ID de Contribution: **22** Type: **Non spécifié**

Arbitrarily accurate, nonparametric coarse graining with Markov renewal processes and the Mori-Zwanzig formulation

Stochastic dynamics, such as molecular dynamics, are important in many scientific applications. Summarizing and analyzing the results of such simulations is often challenging, due to the high dimension in which simulations are carried out (and consequently to the very large amount of data that is typically generated). Coarse graining is a popular technique for addressing this problem by providing compact and expressive representations, but it usually comes at a cost of reduced accuracy. We discuss how to eliminate coarse-graining error using two key ideas by using a Markov renewal process representation of dynamics, parametrized with a data-driven Mori-Zwanzig approach.

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Classification de Session: Result Communication