MedeA Mesoscale Builder

Going Beyond Atomistic Simulations

At-a-Glance

The *MedeA*®[1] *Mesoscale Builder* creates models for simulations on the time and length scale of microseconds and tens of nanometers. The models created can be used with other *MedeA* tools to build more complex systems, such as polymers or thermosets. Mesoscale bead definitions and parameters are provided for the MARTINI[2] and SPICA[3] forcefields.

Key Benefits

- *Quickly build mesoscale models with beads from the scientific literature*
- *Utilize the MARTINI and SPICA forcefields*
- *Define your own beads*
- *Use mesoscale models with Polymer, Amorphous, and Thermoset builders*
- *Use mesoscale models to run MedeA* LAMMPS *simulations on time and lengths scales which exceed atomistic modeling*

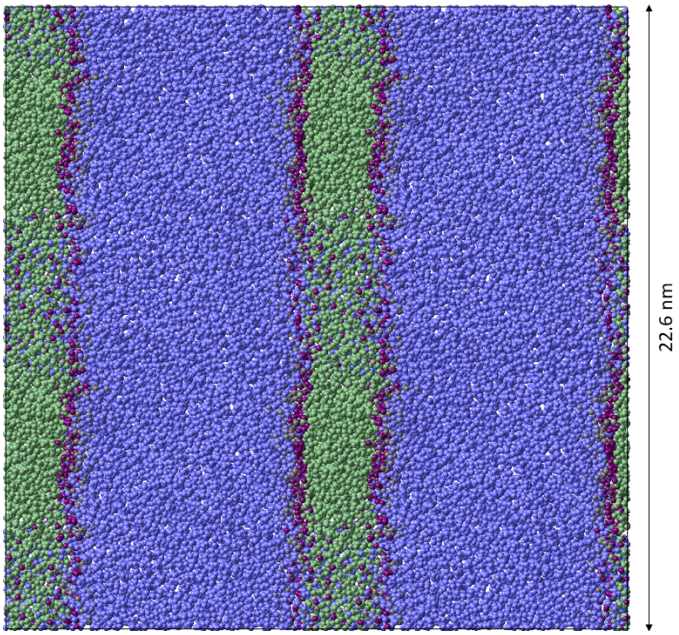

Figure 1: A lipid bilayer has formed in a mesoscale simulation of dipalmitoylphosphatidylcholine molecules (green and purple) in water (blue)

Think Big

The *MedeA Mesoscale Builder* creates mesoscale models using bead definitions from the scientific literature. Use the mesoscale models to build polymers, amorphous systems, or thermosets for modeling on time and lengths scales which are outside the reach of atomistic simulations. Study the phase behavior, mechanical properties, or any other property which can be modeled by forcefields of systems representing millions of atoms.

Mesoscale simulations make it possible to study effects that cannot be observed in atomistic simulations. Self-assembly of molecules, the effect of detergents, explicit solvation, or fluid dynamics become accessible to modeling.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.
[2] http://cgmartini.nl/
[3] https://www.spica-ff.org/

Key Features

- Integrated extensible library with bead definitions and forcefield parameters for
  - MARTINI forcefield[2]
  - SPICA forcefield[3]
- Sketching of mesoscale models using
  - predefined beads, or
  - user-defined beads
- Built systems can be used in mesoscale simulations performed with *MedeA LAMMPS* and gain access to all properties available via *MedeA LAMMPS*

Characteristics & Uses

- Create any desired mesoscale model with the *MedeA Mesoscale Builder*
- Use the models that *MedeA Mesoscale Builder* creates to prepare bulk models for mesoscale simulations of physical properties including:
  - Density and PVT Properties

  - Surface and Interfacial tension
  - Thermal Conductivity
  - Diffusivity

Required Modules

- *MedeA Environment*

Related Modules

- *MedeA Amorphous Materials Builder*
- *MedeA Forcefields*
- *MedeA Diffusion*
- *MedeA Surface Tension*
- *MedeA Thermal Conductivity*
- *MedeA* Mechanical Properties *MT*
- *MedeA Thermoset Builder*
- *MedeA LAMMPS*

Find Out More

To learn more about mesoscale simulations read the following papers:

- S. J. Marrink, A. H. de Vries and A. E. Mark: Coarse Grained Model for Semiquantitative Lipid Simulations, J. Phys. Chem. B **2004**, 108, 750-760
- S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman and A. H. de Vries: The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations, J. Phys. Chem. B **2007**, 111, 7812-7824
- G. Rossi, I. Giannakopoulos, L. Monticelli, N. K. J. Rostedt, S. R. Puisto, C. Lowe, A. C. Taylor, I. Vattulainen and T. Ala-Nissila: A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating, Macromolecules **2011**, 44, 6198-6208
- W. Shinoda, R. DeVane, M. L. Klein: Multi-property fitting and parameterization of a coarse grained model for aqueous surfactants, Molecular Simulation **2007** 33, 27-36
- W. Shinoda, R. DeVane, M. L. Klein: Zwitterionic Lipid Assemblies: Molecular Dynamics Studies of Monolayers, Bilayers, and Vesicles Using a New Coarse Grain Force Field, J. Phys. Chem. B **2010**, 114, 6836-6849
- K. Hall, T. Sirk, M. L. Klein, W. Shinoda: A Coarse-Grain Model for Entangled Polyethylene Melts and Polyethylene Crystallization, J. Chem. Phys. **2019** 150, 244901
- K. W. Hall, T. W. Srik, S. Percec, M. L. Klein, W. Shinoda: Divining the Shape of Nascent Polymer Crystal Nuclei, J. Chem. Phys. **2019** 151, 144901

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