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Vectorization of molecular-dynamics simulations with short-ranged forces

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Molecular-dynamics simulations is a particle-based simulation method that is widely used in computational physics and materials science. The strong increase of available computational power makes it possible to perform materials simulations with many millions of atoms. In order to harness the full power of modern CPUs, it is necessary to make use of the available SIMD instruction sets (e.g. SSE or AVX). Unfortunately, molecular-dynamics simulations with short-ranged forces are not very well suited to take advantage of these vector capabilities. The reason for this is that each particle interacts only with a subset of the total system and the interaction partners are not stored consecutively. In this presentation we present a blocking algorithms that attempts to overcome this problem. The results of our benchmark calculations show that substantial speedups of 2 and above can be obtained for architectures like SSE, AVX and MIC.

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