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Accelerating Molecular Dynamics Simulation on the Many Integrated Core (MIC) Platform HONGSUK YI, HOGYUN JEONG, SEUNGMIN LEE, KISTI — Graphics processing units and Intel Many Integrated Core (MIC) architectures have emerged as alternative computational strategy in computational physics that can significantly speed up high performance computing algorithms. In this paper, we present early experiences on the MIC platform, focusing on porting of molecular dynamics (MD) kernels with the Tersoff potentials for carbon covalent crystals. In particular, we implement our MD code on heterogeneous computing platform consisting of Intel Xeon processors and Intel MIC architecture coprocessors, using offload and OpenMP. The fully optimized MIC version achieves about 8 times speedup over the original CPU version. Furthermore, explicit vectorization on the MIC with 512-bit wide vector registers is found to be critical to achieving good performance of this algorithm in this type environments.

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