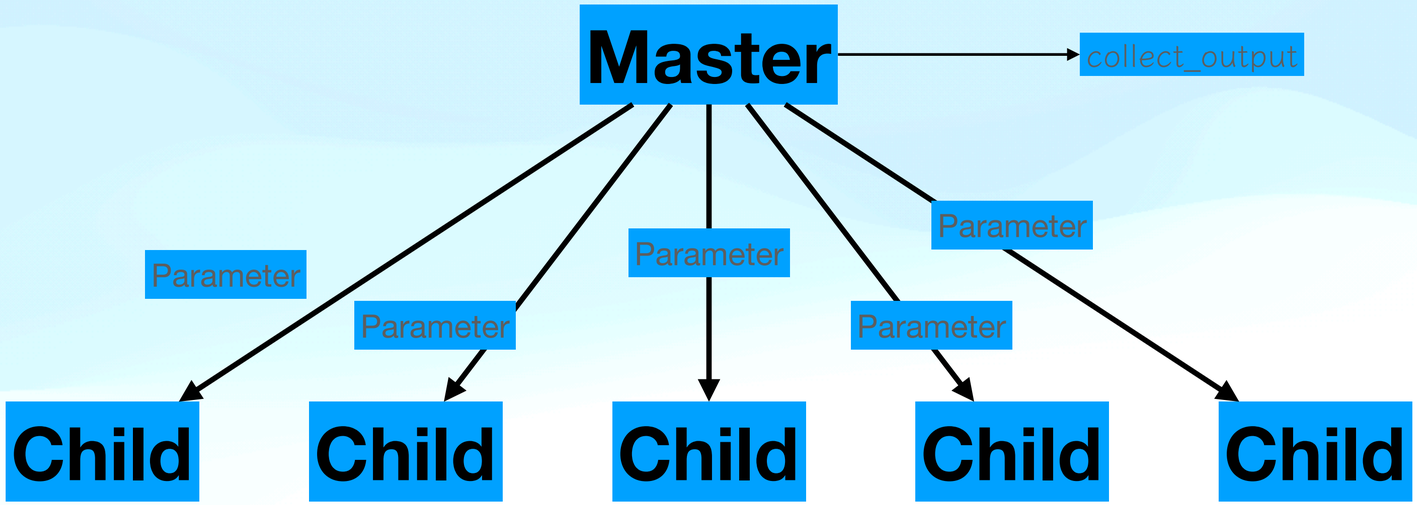
What's inside `pyiron_atomistics`?




LAMMPS
SPHInX
VASP
structure
(calc modes)
potential
potential
interactive


ParallelMaster
GenericMaster
GenericJob
pyiron_base
AtomisticParallelMaster
AtomisticGenericJob
GenericDFTJob
LAMMPS
SPHInX
VASP
base
interactive

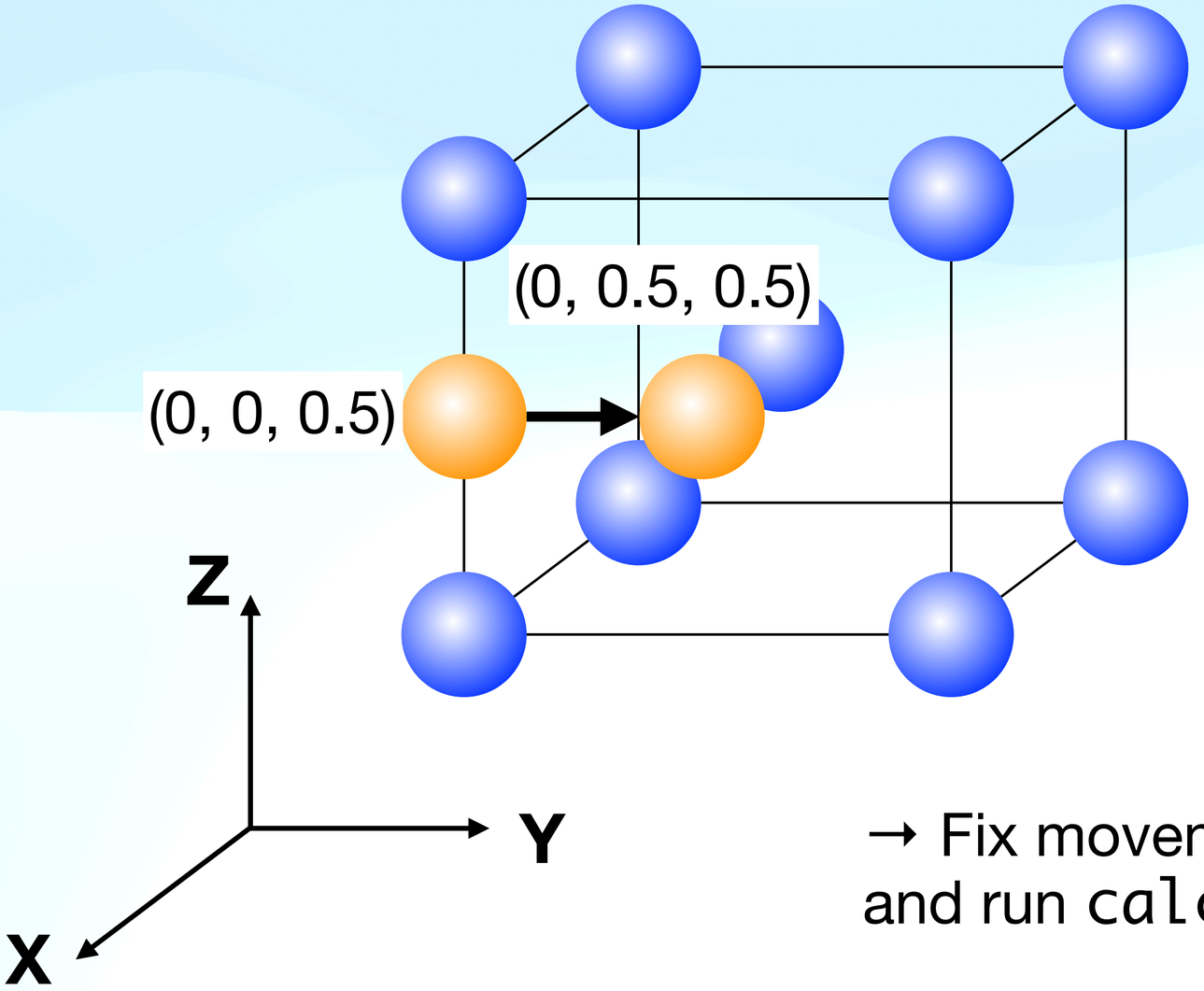
What's `AtomisticParallelMaster` (and why is it interesting)?



Example: Thermal expansion

```
from pyiron_atomistics.atomistics.master.parallel import AtomisticParallelMaster
from pyiron_base import JobGenerator


class MyJobGenerator(JobGenerator):
    @property
    def parameter_list(self):
        return np.linspace(
            self._master.input["min_temperature"],
            self._master.input["max_temperature"],
            int(self._master.input["num_points"]),
        )

    def modify_job(self, job, parameter):
        if parameter == 0:
            job.calc_minimize(pressure=[0, 0, 0])
        else:
            job.calc_md(temperature=parameter, langevin=True, n_ionic_steps=10000, pressure=[0, 0, 0])
        return job


class ThermalExpansion(AtomisticParallelMaster):
    def __init__(self, *args, **argv):
        super().__init__(*args, **argv)
        self.input['min_temperature'] = 0
        self.input['max_temperature'] = 1000
        self.input['num_points'] = 11
        self._job_generator = MyJobGenerator(self)

    def collect_output(self):
        v_lst, T_lst = [], []
        for job_id in self.child_ids:
            job = pr.load(job_id)
            T_lst.append(np.mean(job['output/generic/temperature'][-10:]))
            v_lst.append(np.mean(job['output/generic/volume'][-10:]) / len(job.structure))
        with self.project_hdf5.open("output") as hdf5_out:
            hdf5_out['temperature'] = T_lst
            hdf5_out['volume'] = v_lst
```

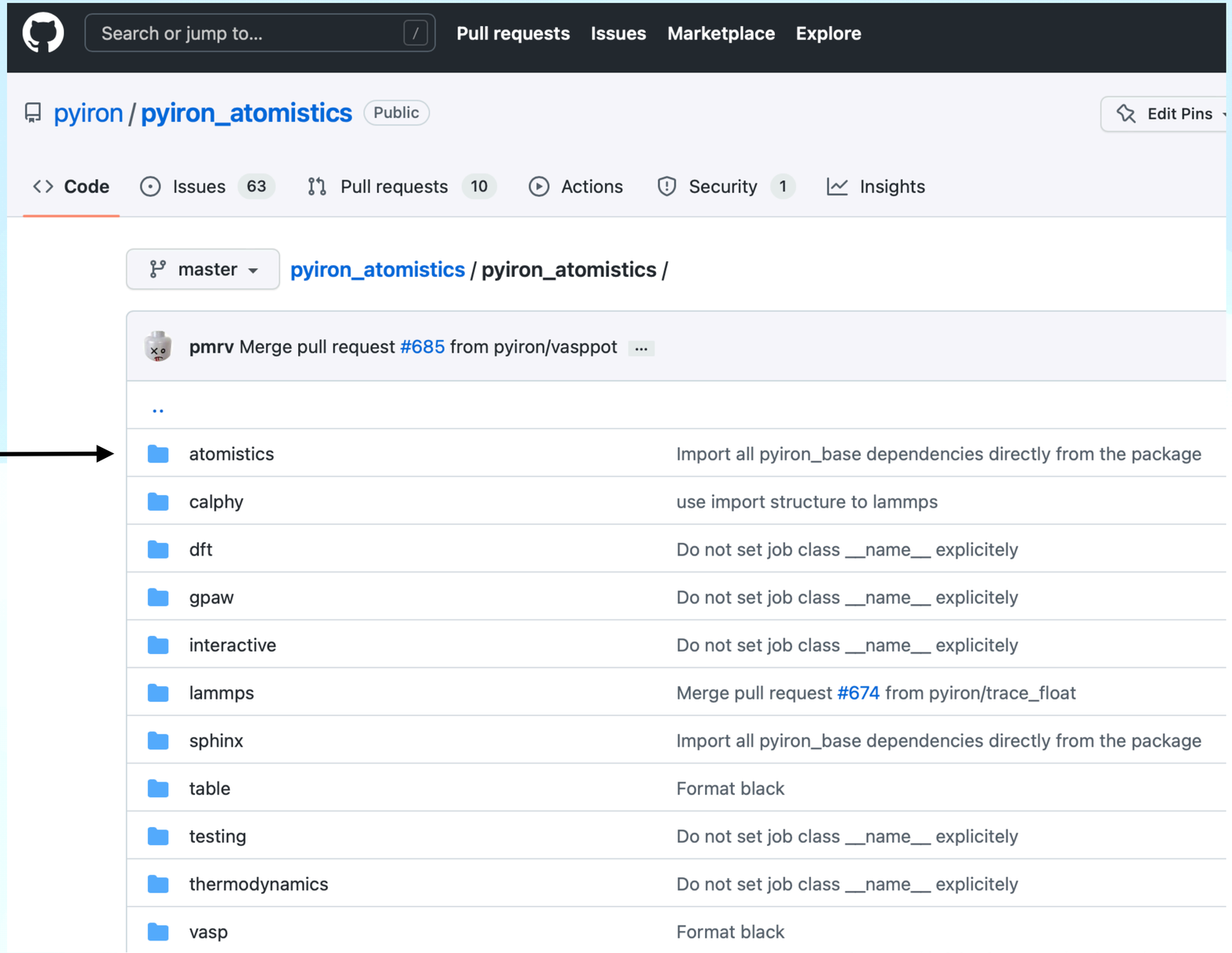
C diffusion barrier in Fe



→ Fix movement along Y-axis
and run `calc_minimize`

I see a problem; what to do?

often →



https://github.com/pyiron/pyiron_atomistics/tree/master/pyiron_atomistics

I see a problem; what to do?

```
lmp = pr.create.job.Lammps('test')
```

```
lmp.output?
```

```
Type:        GenericInteractiveOutput
String form: <pyiron_atomistics.atomistics.job.interactive.GenericInteractiveOutput object at 0x14b48efd75e0>
File:        ~/dev_sam/pyiron_atomistics/pyiron_atomistics/atomistics/job/interactive.py
Docstring:   <no docstring>
```

→ Open it with pycharm and move around

What kind of problems do we have in pyiron?

- LAMMPS potential
  - Pyiron does not know content
- DFT
  - Conversion from generic DFT to code specific input incomplete
- VASP
  - Not taken care of by anyone
- SPHInX
  - Generic DFT input to SPHInX input not properly synchronized
- Master jobs
  - Master job of master job not possible