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Discrete Event-based Performance Prediction for Temperature Accelerated Dynamics CHRISTOPH JUNGHANS, SUSAN MNISZEWSKI, ARTHUR VOTER, DANNY PEREZ, STEPHAN EIDENBENZ, Los Alamos National Laboratory — We present an example of a new class of tools that we call *application simulators*, parameterized fast-running proxies of large-scale scientific applications using parallel discrete event simulation (PDES). We demonstrate our approach with a TADSim *application simulator* that models the Temperature Accelerated Dynamics (TAD) method, which is an algorithmically complex member of the Accelerated Molecular Dynamics (AMD) family. The essence of the TAD application is captured without the computational expense and resource usage of the full code. We use TADSim to quickly characterize the runtime performance and algorithmic behavior for the otherwise long-running simulation code. We further extend TADSim to model algorithm extensions to standard TAD, such as speculative spawning of the compute-bound stages of the algorithm, and predict performance improvements without having to implement such a method. Focused parameter scans have allowed us to study algorithm parameter choices over far more scenarios than would be possible with the actual simulation. This has led to interesting performance–related insights into the TAD algorithm behavior and suggested extensions to the TAD method.

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