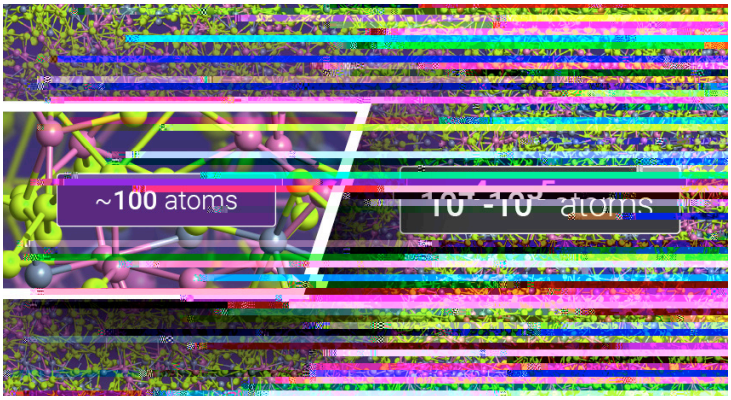
SYNOPSYS®

Machine-Learned Force Fields (ML FFs) provide near-*ab initio* accuracy for large realistic system sizes and dynamical simulation time-scales greatly exceeding those accessible to Density Functional Theory (DFT). Use ML FFs in QuantumATK to generate realistic complex structures of novel crystal and amorphous materials, alloys, interfaces, and multilayer stacks, simulate thermal and mechanical properties, diffusion and surface processes. Benefit from the pre-trained ML FF library or develop new ML FFs using automated and efficient training and simulation workflows. Employ ML FFs for molecular dynamics (MD), force bias Monte Carlo, nudged elastic band (NEB), and geometry optimization simulations.

ML FFs for Dynamical Simulations of Large-Scale Realistic Systems

- 1000 to 10,000x faster than DFT, thus enabling dynamical modeling of realistic novel and complex systems containing even 100,000+ atoms, instead of small model 100-atom systems.
- Provide near-*ab initio* accuracy for multi-element materials, heterogeneous systems like interfaces, and systems far from equilibrium, including amorphous materials, phase transitions, or chemical reactions.
- Often easier to develop than conventional FFs using the automated workflows available in QuantumATK. Accurate conventional FFs for such complex materials would require much more extensive and complicated development processes.



Automated Efficient Generation of ML FFs

Automatic Workflows

Basic workflow
- For crystalline materials
- Automatically generate training configurations, compute training data with DFT, and perform machine learning, i.e., fitting to the training data

Advanced active learning workflow
- For amorphous systems, interfaces, systems at high T, surface processes
- Improve initial ML FFs generated with the basic workflow by actively adding training configurations and DFT training data during MD simulations

Templates & GUI

- Use automatic training tools and GUI templates [1,2] for:
  - crystal & amorphous bulk materials
  - interfaces
  - molecules
- Inspect automatically generated training configurations using GUI
- Validate generated ML FFs by comparing calculated values with available experimental and DFT data:
  - RDF and ADF
  - Elastic constants
  - Neutron scattering factor
  - Chemical composition profile
  - X-ray scattering

QuantumATK Advantages

- Automated user-friendly generation of training data, tailored for specific applications
  - Ensures minimal amount of training data and time needed
  - No computationally expensive *ab-initio* MD is needed in most cases
  - Provides good quality accurate ML FFs for complex systems
- Single interface for different simulation engines
  - Easily switch between training with DFT-LCAO and DFT-PW
  - Combine ML FFs with conventional FFs, DFT or Semi-empirical calculators

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