# The mathematics and algorithmics of long-time atomistic simulations

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Atomic-scale simulations of materials using molecular dynamics (MD) are a cornerstone of computational materials science. These simulations can provide powerful insights into the mechanisms by which materials evolve and respond to external stimuli such as stress or temperature, which are often very difficult to obtain experimentally. The spatio-temporal reach of MD has considerably expanded since its introduction in the 1950's, thanks to the exponential increase in available computing power. However, that growth has been strongly skewed: while sizes have been steadily increasing, timescales have dramatically lagged behind, due to the inherently serial nature of the integration of stochastic differential equations.

In order to address this limitation, our group has been developing so-called Accelerated MD methods, which aim at extending simulation timescales for systems that exhibit metastable dynamics. I will introduce one such method, the Parallel Trajectory Splicing approach, which enables parallelization in the time domain in a way that is ideally suited to massively-parallel computers. I will discuss the mathematical underpinnings of the method, which build on the concept of quasi-stationary distributions, and show that it can provide arbitrary accurate dynamics on extremely long times when deployed at large computational scales. I will finally show how the mathematical framework can also inform the development of accurate discrete-states models of the dynamics.