MedeA 3.9 Release Note:

MedeA 3.9 Highlights:

- **Machine-Learned Atomic Cluster Expansion (ACE) Potentials** based on the PACEMAKER code,
- **Enhanced VASP Quantum Engine** with new density functionals and Projector Augmented Wave (PAW) potentials, designed for performance on the latest graphics processors,
- **Improved atomistic forcefields** enhancing the accuracy of simulations and their applicability in diverse research areas, and
- **Innovative VOTCA module** for seamless parameterization of coarse-grained forcefields from atomistic simulations for mesoscale applications.

Builders and Editors:

- Enhancements in exporting SVG files
- OpenBabel update
- Amorphous Materials Builder:
  - Improved handling of removed components
  - New compress layer functionality for quick and robust use, interactively and in a flowchart, for building layers at the desired density
- Updates to trajectories handling
- Extended Stack Layers builder to allow for stacking triclinic cells
- Ability to create repeat units from SMILES
- Enhancements for mass criterion when creating Subsets
- Microstructure builder:

- Weighted seed & growth to create grains of different volume distributions
- Option to create columnar slab geometries and rotations around z-axis only
- Flowchart stage for builder to be used in a flowchart

Engines:

VASP

- Update to the latest release **VASP 6.4.3** with many enhancements and bug fixes
- New OpenACC-based GPU version which now supports all features of the CPU version
- Added support for new VASP 64 potentials. Users can choose their own default and switch easily between 54 and 64 potentials
- Added support for the revPBE density functional from the user interface
- Added support for further Van der Waals density functionals from the user interface: vdW-DF-cx, rVV10, r2SCAN+rVV10, PBE+rVV10L
- Added support for further meta-GGA functionals from the user interface: SCAN-L, rSCAN-L, r2SCAN-L, v1-sregTM, v2-sregTM, v3-sregTM, v2-sregTM-L, OFR2, local MBJLDA
- Added support for further hybrid functionals from the user interface: HSE03, HSEsol, RSHXLDA, RSHXPBE, SCAN0
- Added support for the van der Waals corrections Many-body dispersion energy /FI and DFT-ulg from the user interface
- Davidson optimization algorithm (non-blocked) available for all simulations
- CSVR thermostat for canonical (nVT) ensemble
- Enhancements for MLFF Molecular Dynamics simulations and trajectory handling
- Substantial speed-up of post-processing of Molecular Dynamics runs
- NMR Calculation enhancements: vGv approximation for evaluating the magnetic susceptibility

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LAMMPS:

Enhancements in NPT, Minimize and Compress Layer stages to allow for the use of variables

GIBBS:

- Several enhancements for GIBBS trajectories and structure list
- visualization
- Enhancements for Sorption stage

Forcefields:

- **MLPs:**
  - Added ZBL parameters to SNAP MLPs
- **MLPG:**
  - New MLP type supported: ACE (New)
  - Fitting Data manager enhancements
  - Enhancements to forces' charts
  - Ability to use variables for hyperparameters
- **VOTCA (New)**: New module for coarse-grained forcefield creation from atomistic simulation input (Iterative Boltzmann Inversion and Force Matching methods)
- **PCFF+:**
  - New atom types and parameters for alkyl borates

- Refinement for quaternary carbon c0 nonbond parameters
- New atom type for alumina and updated for surface atoms
- Addition of bond term and bond increment for alpha carbon in carbonates
- Enhancements for oxalatoborate anions and new atom types

- **ReaxFF:**
  - Added CHONS ReaxFF parameter set (Mattsson et al.)
- **New torsion terms for use with UFF in LAMMPS**

Property modules:

- **UNCLE:**
  - Improvements to message handling, initial and final structure reporting, and checks for the number of requested structures
  - Enhancements for Optimization stage
- **P3C:**
  - Enhancements for computation of X3 and X10 descriptors, and perception of ortho/meta geometries
- **Phonon:**
  - Enhancements for computations using NNP (MLP) forcefields
- **MD Phonon:**
  - Added Etot_QC, sum of MD total energy and the quantum correction of the vibrational energy
  - Added Atotal, the total vibrational Helmholtz free energy, which is calculated with Etot_QC - Svib T
  - Enhanced support of Job restart functionality

- **Polymer Expert:**
  - Enhanced handling of messages and warnings issued
- **Deposition:**
  - Enhancement for use of variables to define regions

JobServer/TaskServer:

- Extended Job submission dialog to include summary regarding the JobServer chosen, the input structure and the active forcefield
- Extended Job submission dialog to include Queuing System options
- Extended TaskServer for GPU device selection
- Enhanced database performance