Contribution ID: **25** Type: **Talk**

Error estimates in molecular dynamics

Thursday 29 August 2024 13:00 (1 hour)

I will provide a brief introduction to molecular dynamics (the computational implementation of the theory of statistical physics) and relate it to Bayesian inference, as these are two situations where sampling a high dimensional probability measure is required. Average properties for these two applications are typically obtained through ergodic averages of discretizations of certain stochastic differential equations. I will provide an introduction to the most popular stochastic dynamics to this end and their numerical analysis – in particular error estimates on the timestep discretization bias, and estimates on the statistical error.

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