DIAMOND: Machine Learning Interatomic Potential demonstrator

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Introduction

The goal of the MLP demonstrator is twofold:

- Delivering an open-access repository of MLPs, to which external users can submit new models and download MLP parameterizations
- Building a platform for the development of new MLPs, including:
  - **Automated generation** of training, validation and test datasets
  - **Common interface** for popular MLP packages
  - **Containerized workflow** solution for MLP development

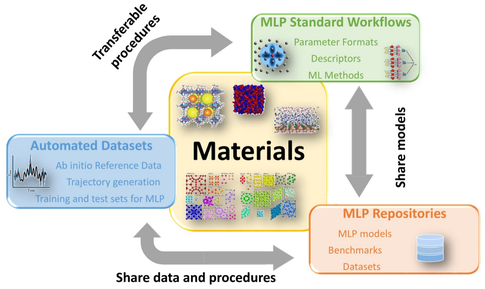

Fig 1. General scheme of the MLP workflow

AiiDA Workflow Management System

- AiiDA [*Uhrin et al., 2021*] is an **open-source**, **high-throughput workflow framework** for computational science with a strong focus on **reproducibility**.
- Workflows in AiiDA are automatically stored in a **provenance graph** with rich **metadata**, including all workflow **inputs** and **outputs**.
- AiiDA is domain agnostic, and any code that can be run over the command line can be integrated through AiiDA's plugin system.

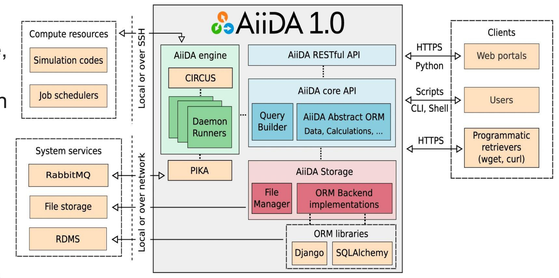

Fig 2. Schematic overview of the architecture of AiiDA 1.0

MLP workflow in AiiDA

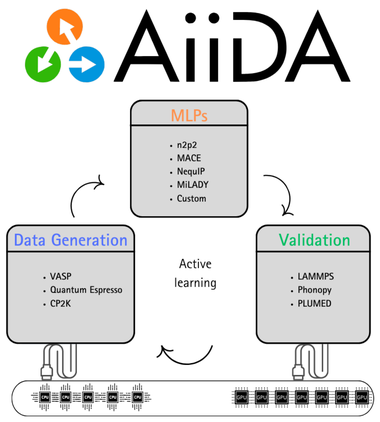

Fig 3. AiiDA workflow for MLPs

Fig 4. Providing a common interface for MLP packages

- ***Ab initio* calculations**: AiiDA provides a plugin interface for software packages such as VASP, CP2K. This will be used to generate training datasets
- **MLPs**: implementation of a **common interface** to train MLPs using different software packages
- **Validation**: methods like (biased) molecular dynamics, phonon-based sampling *etc*

AiiDA-n2p2 plugin

- **n2p2** [*Singraber et al., 2019*] is a software for the parameterization of **Behler-Parrinello neural network** MLPs [*Behler and Parrinello, 2007*]
- We have developed an **AiiDA-n2p2 plugin** to **automate** the process of MLP development
- The plugin features include:
  - Automated selection of optimal weights
  - Validation through molecular dynamics using LAMMPS
  - Semi automated generation of inputs
- Generation of MLPs using AiiDA-n2p2 for aluminium is shown as an example [*Jakse et al., 2022*]

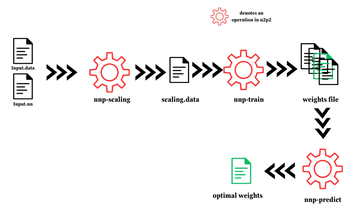

Fig 5. Manual steps in MLP generation for n2p2

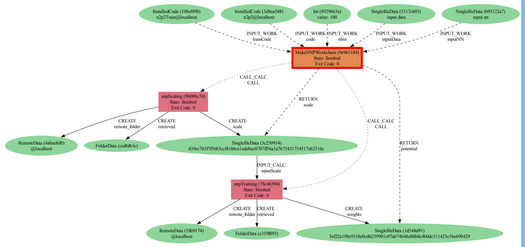

Fig 6. Automated MLP generation for AiiDA-n2p2

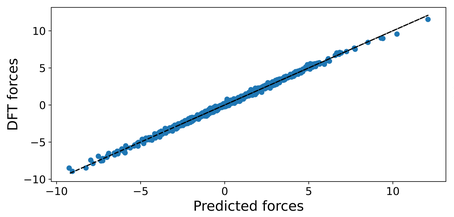

Fig 7. The correlation plot for predicted forces versus *ab inito* forces

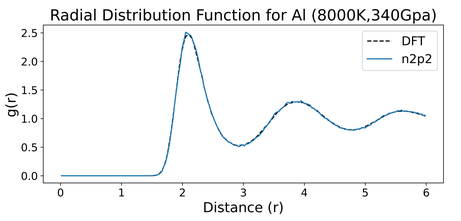

Fig 8. The radial distribution function for liquid aluminium at 8000 K and 340 GPa

Acknowledgements

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