Computing renewable solutions through molecular modeling

The Vermaas lab uses atomic simulation tools to create accurate molecular-scale models for biological phenomena at the nanoscale. In this form of computational microscopy, Newton’s equations of motion track atomic positions for a system over time. The dynamic simulations provide a unique perspective to better understand the connection between form and function for nanostructures found throughout biology. The insights from these simulations can then applied to engineering plants or microbes to facilitate efficient energy conversion and bioproduct production to meet today’s sustainability challenges.

photosyntheticreactioncenterandcofactors.png

*The photosynthetic reaction center of Rhodobacter sphaeroides is an example where multiple research focuses intersect. The complex is composed of 3 protein subunits and is membrane embedded. We want to apply new computational approaches to understand and improve the photosynthetic processes.*

There are three primary research areas for the group, understanding biological membranes and membrane proteins, studying nanostructures and assemblies within photosynthetic organisms, and advancing computational methods to incorporate emerging techniques.

Bpsimagecontest.jpg

*Lipid bilayers are semipermeable to small molecules, such as the guaiacol molecules shown here. To emphasize the biological context, EM images of the bacteria have been overlaid onto the model rendering.*

Lipid bilayers are the fundamental biological structure that partitions cellular structures, creating gradients across the lipid leaflets that drive cellular metabolism and transport processes. We are interested in determining the transport mechanism for small molecules, and determining barriers to transport at the atomic scale. With the transport mechanism in hand, we can work with experimental groups to modulate transport barriers through protein mutation or lipid modification to influence cellular metabolism.

Coarsedemo.png

*Coarse grained cell wall model, with green beads representing cellulose fibrils, blue beads representing hemicellulose strands, and orange beads for the lignin.*

Nature has created many nanostructures to fulfill specific cellular functions. The cell walls of terrestrial plants provide structure and defense to plant tissues through a network of complex carbohydrates such as cellulose, hemicellulose, and pectins and polyaromatic lignin molecules. Understanding the resulting complex structure at the nanoscale provides insight into deconstruction and materials engineering pathways to use these renewable materials at industrial scales.

carboxysomesurface.png

*One of the nanostructures we study is the carboxysome, which is composed of a protein shell around critical metabolic enzymes to trap intermediate molecules and increase catalytic efficiency.*

Similarly, computational models of the complex nanostructures nature uses to organize metabolism offers unique insight into the design constraints evolution needs to respect. As an example, bacterial microcompartments accelerate metabolic processes by trapping substrates and increasing the concentration of intermediate products. Through simulation, we can track individual molecules and quantify the impact of this confinement.

lignindeconstruction3.gif (this is the same as test.mp4, but gifified.

*Using machine-learned atomic potentials, we can track deconstruction events in biomolecules, such as the lignin polymer here.*

As a longer term strategic goal, we want to develop solutions to adapt and evolve our current computational models to the changing computational landscape. With the increased computing power offered by GPUs, we foresee a future where classical forcefields are replaced by potential energy surfaces based on machine learning. These machine-learned force fields would be able to combine the long simulation timescales offered by classical methods with the accurate chemistry and reactivity of quantum methods. Students with an interest in applying computation to study biological processes in photosynthetic organisms are encouraged to contact Josh directly to discuss current projects in the group.