Abstract Submitted
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Ultra-coarse-grained (UCG) models for biomolecular simulations[1] JOHN GRIME, GREGORY VOTH, The University of Chicago — Computational molecular dynamics (MD) is a well-established complement to traditional experimental techniques and can provide information at very high spatial and temporal resolutions. Traditional MD has typically used atomic-level molecular representations, but the use of "coarse-grained" models (which require fewer degrees of freedom) can provide access to significantly larger time and length scales. The use of coarse-grained models at very large scales can introduce unique challenges that require novel theoretical approaches and software algorithms to overcome. In this talk, recent successes in the application of "ultra-coarse-grained" (UCG) models will also be described in the context of a medically relevant viral system: self-assembly of the capsid protein of type 1 Human Immunodeficiency Virus (HIV-1).

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