Toward Event-Driven Reformulations of Particle Interactions for Neuromorphic Computing

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Particle-based simulations, such as molecular dynamics simulations, are central to science and have countless real-life applications in fields such as pharmacology, material science, and biotechnology. The development of specialized hardware [Shaw et al., 2021] demonstrates their relevance. However, these simulations rely on computational patterns that are not well aligned with emerging neuromorphic and event-driven hardware. Although neuromorphic computing has been extensively studied in the context of neuroscience and machine learning, its potential for broader scientific applications has only recently begun to be explored [Schuman et al., 2022; Diaz-Pier et al., 2024]. Recent work has examined the use of spiking neural networks for molecular dynamics via learning-based approaches [Pham et al., 2024] rather than reformulating the underlying interaction dynamics. Bridging this gap requires rethinking how core simulation primitives are expressed computationally.

Molecular dynamics simulations compute interactions via explicit geometric relations between particles, which typically requires distance evaluation and coordinated pairwise computations. These operations introduce non-local dependencies and arithmetic complexity that are not naturally compatible with neuromorphic systems, which operate through local, event-driven interactions. Thus, the question arises as to whether particle interactions can be reformulated so that distance-dependent forces emerge from local interaction rules rather than from explicit distance calculations.

In this study, we examine a reformulation of short-range particle interactions that uses lookup-table approximations of inter-particle forces. Using a simple Lennard–Jones fluid as a reference, we analyze how these approximations affect force evaluation and long-horizon simulation behavior, in particular with respect to energy conservation. Next, we examine alternative ways of expressing distance-dependent interactions through local or distributed formulations. These approaches are being investigated further.

Our results provide initial insight into which components of particle-based simulations may be reformulated and highlight open questions about the appropriate representation of interactions in molecular dynamics simulations running on neuromorphic hardware.

Schuman et al., Nat. Comput. Sci., 2(1), 10–19, 2022.
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Shaw et al., Proc. SC21, 1–11, 2021.
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