MedeA 3.10 Release Note:

Key features in MedeA 3.10

- **Phase Field Modeling:**

  Study the evolution of microstructures with the powerful new *PhaseField* tool, to simulate processes such as grain growth, corrosion/oxidation, hydriding, phase separation (e.g., spinodal decomposition), precipitation, and solidification. *MedeA PhaseField* allows you to use properties computed using atomistic simulation methods (free energies, diffusion coefficients, and elastic constants) to simulate and understand materials behavior over substantial length and time scales, dramatically extending the scope and range of the *MedeA* materials simulation environment.

- **Enhanced Materials Modeling:**

  Explore the rich landscape of magnetic materials with support for non-collinear magnetic structures in VASP and throughout the *MedeA* interface.

- **Advanced Simulation Engines:**

  Leverage the power of VASP, LAMMPS, and GIBBS with new features and optimizations for faster and more reliable simulations.

- **Cutting-Edge Forcefields:**

  Benefit from enhancements to *MedeA* forcefields for *MedeA* simulations based on classical forcefields, and improved capabilities for machine-learned potential generation and usage.

- **Powerful Analysis Tools:**

  Gain deeper insights into your materials with enhanced options for structural analysis, phonon dispersion, band structure, and density of states analysis.

- **Polymer Property Analysis and Design:**

  The *MedeA* Polymer Expert module has been substantially extended and now includes a synthetic difficulty score for any returned polymer system. The Polymer Expert Analog Repeat-unit Library (PEARL) database has been extended to include more than 3 million unique entries, making PEARL the largest compendium of synthetically accessible polymer systems commercially available today.

MedeA 3.10 Release Note:

Builders and Editors:

- **Building and editing periodic structures:**
  - Create non-collinear magnetic structures with spin vectors assigned to atoms
  - Switch between collinear (scalar) and non-collinear (spin vector) magnetic structures and vice versa in the Edit Atom tab of the Edit structure... menu
  - Automatically initialize non-collinear magnetic moments upon switching to non-collinearity
  - Edit non-collinear magnetic moments (spin vectors) in the Edit Atom tab of the Edit structure... menu or the Atoms spreadsheet
  - Process non-collinear magnetic structures in *MedeA*'s Builders and Editors
  - Handle non-collinear magnetic moments to initialize non-collinear and spin-orbit magnetic VASP calculations

- **Polymer builder:**
  - Enhancement for repeat units' recognition

- **Thermosets:**
  - Enhancement for retrieving build cycle trajectories

- **Amorphous Materials builder:**
  - Added ability to use a custom forcefield and ship it to the Job Server to be used, even if no other stage is present in the flowchart

- **Flowchart:**
  - New "Append to list" stage

- **Subsets:**
  - Enhanced user interface for the creation and use of pair/triplet/quadruplet

subsets
  - Enhancements in the visualization of pair subsets
  - Extension of operations in the Subset Manager (combine subsets)

- Enhancements for the use of variables to define subsets in "For" loops
- Extensions for the creation of supercells in Flowcharts
- Enhancement for ring catenation checks
- Enhancement for speed-up of duplicate checking when importing lists in the Fitting Data Manager
- Random Substitution:
  - Enhancement for use of isotopes
- Enhancements for sorting of columns in the Atoms spreadsheet
- Extended information provided when Forcefield Optimizer is used with a forcefield which contains "bond-increments" for the charge assignments
- Microstructure Builder:
  - Enhanced printing of information, help messages and warnings
- Added support for space group Pn as an alias for P1n1

Databases:

- Enhanced space group handling for ICSD
- New Polymer Expert databases

MedeA 3.10 Release Note:

Compute Engines:

VASP:

- Initialize non-collinear magnetic moments from non-collinear magnetic initial structures when running non-collinear or spin-orbit magnetic calculations
- Run automatically non-collinear magnetic calculations for non-collinear magnetic initial structures, if Magnetism is set to "Defined by model"
- Addition of an approach to constrain non-collinear magnetic moments via a penalty contribution to the total energy and Hamiltonian, including an automatic stepwise increase of the weight of the penalty terms to converge the total energy of the constrained magnetic structure
- Addition to structure optimizations in VASP 6: Enable selective optimization of cell vectors that are orthogonal to all other cell vectors
- Extension to density of states calculations: enable l,m-projected partial density of states with respect to the Cartesian coordinate system for each individual atom
- Enhancement to VASP 5 user interface for restoring options from VASP 6 jobs
- Enable MLFF for VASP-NEB and VASP-VTST
- User interface enhancement for setting per-site potentials
- Enabled choice for the number of grid points for all optical spectra techniques (including TD-DFT, GW, time evolution approach etc.)
- Enhancement to VASP GPU executables for performance on a wide range of hardware components
- Access to legacy potentials
- Default potentials version set to 6.4

MedeA 3.10 Release Note:

New PhaseField module:

- Evolves a microstructure in either 2D or 3D over seconds, days, or years using phase field equations.
- Enables the simulation of multiple phases and grains of phases thanks to efficient parallelization.
- Implements mechano-elastic effects when phases grow or shrink.
- Allows the setting of bulk diffusion for every phase and grain-boundary diffusion at the interfaces for the diffusing species.
- Uses a robust and efficient finite-element framework with adaptive meshing and adaptive time stepping for optimal performance and high numerical stability and accuracy.
- Supports periodic boundary conditions as well as the presence of free surfaces with custom constraints.
- Provides several initial scenarios to simulate different microstructure problems, e.g., tessellated grain structures (periodic or columnar), small, nucleated particles, or perturbed fields to model spinodal decomposition.
- Uses the *MedeA* task server and job server and is fully integrated into the *MedeA* platform, leveraging the calculation of materials properties from first principles and atomistic simulations within the same computational environment.

LAMMPS:

- New LAMMPS 17Apr2024 binaries
  - Enhancements for speed-up of large input file generation
  - Enhancements when adding analysis items in a LAMMPS stage with existing analyses present
- New LAMMPS on-the-fly analysis of the radius of gyration (Rg) in the LAMMPS NVT,

NPT and NVE stages

- Enhancements in Viscosity and Thermal Conductivity when the Mueller-Plathe method is used, to assist with the selection of number of layers
- Updated long-range electrostatics methods in flowcharts in the flowchart library to PPPM
- Extend reporting associated with attempts to perform NPT simulations on systems with fixed atoms
- Unified GPU support for Windows

GIBBS:

- Enhancement for update of atoms to be excluded from the energy grid computation in a sorption simulation
- Setting increased tolerance for rigid molecules

MOPAC:

- New MOPAC TS flowchart added to the flowchart library

Forcefields:

- Set Forcefield stage:
  - Added ability to use a variable for the forcefield file name
- PCFF+:
  - Refinement for formic acid (new atom type)
  - Minor adjustment of phenyl-sulfonate bond increment
  - Addition of missing bond increment for hydroxylated alumina O-H bonds

- Addition of missing bond increment for cp - n_4c atom types
- Minor adjustment of charges on the carbonate anion

- MLPG & MLPs:
  - Improved reporting during generation of ACE potentials
  - Addition of optimal design analysis function for the Fitting Data Manager
  - Added fitting training sets as a choice to initialize structure lists
  - Enhancements in the Analysis user interface
  - Extensions to handle cases when charges are defined and an MLP is being used
  - Extensions for reporting on the quality of fitting datasets
  - Addition of a machine-learned potential (MLP) in the ForceFields library which allows for prediction of phase diagrams for Si/O phases
- Display of the active forcefield in Job.out, if there is a flowchart stage requiring the use of a forcefield.
- Added reporting forcefield version number in Job.out (except for EAM and ReaxFF forcefields)

Property Modules:

- Polymer Expert:
  - Enhancement for speed-up of writing a structure list file using Polymer Expert in a flowchart stage
  - Addition of synthesis difficulty score (SD-Score) information to the Polymer Expert output, allowing users to select repeat units on the basis

of synthetic accessibility

- The Polymer Expert Analog Repeat-unit Library (PEARL) database has been extended to include over 3 million entries, enhancing the ability of Polymer Expert to identify polymers based on desired properties.

- Docking:
  - Enhancement for cases where the guest molecule does not have a forcefield assigned

Analysis:

- New Structural Analysis with additional functionality and extensions for also treating structure lists and trajectories, including the ability to save and reuse an analysis protocol
- New summary/monitoring plots in the job (accessible from the JobServer) for different types of jobs (e.g. LAMMPS, GIBBS, MLPG) with export options

- Enhancement for plots printed after job and analysis completion (on Windows)

- Updated Phonon Dispersion plot tool
  - Customize plot style (line type, line width, symbol, symbol size)
  - Add/modify legend
  - support for Greek characters
    - Added structure name to plot title

- Added k-point and frequency to plot animation window title

- Updated Band Structure plot tool
  - Customize plot style (line type, line width, symbol, symbol size)
  - Add/modify legend
    - support for Greek characters
  - Display site and orbital projections (so-called fat bands)
    - Scale projections by symbol size and/or color
    - Define color scheme and symbol type

- Updated Density of States plot tool to display l,m-projections for each individual atom. This includes the following projections with respect to the Cartesian coordinate system:
  - px, py, and pz projections
  - dxy, dyz, dz2, dxz, and dx2-y2 projections
  - fy3x2, fxyz, fyz2, fz3, fxz2, fzx2, and fx3 projections

- Enhancements for Fermi surface rendering

JobServer & TaskServer & Maintenance & Infrastructure:

- Improved handling of task termination in asynchronous mode
- Extension to allow user ids (for JobServer/TaskServer encrypted connection) to contain "." characters
- Updated Linux post-install for LAMMPS symlink creation
- Updated Open MPI to 20240725
- Addition of an editable option to set JobServer timeout (default 10 sec)