MedeA 3.1 features:

- VASP 6 with a dedicated GUI
- A mesoscale builder for creation of coarse-grained molecules
- Extensions to builders for handling coarse-grained systems (polymer builder, amorphous materials builder and thermoset builder)
- Flowchart support for mechanical modification of arbitrary systems through the Deformation module
- The direct simulation of emissivity
- The ability to start GIBBS Monte Carlo simulations from existing configurations
- Numerous PCFF+ forcefield enhancements
- Support for the latest version of LAMMPS
- A streamlined installation and administration interface
- The UNIFAC correlative simulation method
- A diverse array of high throughput simulation environment updates
- Numerous enhancements throughout MedeA's infrastructure support the key themes of this release: accuracy and realism

Description of *MedeA* 3.1 new features and enhancements

Builders and Editors

- Mesoscale Builder: NEW builder for building coarse-grained molecules, using pre-defined beads or introducing new types of beads
- Polymer Builder: ability to build coarse-grained polymers
- Amorphous Builder: ability to build coarse-grained systems
- Thermoset Builder: ability to build coarse-grained thermosets

Engines

- ***MedeA VASP***
  - VASP 5.4.4 and VASP 6.1.1 executables
  - Dedicated VASP 6 GUI enabling easy access to newly implemented functionality of VASP 6.1.1 as listed below
  - Space-time based approach for the calculation of polarizibility, providing essentially cubic rather than quartic scaling with system size, facilitating the study of larger systems
  - Accurate energy, forces and phonon modes from adiabatic connection applying the space-time algorithm (Low Scaling ACFDT/RPA)
  - Automatic optimization of atom position on the ACFDT/RPA level of theory applying the space-time algorithm
  - Accurate energy from Moeller-Plesset perturbation theory (MP2)
  - Dielectric-dependent hybrid functionals (DDH/DSH)
  - Electron-phonon interaction from full Monte-Carlo sampling of displacements or a single-configuration (Zacharias-Giustino approach)
  - X-ray absorption spectroscopy (XAS)
  - GUI access for applying electric fields
  - Enhancements for NMR calculations
- ***MedeA LAMMPS***
  - LAMMPS 3-March 2020
  - Several enhancements on existing functionality
  - Additional LAMMPS packages included in the build (LATTE, USER-COLVARS)
  - Support for NVIDIA GPUs up to compute capabilities of 7.0
- ***MedeA GIBBS***
  - GIBBS 9.7.3
  - Ability to start a single-phase simulation from a pre-built initial configuration
  - Extended, and fully automated, Pivot move control

Property Modules

- Brand new Deformation Module to apply systematic stresses and strains to atomic models in a defined manner
- Molecular Descriptors: addition of new molecular descriptors facilitating correlative model creation
- Brand new UNIFAC capability for vapor−liquid equilibria simulation based on correlations

Forcefields

- Extension of nonbond interactions in frc files to handle defined pair-interactions instead of using mixing rule (LAMMPS)
- **New Mesoscale Forcefields:**
    - MARTINI
    - SPICA
- **pcff+ : Forcefield extensions for:**
    - Optimized parameters for Ba (based on BaCO3)
    - New parameters for divalent Mg and Sr cations
    - Improved parameterization of urea
    - Extensions for -OCH3 terminated oligo-ethyleneglycols
- **EAM:**
    - Combination of Morse Forcefield with Streitz-Mintmire charge equilibration
- **TraPPE-UA+:**

Flowcharts:

- Subset Manager stage: providing the ability to create a subset in a flowchart
- Flowchart Library: several updates to existing flowcharts and addition of new flowcharts

Analysis Tools:

- **Optical Spectra:**
  - Display of blackbody radiation as a function of frequency
  - Spectral emissivity
  - Total emissivity as a function of temperature
  - CIE 1931 and 1964 color spaces upon reflection and transmission, now both for spectral power distribution of Standard Illuminant D65 and of fluorescent lamp FL2

MedeA's JobServer & TaskServer & Maintenance:

- Update of maintenance program (efficiency and robustness improvements)
- Ability to install fully from command line