A GPU Implementation of Coulomb Interaction in Molecular Dynamics

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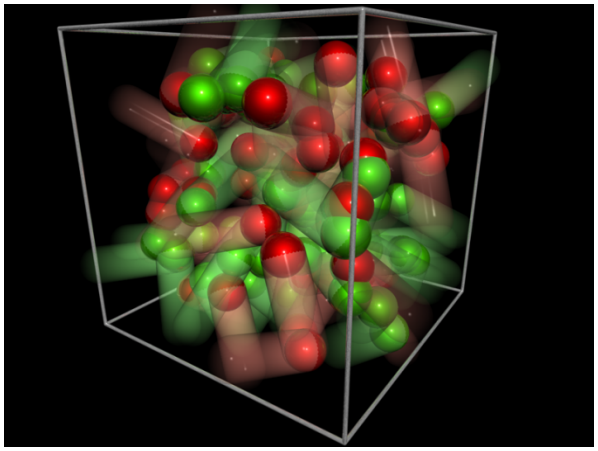
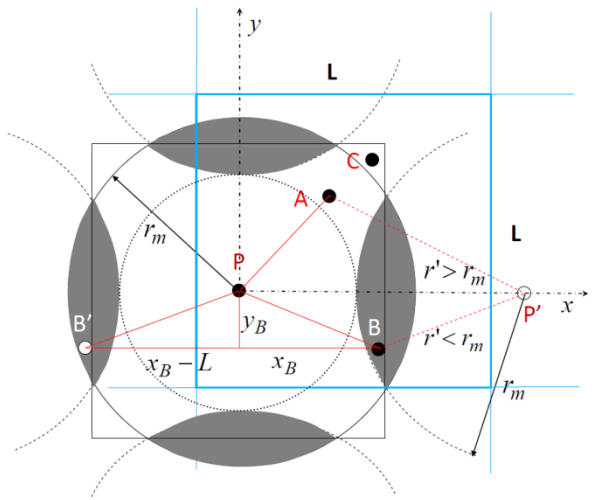
Ever increasing market demand for fast and realistic graphics has driven a rapid development of inexpensive GPU devices, with a doubling of computational power every 12 months. In recent years, the GPU hardware has become available to non-graphical applications through the advent of general-purpose programmability of the device. A notable example is molecular dynamics (MD) with reports of GPU implementations achieving speed-ups in excess of 100 times compared to standard MD codes.

We report a GPU implementation of long-range electrostatic interactions. Our implementation is significantly faster than the CPU implementation of the standard Ewald method for small to a sizable number of charged particles (~10^5) in electrolyte solutions.





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Journal of Chemical Theory and Computation **2010** *6* (10), 3058-3065