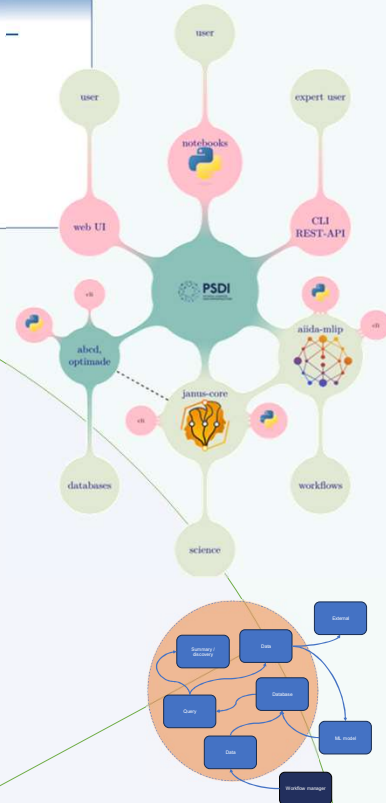
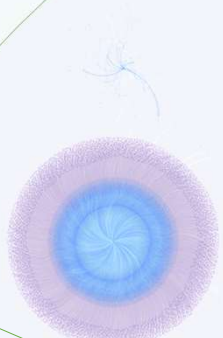


Introduction

- o **design and deploy the hardware infrastructure** to host both training data for machine learnt interatomic potentials –
- o MLIP and potentials themselves
- o **Features:** *Curate, store, distribute and interrogate* MLIPs and training data
- o **Visualisation and training workflows**
- o **Benchmarking and validation**
- o **HPC integration**



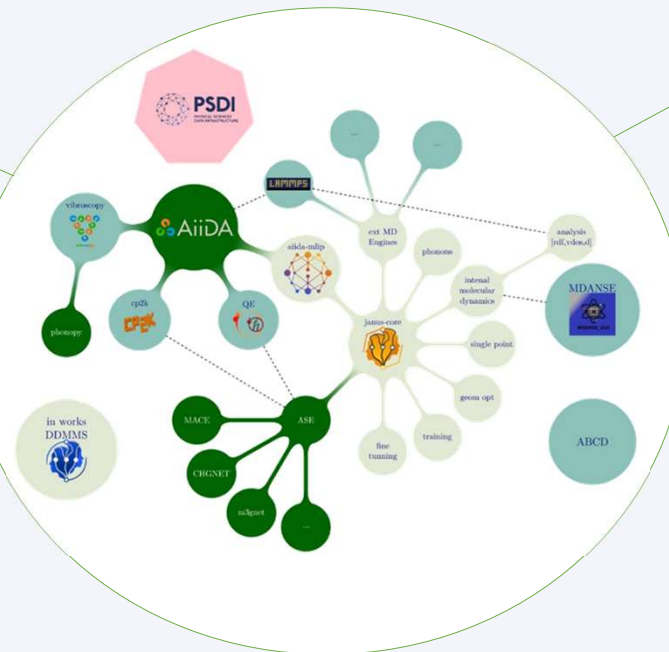
- AiiDA plugin for janus-core
- Data provenance tracking, reproducibility and shareability of processes and data.
- Automatisation of complex workflows
- Common calculations and workflows implemented as AiiDA `Calcjob` and `Workchain` types



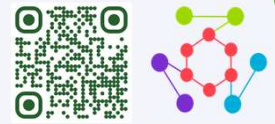
Janus-core



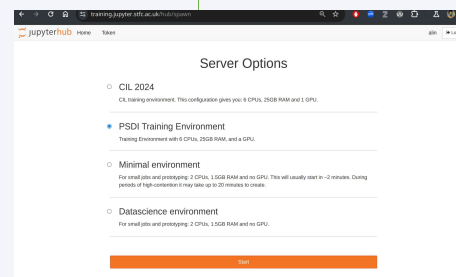
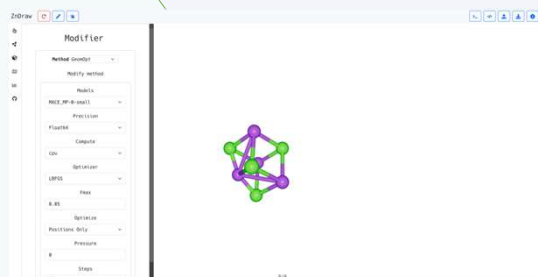
- Converting proof-of-concept tools for MLIPs to production
- Integration of modern MLIPs (MACE, CHGNET, M3GNET)
 - Training/fine-tuning
- Results analysis
- Active learning
- Integration with abcd, aiiida-mlip, PSDI



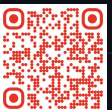
abcd



- Specialised scalable database for MLIPs data training management
- OpenSearch implementation 100 times faster for 500k documents than MongoDB



janus-tutorials



Set of tutorials to use MLIPs:

- [Single Point](#) [Open in Colab](#)
- [Equation of State](#) [Open in Colab](#)
- [Phonons](#) [Open in Colab](#)

