RUTGERS UNIVERSITY

CASS Brown Bag Seminar

Friday, March 8, 2024, 11:30 am to 12:30 pm
Location: Room 330W Physics and Astronomy Building
(Busch Campus) Map
Boxed lunches will be available.

Meenakshi Dutt
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"Pipelines for Automating Compliance-based Elimination and Extension (PACE2): A Systematic Framework for High-throughput Biomolecular Material Simulation Workflows"

Abstract: The formation of biomolecular materials via dynamical interfacial processes such as self-assembly and fusion, for diverse compositions and external conditions, can be efficiently probed using ensemble Molecular Dynamics (MD). However, this approach requires a large number of simulations when investigating a large composition phase space. In addition, there is difficulty in predicting whether each simulation is yielding biomolecular materials with the desired properties or outcomes and how long each simulation will run for. These difficulties can be overcome by rules-based management systems which include intermittent inspection, variable sampling, premature termination and extension of the individual MD simulations. The automation of such a management system can significantly improve runtime efficiency and reduce the burden of organizing large ensembles of MD simulations. To this end, a computational framework – the Pipelines for Automating Compliance-based Elimination and Extension (PACE2), for high-throughput ensemble biomolecular materials simulations is proposed. The PACE2 framework encompasses Candidate pipelines, where each pipeline includes temporally separated simulation and analysis tasks. When a MD simulation completes, an analysis task is triggered which evaluates the MD trajectory for compliance. Compliant simulations are extended to the next MD phase with a suitable sample rate to allow additional, detailed analysis. Non-compliant simulations are eliminated, and their computational resources are either reallocated or released. The framework is designed to run on local desktop computers and high performance computing resources. Preliminary scientific results enabled by the use of PACE2 framework, which demonstrate its potential as well as serve to validate PACE2, is presented. In the future, the framework will be extended to address generalized workflows and investigate composition-structure-property relations for other classes of materials.

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