MedeA VOTCA

Forcefields Beyond Atomistic Simulations

At-a-Glance

The *MedeA*®[1] *VOTCA* interface provides access to the Versatile Object-oriented Toolkit for Coarse-graining Applications (VOTCA)[2] from *MedeA*. VOTCA is a coarse-grained modeling package, which focuses, among other things, on the development of systematic coarse-graining techniques. The interface makes it possible to use the coarse-graining toolkit (VOTCA-CSG) to create coarse-grained forcefields from atomistic molecular dynamics simulations by using iterative Boltzmann inversion or force matching.

Key Benefits

- **Derive mesoscale forcefields** from atomistic simulations with precision
- **Develop custom forcefields** tailored to your specific materials and systems
- **Execute large-scale simulations** in *MedeA* LAMMPS across time and length scales beyond atomic-level modeling

Move seamlessly from atomistic to mesoscale simulations

The Versatile Object-Oriented Toolkit for Coarse-Graining Applications (VOTCA) has gained widespread adoption across computational chemistry, molecular simulation, and multiscale modeling communities. This toolkit emphasizes coarse-graining methodologies and property prediction spanning multiple length scales, particularly in soft matter research, organic semiconductor development, and various materials design projects.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] http://www.votca.org/

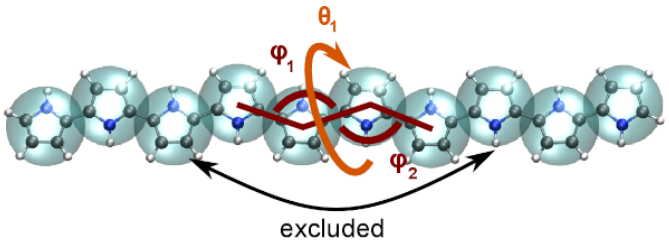

Fig. 1: Interactions in a mesoscale forcefield

Key Features

- Specialized for Coarse-Graining
  - Provides systematic methodologies for deriving coarse-grained models from atomistic simulations
  - Implements multiple coarse-graining algorithms (e. g., Iterative Boltzmann Inversion, Force Matching)
  - Facilitates transferability and accuracy of coarse-grained forcefields
- Multiscale Modeling
  - Bridges atomistic and mesoscopic scales within a unified framework
  - Allows fluid transitions between detailed molecular models and coarse-grained representations
- Integrated Workflows
  - Automates the workflow from atomistic simulations to coarse-grained parameterization and validation
  - Offers comprehensive tools for analyzing structural, thermodynamic and dynamic properties
  - Interfaces seamlessly with *MedeA* LAMMPS
- Community and Documentation
  - Actively developed by an international research community
  - Well-documented with tutorials, examples, and validation cases
  - Extensively cited and established within computational chemistry and soft matter fields
- Performance and Parallelization

  - Optimized for high-performance computing environments
  - Scales efficiently with large systems and long simulations

In short: *VOTCA*'s biggest strengths are its flexibility, extensibility and specialized focus on systematic coarse-graining combined with multiscale modeling. It provides an efficient, validated framework to reduce complexity while preserving essential physics in simulations.

Required Modules

- *MedeA Environment*

Related Modules

- *MedeA Mesoscale Builder*
- *MedeA LAMMPS*

Find Out More

To expand your knowledge of *VOTCA*, consider these foundational papers:

- V. Rühle, C. Junghans, A. Lukyanov, K. Kremer and D. Andrienko: Versatile Object-oriented Toolkit for Coarse-graining Applications, J. Chem. Theor. Comp. **2009**, 5(12), 3211-3223
- V. Rühle and C. Junghans: Hybrid Approaches to Coarse-Graining using the VOTCA Package: Liquid Hexane, Macromolecular Theory and Simulations **2011**, 20(7), 472–477
- S. Y. Mashayak, M. N. Jochum, K. Koschke, N. R. Aluru, V. Rühle and C. Junghans, Relative entropy and optimization-driven coarse-graining methods in VOTCA, Plos One **2015**, 10(7), e131754
- C. Scherer and D. Andrienko, Understanding three-body contributions to coarse-grained force fields, Phys. Chem. Chem. Phys. **2018**, 20(34), 22387–22394

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