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Fast Kinetic Monte Carlo Methods for Novel Solar Cell Design

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Kinetic Monte Carlo (KMC) methods [1] are widely used to simulate the surface adsorption, diffusion, growth, statistical physics, radiation damage annealing, bioglogical systems, amongst other applications by evolving systems dynamically from state to state. In our application to solar cells, KMC are required to predict device behaviour from the material properties at the microscopic scale. Our work has mainly focussed on atomistic studies of the microscopic processes, such as charge and exciton hopping, recombination rates and light absorption. Using the parameters obtained from the atomistic simulations, we focus on KMC simulations at the mesoscale, computing current-voltage characteristics, charge mobilities and parameters for calculating recombination that subsequently feed into faster device design offered by continuum models where current-voltage characteristics are obtained.

The KMC method is equivalent to the Gillespie algorithm [2] which simulates the trajectories consistent with the "exact"dynamical evolution of a system. The advantage of KMC method is the probability that we see a given sequence of states and transition times is the same as the probability for seeing that same trajectory in the molecular dynamics which is much more expensive since one propagates equations of motion forward in time. However, the computational cost is still very high in many practical applications such as solar cell design, bioglogical systems.

In order to accelerate atomistic simulations, we apply the idea of multilevel Monte Carlo (MLMC) methods [3] to reduce the computational time significantly but still retain the accuracy based on controlling statistical errors. The first results we have obtained with r-leaping and tau-leaping show the efficiency when skipping expensive computations such as the update of the electrostatic potential (the most expensive) and propensity functions in such a way that the statistical errors are still acceptable (less than 10%).
In particular for solar cell designs, this development will be coupled with fast and massively parallel Poisson solvers for the modelling of long-range interactions.

[1] U. Neupane, B. Bahrami, M. Biesecker, and Baroughi M.F. Kinetic monte carlo modeling on organic solar cells: Domain size, donor-acceptor ratio and thickness. Nano Energy, 81:128–137, 2017.

[2] D.T. Gillespi. Exact stochastic simulation of coupled chemical reactions. Journal of Physical Chemistry, 81(25), 1977.

[3] C. Lester, R.E. Baker, M.B. Giles, and Yates C.A. Extending the multi-level method for the simulation of stochastic biological systems. Bull Math Biol, 2016

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