
11th i-CoMSE Workshop: Mesoscale Particle-Based Modeling

**Mississippi State University
July 21–25, 2025**

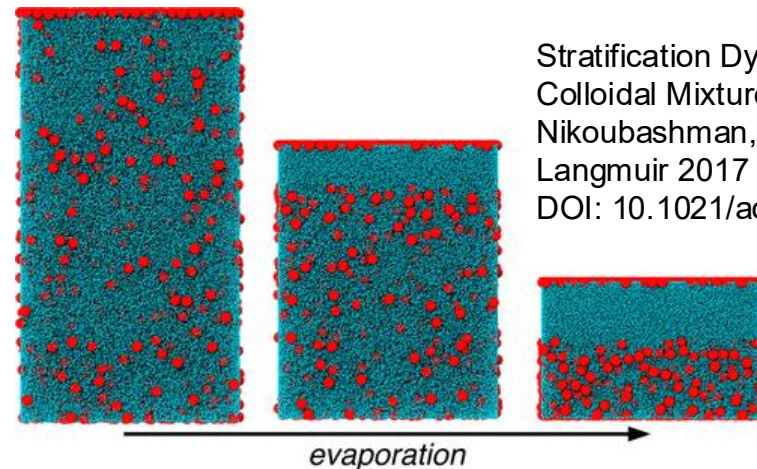
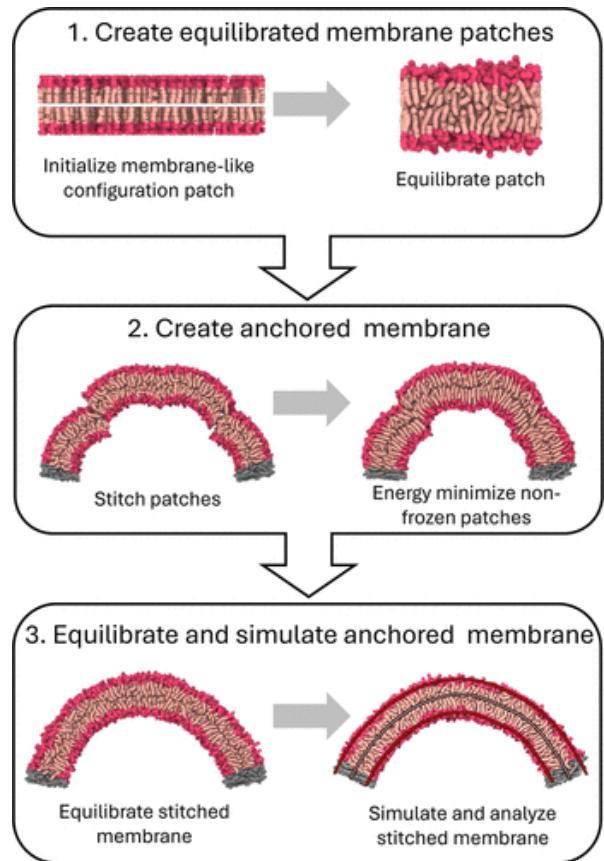
Session 4: Visualization



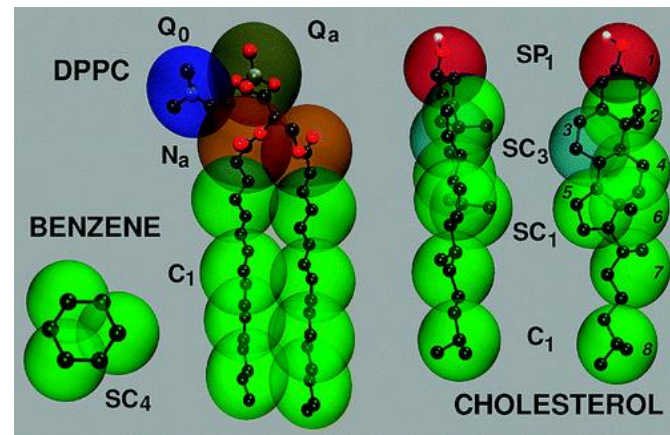
Visualization

- **Why do we need to visualize our simulations?**
 - Does the system behave as expected? (sanity checks):
 - Are all particles in the simulation? Are types, bonds, etc. correctly defined?
 - Do dynamics seem reasonable?
 - Is it phase separating/homogeneous?
 - Illustration for publications/talks/posters
 - Schematics to explain the model components and simulation setup
 - Snapshots to draw attention for table of content figures, covers, etc.

Visualization



Stratification Dynamics in Drying Colloidal Mixtures, M. Howard, A. Nikoubashman, A. Panagiotopoulos
 Langmuir 2017 33 (15), 3685-3693
 DOI: 10.1021/acs.langmuir.7b00543



Simulating Curved Lipid Membranes Using Anchored Frozen Patches, J. Tallman, A. Statt, JPC B 2025 129 (24), 6009-6022 DOI: 10.1021/acs.jpcb.5c02518

The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations, S. Marrink, H. Risselada, S. Yefimov, D. Tieleman, and A. de Vries, JPC B 2007 111 (27), 7812-7824, DOI: 10.1021/jp071097f

Visualization

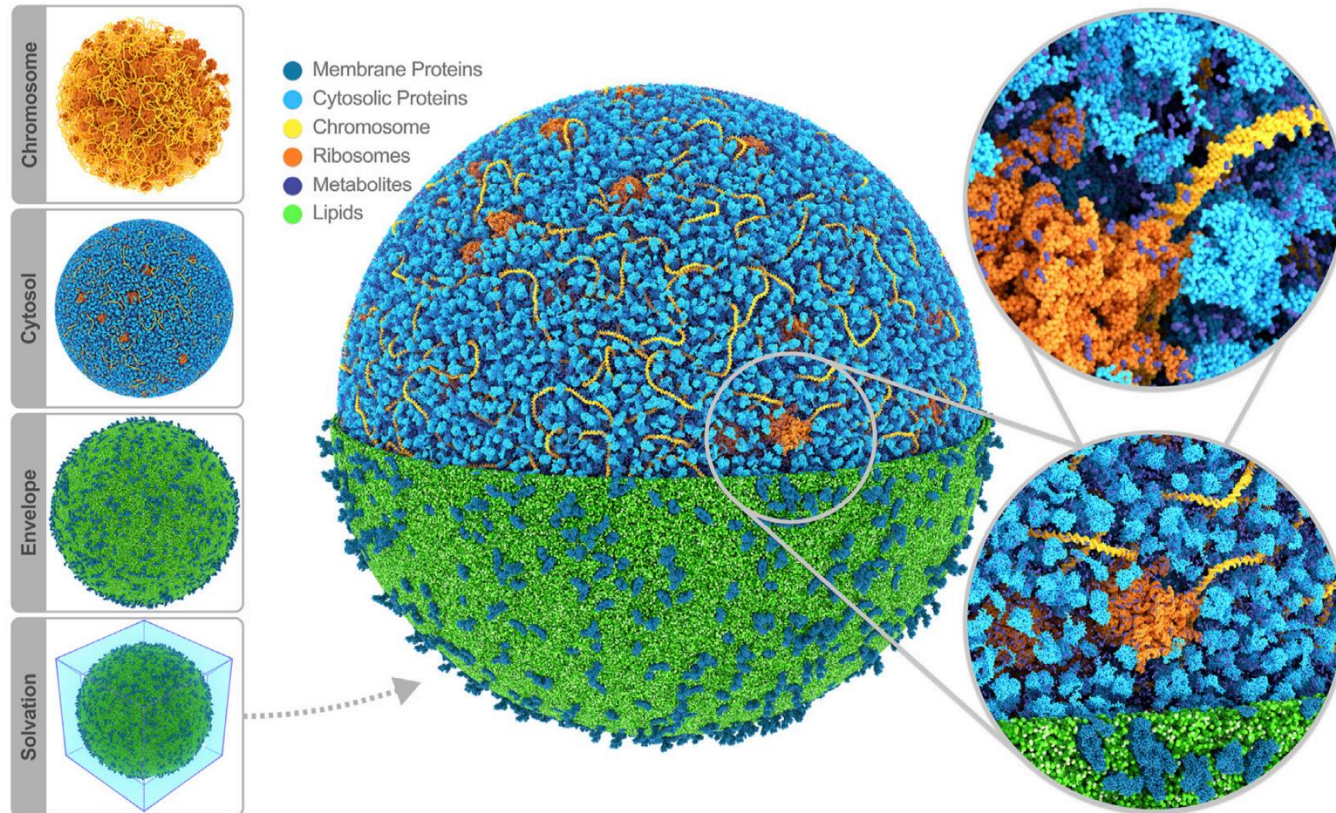


FIGURE 2

Whole-cell Martini model of JCVI-syn3A. The four stages of cell building are shown on the side. The final system contains 60,887 soluble proteins (light blue), 2,200 membrane proteins (blue), 503 ribosomes (orange), a single 500 kbp circular dsDNA (yellow), 1.3 million lipids (green), 1.7 million metabolites (dark blue), 14 million ions (not shown) and 447 million water beads (not shown) for a total of 561 million beads representing more than six billion atoms. Image rendered with Blender ([Blender Online Community, 2022](#)).

Visualization

The Journal of Chemical Physics



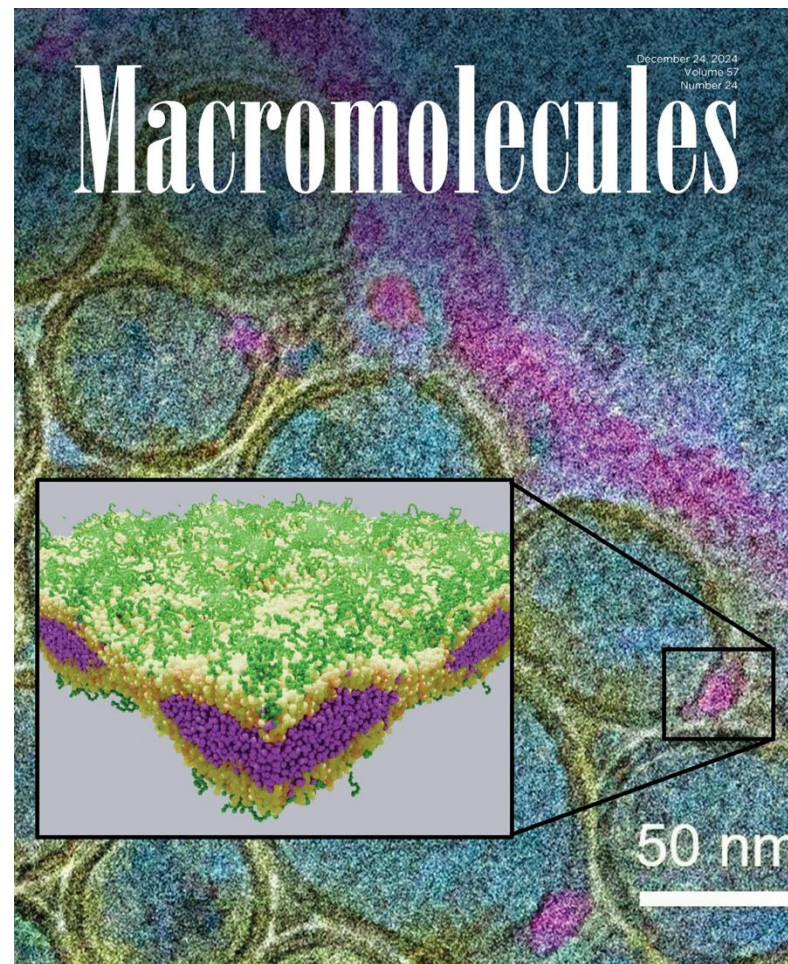
Vol. 160, Iss. 24, 28 Jun. 2024

**Molecular dynamics simulations of anisotropic
particles accelerated by neural-net
predicted interactions**

B. Ruşen Argun, Yu Fu, and Antonia Statt



Available Online: pubs.aip.org/aip/jcp



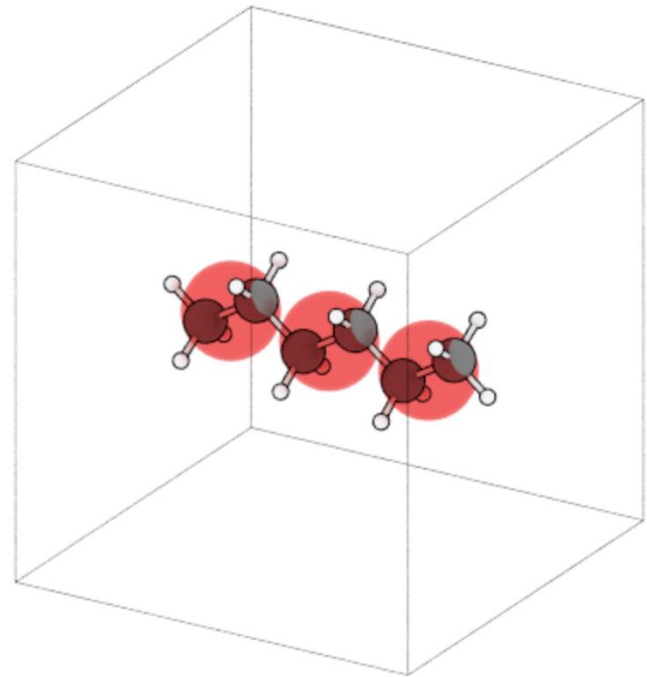
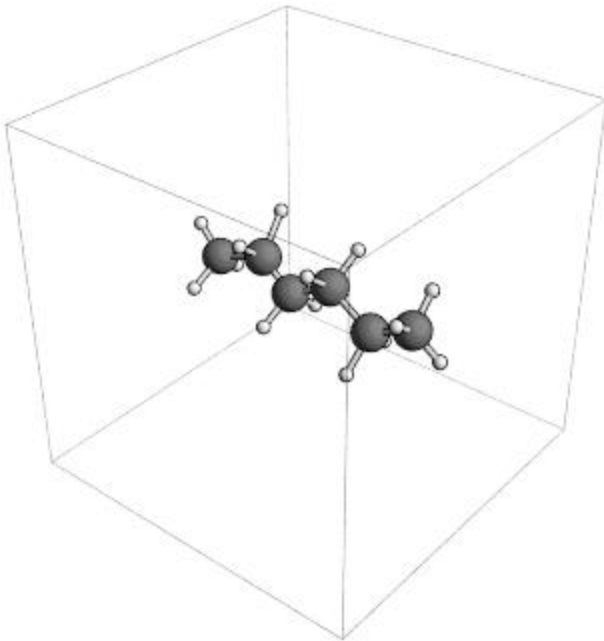
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Ovito + Gimp

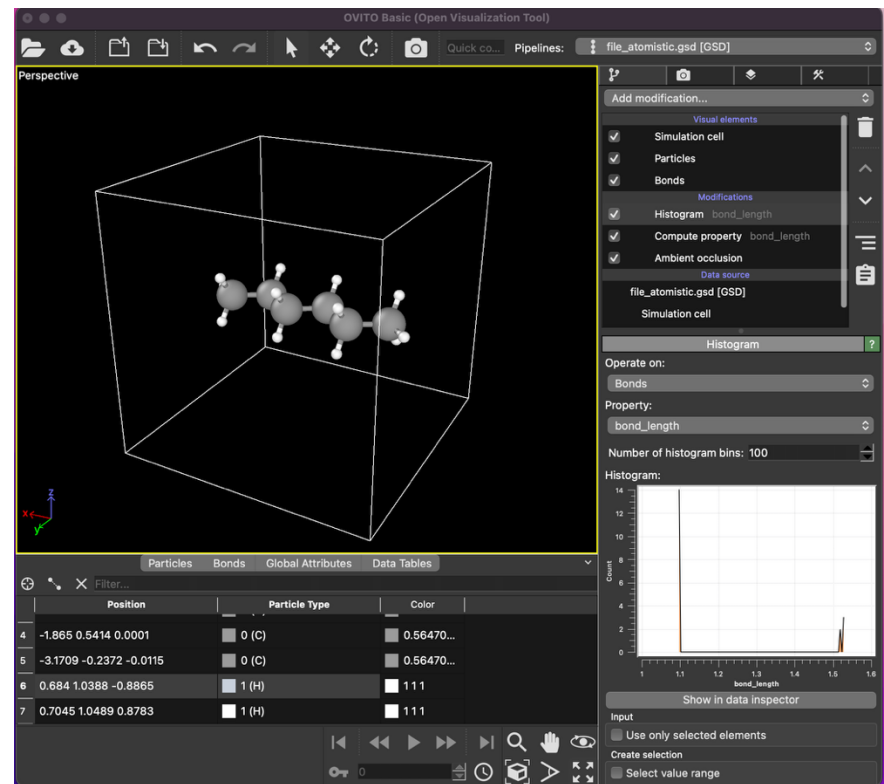
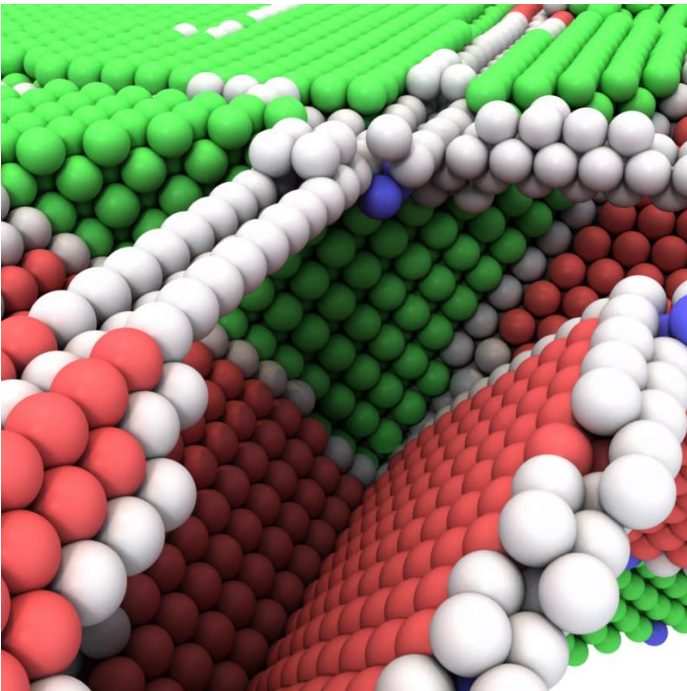
Exercise

- **Objectives:**
 - Use fresnel to render simple snapshots and movies
 - “Coarse grain” simple molecule and visualize the result



Alternatives

- **OVITO** <https://www.ovito.org>
 - Runs on macOS, Linux, Windows
 - Has Python interface to write scripts for rendering/movies
 - Quasi-open source (paid pro version)



Alternatives

- **VMD** <https://www.ks.uiuc.edu/Research/vmd/>
 - Runs on mac, Linux, windows
 - Must install GSD plugin <https://github.com/mphowardlab/gsd-vmd>
 - Open source

