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Predicting the atomic kinetics of materials with uncertainty

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I will discuss two methods to coarse-grain and predict atomic kinetics generated by molecular dynamics, with application to diffusion and plasticity in metals. When the energy landscape is metastable, atomic kinetics can be mapped to a discrete Markov chain with robust Bayesian bounds on unseen transitions. These bounds are used to allocate resources in massively parallel computation and measure the convergence of coarse-grained properties such as transport coefficients.
However, in many important cases kinetics are driven and show no clear signature of metastabilty. I show how many-body basis functions used in atomic machine learning form a medium dimensional, metric latent space ideal for coarse-graining and analysis. A vector autoregressive model can resample and forecast latent space trajectories using a Mahalanobis distance to qualify forecast uncertainty. Finally, the descriptor manifold is analyzed in the context of the yielding transition.

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Classification de Session: Challenge and Perspective