



Science and  
Technology  
Facilities Council

Scientific Computing

# Machine-Learnt Interatomic Potentials Modelling Workflows

Alin M Elena  
scientific computing department

March 17, 2026



Data-driven Materials  
and Molecular Science

**CCP5**  
Collaborative  
Computational Project  
Computer Simulation of Condensed Phases



**PSDI**  
PHYSICAL SCIENCES  
DATA INFRASTRUCTURE

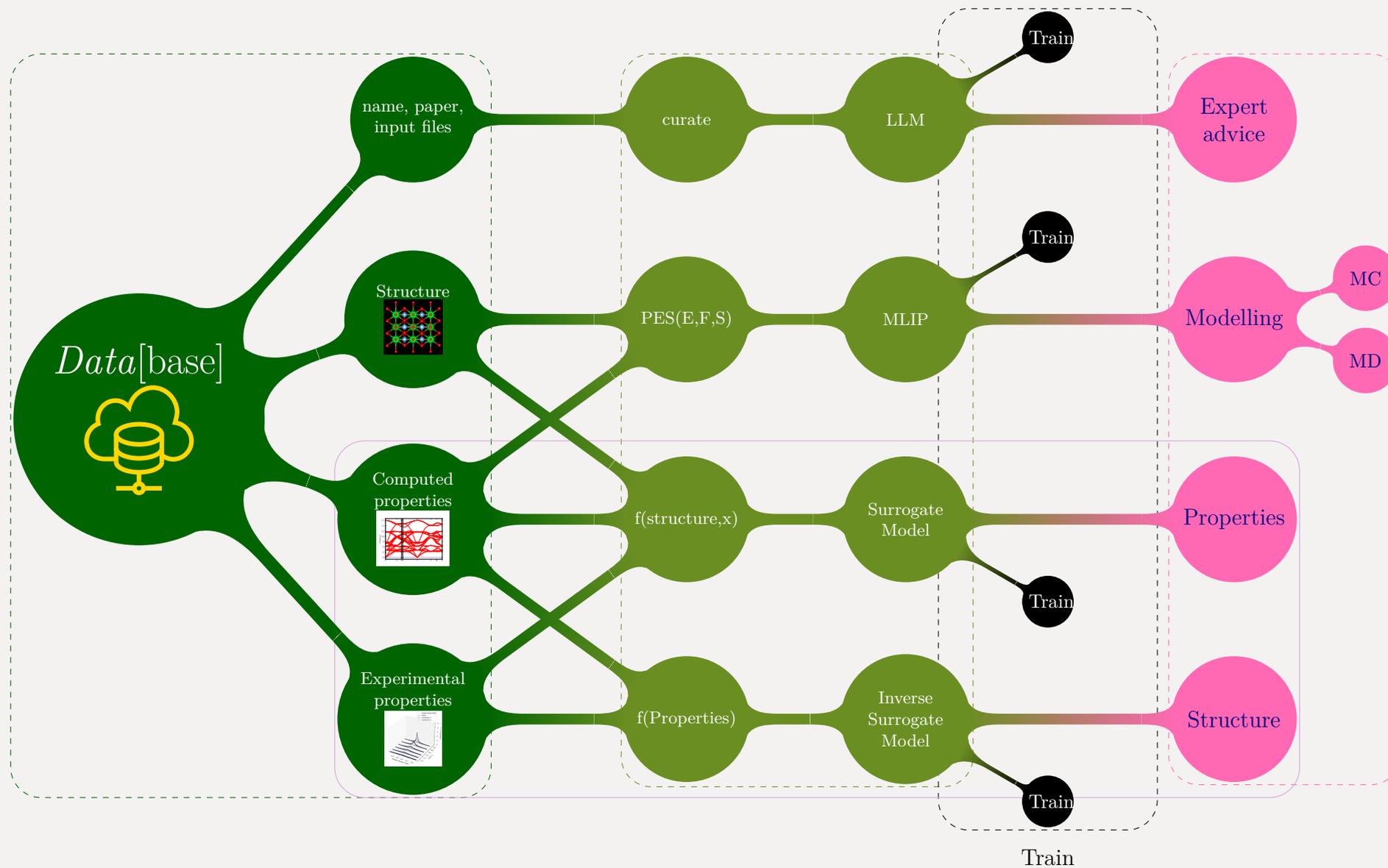


Science and  
Technology  
Facilities Council

Ada Lovelace Centre

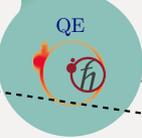
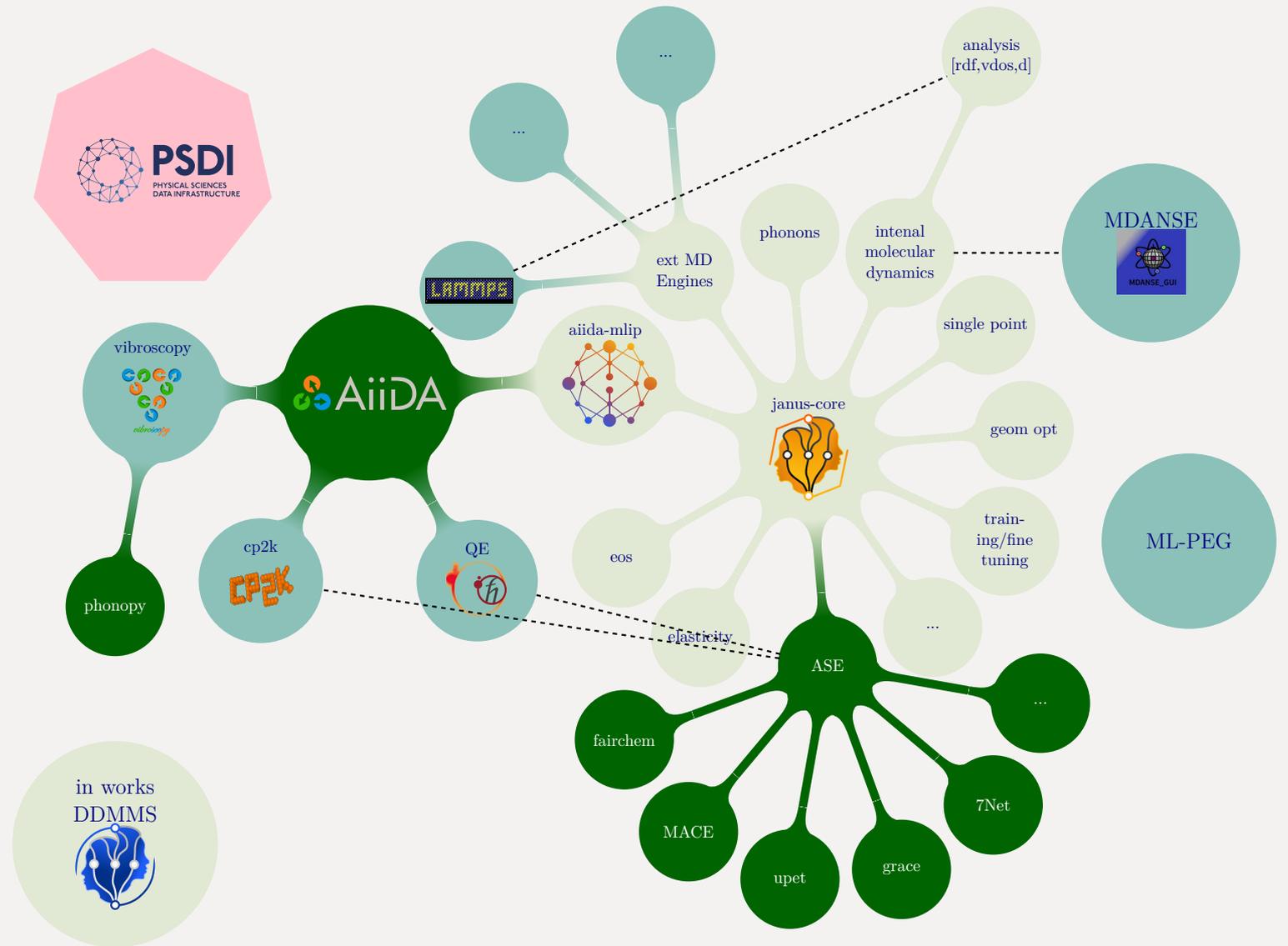


# ML and Materials Landscape





# MLIPs workflows for modelling





# MLIP workflows for experiments: Exafs

## EXAFS Pipeline Processing

Interactive EXAFS processing using the new PipelineProcessor architecture

### Three-Stage Workflow:

- **Stage A: Input Generation** - Create FEFF input files
- **Stage B: FEFF Execution** - Run FEFF calculations
- **Stage C: Analysis** - Process results and create plots

Upload File Uploaded 1 file. [Click to clear files.](#)

Sampling Method

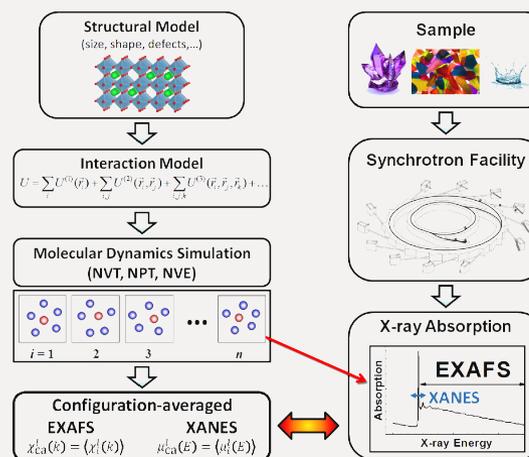
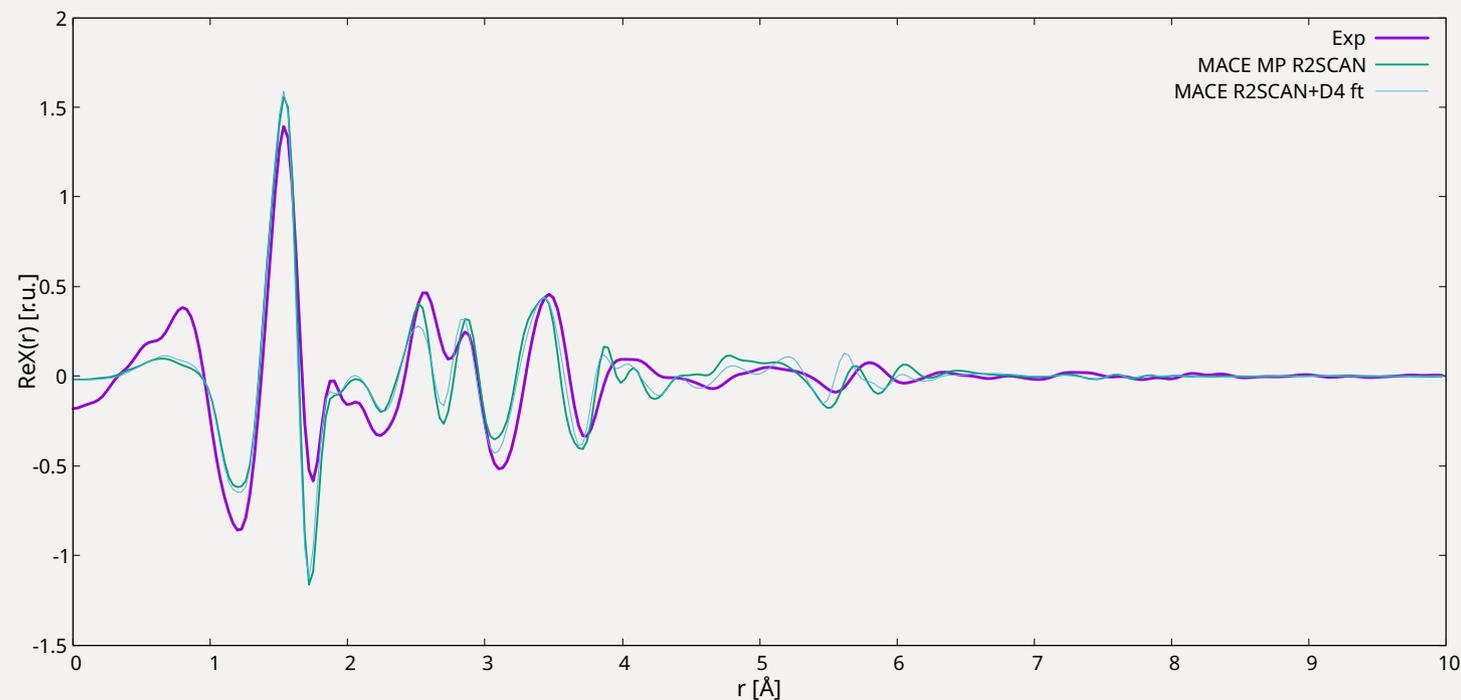
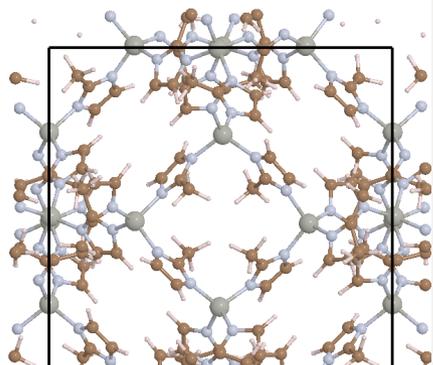
Input Kwags (as dict)

e.g., {'format': 'xyz', 'index': 0}

the uploaded file with current settings

Read Structure

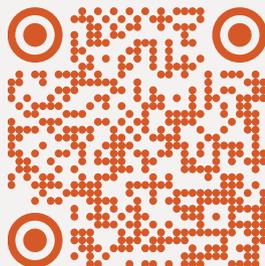
Loaded 100 structure(s).





# Software

**janus\_core**



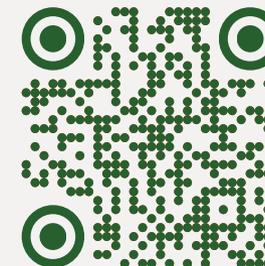
[github.com/stfc/janus-core](https://github.com/stfc/janus-core)

**aiida-mlip**



[github.com/stfc/aiida-mlip](https://github.com/stfc/aiida-mlip)

**pack-mm**



[github.com/ddmms/pack-mm](https://github.com/ddmms/pack-mm)

**alc-dls-exafs**



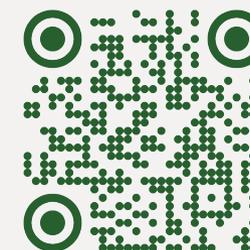
[github.com/stfc/alc-dls-exafs](https://github.com/stfc/alc-dls-exafs)

**data-collections-api**



[github.com/PSDI-UK/data-collections-API](https://github.com/PSDI-UK/data-collections-API)

**ML-PEG**



[ml-peg.stfc.ac.uk](https://ml-peg.stfc.ac.uk)

# acknowledgments



Joshua Elliott, Thokozile Kathyola, Shu Hayama

Prathami Kamath, Théo J Inizan and Kristin Persson

Ilyes Batatia and Gábor Csányi

Gábor Csányi

Elliott Kesoar, Jacob Wilkins, Kane Shenton, Andy Duff



Scientific Computing





Science and  
Technology  
Facilities Council

Scientific Computing

# Questions?





Science and  
Technology  
Facilities Council

Scientific Computing

# Thank you

[scd.stfc.ac.uk](http://scd.stfc.ac.uk)