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Asynchronous Event-Driven Particle Algorithms in Computational Materials Science.

I will present, in a unifying way, the main components of asynchronous event-driven (AED) algorithms for simulating physical systems of interacting particles [arXiv:cs/0703096]. Event-driven algorithms are not as widely used as time-driven algorithms even though they offer substantial efficiency improvements for a variety of algorithms. I will briefly sketch two examples where AED algorithms have proven to be vastly superior to more traditional alternatives: the well-known hard-particle Molecular Dynamics, as well as a recently-developed diffusion Kinetic Monte Carlo algorithm.

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