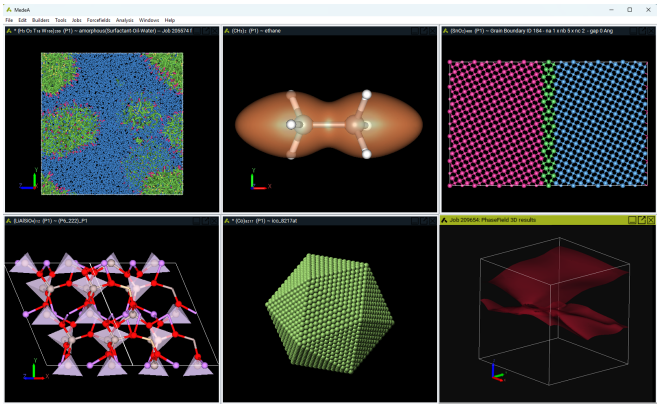
What's New in MedeA 3.12

Train.Deploy.Discover

Materials Design announces the *MedeA* 3.12 materials simulation environment, delivering a revolutionary integration of machine learning capabilities that transform materials modeling workflows. The *MedeA* 3.12 release establishes a comprehensive machine-learned potential ecosystem spanning training, refinement, deployment, and analysis, while introducing powerful new builders for complex microstructures and enhanced tools for materials discovery.



MedeA *3.12 - Train.Deploy.Discover*

At-a-Glance

Key Features of MedeA 3.12

- **Complete MLP Workflow Integration**: Seamless pipeline from VASP MLFF training to LAMMPS deployment with automatic .frc file generation
- **Foundational Model Support**: GRACE-1L-OMAT, GRACE-2L-OMAT, GRACE-1L-OAM and GRACE-2L-OAM universal machine-learned potentials available for immediate use in LAMMPS
- **MLPG Enhancements**: Direct fitting of GRACE potentials (1L/2L) within the MLPG module for custom forcefield development
- **Advanced MLFF Capabilities**: Descriptor reduction, spilling factor quality assessment, and enhanced training set management in VASP
- **Perturbation Builder**: Systematic generation of diverse training sets with controlled perturbations of lattice parameters, positions, and magnetic moments
- **High-symmetry Grain Boundary Builder**: Comprehensive CSL database for nine crystal lattice types enabling systematic interface studies
- **Enhanced Analysis Tools**: New Similarity Analysis for intelligent structure selection from large MLP training datasets
- **Temperature-dependent P3C**: Advanced polymer property predictions with PEARL library exceeding 3 million repeat units

Dr. Clive Freeman, CEO of Materials Design comments:

The MedeA 3.12 environment delivers a complete machine learning workflow for materials modeling. Researchers can now generate training sets with the Perturbation Builder, develop MLFFs in VASP with quality assessment tools, and seamlessly deploy those forcefields in LAMMPS for large-scale simulations. The foundational GRACE models provide immediate access to universal potentials, while MLPG enables custom forcefield fitting. Combined with the new high-symmetry grain boundary builder and Similarity Analysis tool for managing large datasets, this release provides practical solutions for the full spectrum of materials discovery challenges. We're excited to see how these integrated capabilities accelerate research workflows across the community.

About Materials Design:

Materials Design, Inc. is the leading atomistic modeling and simulation software and services company for materials. Materials Design helps customers across diverse industries design and optimize materials and processes, predict materials properties, and generate value through innovation. The company is dedicated to providing efficient access to the world's leading atomistic and electronic scientific simulation methods.

The advanced MedeA®[1] materials modeling and simulation environment is used by thousands of customers at more than 800 institutions worldwide. Scientists and engineers in industry and research institutions rely on the MedeA

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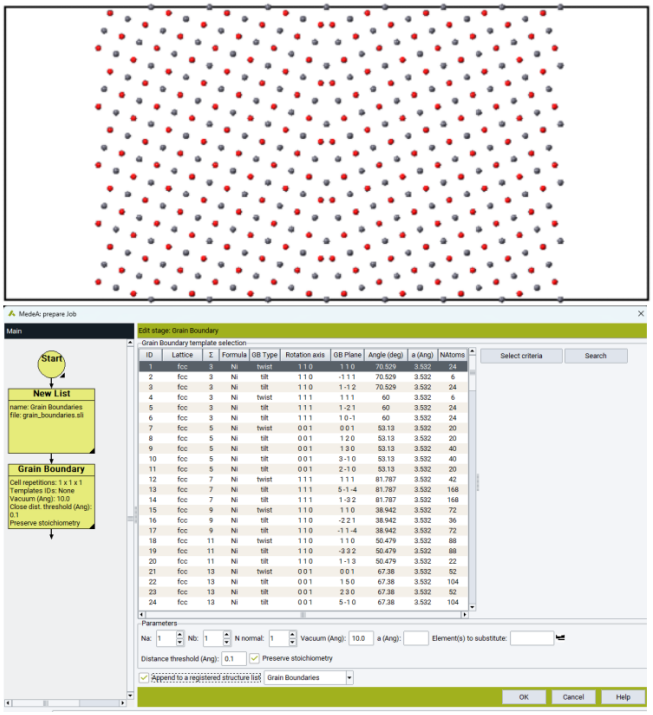
Environment to simulate materials properties and understand diverse phenomena. The MedeA Environment enables users to create better products while saving valuable research and development time and cost.

The MedeA Environment integrates world-leading structural databases (totaling over 1.2 million entries), electronic structure engines (VASP, Gaussian, MOPAC), molecular dynamics (LAMMPS), Monte Carlo methods (GIBBS), and Continuum methods (PhaseField) with a host of powerful building, editing, and analysis tools in a unified environment, allowing the creation of efficient workflows. Its innovative high-throughput (HT) capabilities enable the use of computational resources to achieve exceptional results.

Overview of MedeA 3.12

An overview of updates in this *MedeA* release is provided below.



Create High-symmetry grain boundaries with the Interface Builder

Builders and Editors

- Microstructure Builder
  - Insertion of interstitial atoms at grain boundaries
  - Easy creation of multiple slab structures
  - Rotations can be specified as hkl indices
- Custom supercell builder: a warning is issued if the resulting supercell is left-handed (the system is still built)
- Interface Builder
  - High-symmetry grain boundary builder (NEW)
    - A database of Coincidence-Site-Lattice (CSL) grain boundary models for both twist and tilt types, with Σvalues up to Σ13, is included. The following crystal lattice types are supported
      - face-centered cubic (fcc),
      - body-centered cubic (bcc),
      - hexagonal close-packed (hcp),
      - simple cubic (sc),
      - rocksalt,
      - zincblende,
      - wurtzite,
      - nickeline, and
      - fluorite
    - Models can be customized by specifying size, lattice parameter, and atom types (elements)
    - Multiple grain boundary models can be built simultaneously and saved in a structure list
    - The builder is accessible both as an interactive tool and as a flowchart stage
- Perturbation Builder (NEW)
  - Particularly useful for creating training sets for forcefield fitting and machine learning
    - Lattice parameters (cell lengths and angles) can be randomly perturbed
    - Magnetic moments for all or selected atoms can be set
    - Atomic positions (x, y, z) can be randomly perturbed
    - Magnetic moments can be randomly perturbed
  - The builder is available as an interactive tool and as a flowchart stage
- Amorphous Materials Builder
  - Enhancements for the detection of molecules with large cycles

Engines

- VASP
  - New binaries (VASP 6.5.1) are provided with additional features
    - Export of machine-learned forcefields (MLFF) as .frc files which can be used in *MedeA* LAMMPS simulations
    - Support for data exchange via HDF5 files
    - Support for exchange-correlation functionals from the libXC portable library of functionals at libxc.gitlab.io (DFT, metaGGA, and hybrid func-

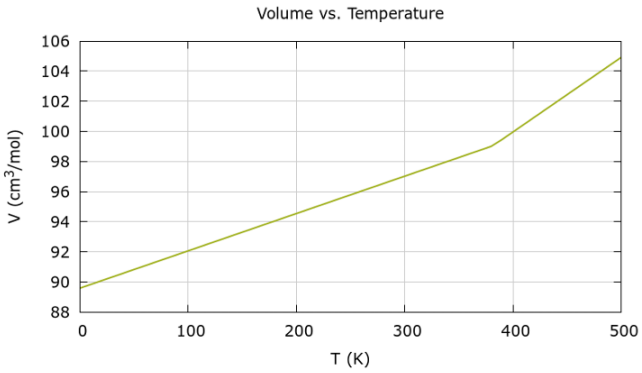
tionals)
    - Support for DFT-D4 van-der-Waals interactions
    - Access to the library for Many-Body Dispersion interactions provided by libMBD
  - MLFF enhancements
    - Controls to reduce the complexity of atomic environment information for increased efficiency have been added: element-reduced three-body descriptors and angular descriptors
    - Quality assessment is now provided using the spilling factor, both in applications and during on-the-fly training
    - Use of structure lists for the entire training set now makes this independent of trajectory file frequency settings
    - Enhanced help text for MLFF options with keyword links
  - Flowchart enhancements:
    Ability for a VASP flowchart stage to access files from previous stages and/or jobs, enabling improved access to:
    - Wave functions and charge densities for restart
    - Final configuration and velocities for MD continuation
    - Trainings sets for continued on-the-fly training or refit
    - Machine-learned forcefields for application
  - Core-level energies are now computed and reported in the ListOfResults.sli structure list
  - A system-independent non-default user choice of the number of bands has been implemented
  - Improved performance by offering greater flexibility for ScaLAPACK
  - Integrated DOS data and related parameters has been added to DOS data for use in the training of machine-learned potentials
  - Enhanced autocorrection procedures to allow user intervention
  - Submission of left-handed systems is prevented with informative warnings
- PhaseField
  - Temperature evolution over time is computed as a function of heat capacity and thermal conductivity
  - Temperature dependencies of material properties (bulk/grain boundary diffusion, free energy, eigenstrain) are supported
  - Boundary conditions and initial temperature scenarios can be defined
  - Visualization of 3D PhaseField results is enabled in Analysis
- LAMMPS
  - New binaries (Jul2025) are provided
    - Machine-learned potentials (MLPs) created by VASP on-the-fly training (MLFF) are supported
    - ACE & GRACE (1L/2L) machine-learned potentials are supported
  - Stress uncertainty evaluation for non-standard orientations is enhanced
  - On-the-fly computation of angle and dihedral distributions
  - On-the-fly computation of the radius of gyration of molecules
- GIBBS
  - Enhancement for sorption simulations on systems with very large solids (unit cell replicated multiple times in each direction); output structures include only the sorbed species

Forcefields

- MLPs
  - GRACE 1L and 2L MLPs are supported in LAMMPS
  - VASP-generated MLPs (MLFF) can be used in VASP and/or LAMMPS
  - Foundational (universal) machine-learned potentials GRACE-1L-OMAT, GRACE-2L-OMAT, GRACE-1L-OAM and GRACE-2L-OAM are available for use with LAMMPS
- MLPG
  - Fitting GRACE potentials (1L/2L) is enabled within the MLPG module
- PCFF+
  - New parameters for boric acid, borate and silicate ions, with refined treatment of fused-ring aliphatics

Property Modules

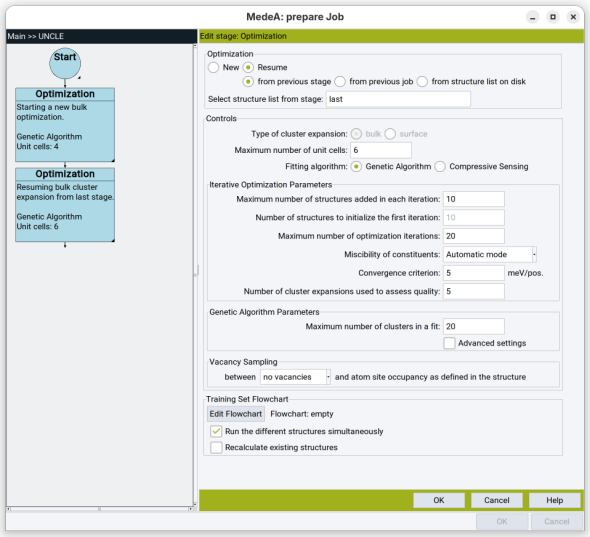
- P3C
  - Temperature-dependent property calculations have been added to the Flowchart P3C stage; graphs for computed temperature dependencies are generated automatically
  - Copolymer property enhancements
    - Properties are reported as described in Chapter 18 of Prediction of Polymer Properties (Jozef Bicerano): Tg, Td12, aT, Density, cp, solubility1, g1, Ref, diel, vpoisson298K, B298K, Eyoung298K Gshear298K,Bf298K, Sy298K, Eavis, PO2, PCO2, and Tc



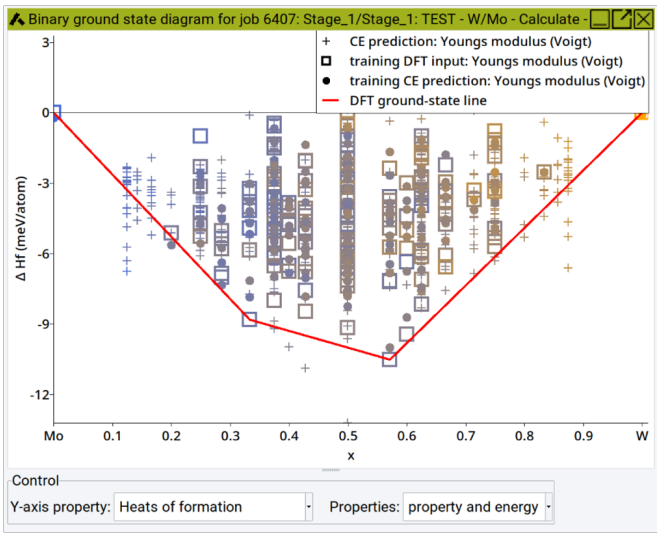
  - Specific heat capacity (cp) is now reported for copolymers
  - Updates for g1, Eyoung298K, Gshear298K, vpoisson298K, V, B298K, Bf298K improve agreement with reference data
  - Td12 and EyoungTgp30K calculations have been improved
- Documentation updates
  - Reporting of temperature-dependent properties
  - Copolymer property enhancements
  - Quality of statistical fits is described
  - Tabulated flowchart variables for properties and descriptors

- Polymer Expert
  - The PEARL (Polymer Expert Analog Repeat unit Library) now includes more than 3 million repeat units. Latest version: 2025-07-28

- UNCLE
  - Optimization stage
    - The ability to resume cluster expansion optimizations from a previous stage, job, or UNCLE structure list has been added
    - Reference energies for all elements in the model are now calculated automatically, ensuring accurate heats of formation for all enumerated structures
    - The vacancy sampling range can now be set from “no vacancy” to the defined occupancy, or from “vacancies only” to the defined occupancy
    - The state of the training set flowchart is displayed in the UI
  - Calculate property stage
    - Support for accurate heats of formation calculations has been added
    - The display of training set flowchart information has been enhanced



Resume an UNCLE optimization from a previous run or stage

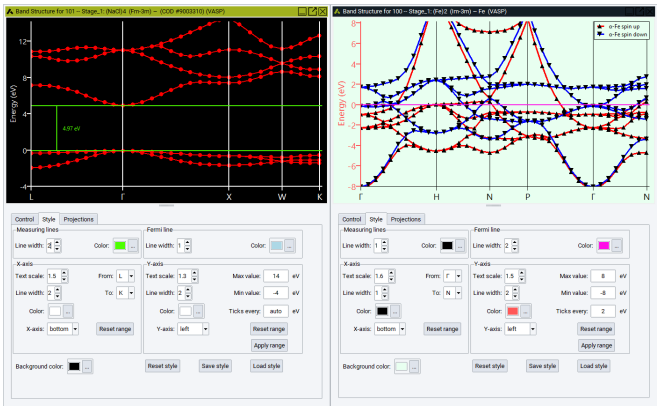


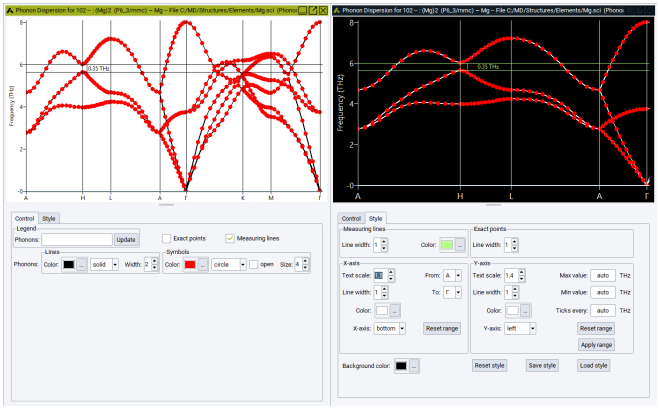
Compute accurate heats of formation with automatic calculation of the reference energies of all the elements in the model

- General improvements to all UNCLE stages

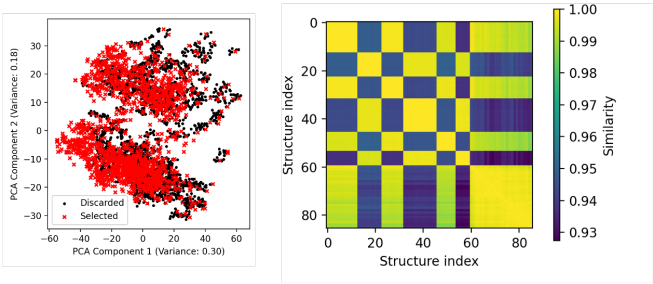
Analysis

- Binary Ground State Diagram Analysis (UNCLE)
  - A control for switching the y-axis between “Total energy,” “Pseudo heats of formation,” and “Heats of formation” has been added
  - Support for plotting data from the Calculate Property Stage with color-coded properties has been added
  - The random mixing energy curve is plotted when available
  - High-resolution screen support has been improved
- Monte Carlo Temperature Profiles
  - Support for high-resolution screens has been improved
- Band Structures and Phonon Dispersions Plot
  - A Style panel has been introduced, allowing customization of color, scale, and size of measuring lines, Fermi line, and axes. The plotting range and axis placement can be fine-tuned, and the background color can be changed. Styles can be reset, saved, or loaded
  - Support for high-resolution screens has been improved





- Similarity Analysis (NEW)
  - Structural similarity in lists (sli, fts, trj) can be checked
  - Smaller subsets including representative structures can be generated
  - Implemented as an interactive builder and as a flowchart stage



Use similarity analysis to reduce the size of an MLP training set

- Radius of Gyration (NEW)
  - Computation of the radius of gyration for selected molecules from an MD trajectory or a structure list
  - Implemented as an interactive builder and as a flowchart stage
- Geometrical distributions (NEW)
  - Computation of distances, angles and torsions for selected subsets of atoms (single, pair, triplets)
  - Implemented as an interactive builder and as a flowchart stage
- Constitutional descriptors’ list updated to consist of Joback & P3C descriptors

JobServer & TaskServer

- TaskServer SLURM Wrapper Script: Monitoring capabilities have been introduced to track the state of submitted tasks in the SLURM queue, ensuring smooth execution
- Enhancements for transfer of large files to the JobServer

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