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The predictive integration method for dynamics of infrequent events EKIN CUBUK, AMOS WATERLAND, EFTHIMIOS KAXIRAS, Harvard University — With the increasing prominence and availability of multi-processor computers, recasting problems in a form amenable to parallel solution is becoming a critical step in effective scientific computation. We present a method for parallelizing molecular dynamics simulations in time scale, by using predictive integration. Our method is closely related to Voter's parallel replica method, but goes beyond that approach in that it involves speculatively initializing processors in more than one basin. Our predictive integration method requires predicting possible future configurations while it does not suffer from restrictions due to correlation time after transitions between basins.

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