Electrostatics: Numerical algorithms and biological applications
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Fast Electrostatic Calculation in Molecular Simulation

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Molecular dynamics is a well-established technique for simulating complex systems in physics, chemistry, biology and materials science. However, fundamental hurdles remain in order for molecular dynamics to reach either spatial or temporal scale of most realistic systems. The biggest challenge is the lack of efficient and scalable algorithms for treating long-range interactions, i.e. Coulomb interactions, which mostly relies on fast convolution methods. In this talk, I will discuss some recent progress and challenges toward fast convolution algorithms with their application to molecular dynamics on emerging heterogeneous platforms.