Contribution ID: **4** Type: **not specified**

The Minimal Cell under a Computational Microscope

Thursday 26 September 2024 09:45 (45 minutes)

Molecular dynamics (MD) is a well-established simulation method that has successfully been applied to study a wide range of biomolecular processes. As a result of continuous improvements in both modeling methods and computational infrastructures, the study of mesoscopic, multi-component systems has become more attainable. However, the intricacies involved in setting up MD simulations for these systems remain daunting, requiring the integration of diverse data from both experimental and in silico sources.
Here we present how the coarse-grained Martini force field and its associated tools, form an ideal ecosystem for facilitating a integrative modeling pipeline. Employing a CG resolution, typically representing four heavy atoms by one CG bead, significantly reduces the computational cost inherent in simulating large-scale MD models. Furthermore, a key feature of the force field is its universality, which allows us to create CG models of all major biological components and construct complete cellular environments.
The Martini force field's capabilities are showcased in an ongoing effort to simulate a genetically minimal cell: JCVI-syn3A. We constructed the first near-atomistic MD model of a cell based on data from kinetic models, Cryo-Electron Tomograms, and omics experiments. Studying entire cells under the computational microscope will allow us to look into a wide range of problems, ranging from drug design to understanding the internal organization of cellular environments.

Presenter: STEVENS, Jan (University of Groningen)

Session Classification: Multiscale Models in Cell Biology II (Chair: Sebastian Thallmair)