MedeA 3.5 Release Note:

MedeA new features:

Description of MedeA 3.5 New Features and Enhancements

Flowcharts:

- **A brand-new flowchart interface with improved ease of use for all flowchart stages**
- **Copy/paste functionality for all flowchart stages**
- **Ability to retrieve flowcharts from VASP runs submitted through the (non-flowchart) VASP interface**
- **A new Interfaces stage**

Builders and Editors:

- **Structure Lists for calculation automation and information management are now available with the standard MedeA Environment**
- **Structure Lists can be directly created from several flowchart stages, such as:**
  - VASP
  - GIBBS
  - Phonon
  - MT
  - TSS
  - LAMMPS Deposition
  - UNCLE
- **Numerous enhancements for large PDB files**
  - Enhanced connectivity information handling
  - Added ability to write large PDB files with hybrid36 extension (for systems containing 100,000 atoms or more)
- **Added ability to read mmCIF files through OpenBabel**

MedeA 3.5 Release Note:

Engines:

VASP

- **Full VASP 6.3.1 support via MedeA**
- **On-the-fly machine-learned forcefields (MLFF):**
  - Accelerates ab initio molecular dynamics simulations employing machine learning, massively increasing accessible simulation times
  - Creates a machine-learned forcefield using ab-initio molecular dynamics trajectories as training set as the simulation proceeds
  - Continues machine-learned forcefield optimization running additional molecular dynamics simulations (for other systems)
  - Applies machine-learned forcefield without further running ab-initio simulations
- **Various improvements and optimizations for non-collinear VASP 6 and 5.4 calculations**
- **Enhanced of parsing efficiency of large OUTCAR files**
- **Further support of MetaGGAs (rSCAN, r2SCAN)**
- **Structure lists (ListOfResults.sli) with final structures and including calculated properties, suitable for forcefield fitting, are now created automatically further enhancing efficiency, analysis, and post-processing options**

LAMMPS

- **Updated to the 7Jan22 version**
- **Added support for new packages:**
  - PYTHON: both Linux and Windows, on CPUs and GPUs
  - SPIN: both Linux and Windows, on CPUs and GPUs
- **Improved GPU support:**
  - Support for Nvidia GPU cards with compute capabilities from 3.5 to 8.6 on both Linux and Windows
  - Approximately 40% computation performance improvement for potentials using

long-range Coulombic interactions

- **Use new rigid pcff+ H2O model employing shake (which is now the default) providing superior rdf, and surface tension for water at ambient conditions**

Forcefields:

PCFF+

- Improved water model

Property Modules:

Phonon

- **Structure list (DisplacedStructures.sli) created, suitable for forcefield fitting**

MT

- **Structure list (StrainedStructures.sli) created, suitable for forcefield fitting**

TSS

- **Structure list (EnergyProfileStructures.sli) created, suitable for forcefield fitting**