MedeA 3.8 Release Note:

MedeA new features:

Description of MedeA 3.8 New Features and Enhancements

Builders and Editors:

- **Microstructure Builder (New)**
  - The MedeA Microstructure Builder creates microstructure models for atomistic simulations using a Seed & Growth algorithm with starting points either placed randomly or at user-specified coordinates within a supercell. Each such point is used as an origin to grow a crystalline grain by adding atoms from that seed point outwards until a grain boundary is encountered.

  - The models created by the MedeA Microstructure Builder can be used with other MedeA tools to explore microcrystalline materials' structural, energetic, and dynamic characteristics.

  - Enhancements for exporting structures to extxyz
  - Enhancements for bond computation
  - Enhancements for assigning element colors
  - Addition of the ability to use a variable for density in the amorphous builder stage
  - Added an automated orthorhombic construction mode to the Supercell Builder

MedeA 3.8 Release Note:

Engines:

- **VASP:**
  - Update to latest VASP 6.4.2 executables for Linux and Windows
  - All combinations of constraints for atom positions, cell volume and shape are enabled for structure optimization Added user interface support for many molecular dynamics features through (thermostats, constraints, monitoring)
  - Added support for isoenthalpic isobaric (nPH) ensemble
  - Added ability to refit machine-learned forcefields
  - New user interface for fine-tuning and optimizing the process for on-the-fly machine learning and refitting of forcefields.
  - Faster loading of machine-learned forcefields.

- **LAMMPS:**
  - Update of automatically produced plots (post-processing)
  - Addition of an option for writing a trajectory in native LAMMPS format
  - Addition of warning if there are frozen atoms during an NPT run

- **GIBBS:**
  - GIBBS 9.7.8 executables for Linux and Windows

- **GAUSSIAN:**
  - Optimization of transition states accessible in flowcharts

MedeA 3.8 Release Note:

Forcefields:

- **MLPG:**
  - Enhancement to allow for manual assignment of structures to training/validation sets
  - Addition of "Coordinates" property when importing into the Fitting Data Manager
- Enhancements on forcefields handing in **FFO**
- **PCFF+:**
  - Refined nonbond parameters for carbon in acetal groups

Property modules:

- **Polymer Expert (New)**
  - Polymer Expert is a new module in the MedeA Environment in MedeA 3.8. The innovative Polymer Expert capability facilitates de novo polymer design through high-efficiency access to a substantial (>1.1 million entries) database of polymer properties, PEARL (Polymer Expert Analog Repeat unit Library). Polymer Expert allows you to identify novel polymers by querying the PEARL database based on properties and property ranges. You can also search for biologically derivable analogs within the PEARL database. Polymer Expert was developed in collaboration with Jozef Bicerano, the author of Prediction of Polymer Properties, Marcel Dekker, Inc. (2002) and is described in the paper: J. Bicerano, D. Rigby, C. Freeman, B. Leblanc, and J. Aubry, Polymer Expert - A Software Tool for De Novo Polymer Design, 2023 (submitted for publication).

MedeA 3.8 Release Note:

- **P3C:**
  - In consultation with Jozef Bicerano, various upgrades to P3C have been made, extending and adding correlations, allowing MedeA P3C to report polymer properties for larger systems and presenting results to users in an improved and more intuitive manner.
- **Deposition:**
  - Enhancements for subsets used in deposition
- **MT:**
  - Faster loading of machine-learned forcefields
  - Output enhancements

Analysis:

- Enhancement for pair correlation panel

Infrastructure:

- Addition of the MedeA Python environment
- Update of IntelMPI to the 2019 version on Linux