Seventeenth International Conference Zaragoza-Pau on Mathematics and its Applications
Jaca, September 4–6th 2024

Fast neighborhood iterators for particle and particle-mesh codes on parallel computers

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SUMMARY

Fast neighborhood iteration is essential for scalable and efficient numerical simulations. OpenFPM is an open-source C++ framework that provides infrastructure for shared-memory and distributed-memory implementations of particles-only and hybrid particle-mesh simulations of both discrete and continuous models. The transparently parallelized data structures of OpenFPM are complemented by numerical routines required for efficient execution of particle and particle-mesh codes, as well as interfaces to state-of-the-art third-party numerical libraries. We present a general overview of the architecture and design of OpenFPM with a focus on the underlying abstractions for fast neighborhood iterators optimized for the use on central processing units (CPUs) and graphics processing units (GPUs). We show benchmark results in several applications that particularly benefit from fast neighbour lists, including Smoothed Particle Hydrodynamics (SPH) and Molecular Dynamics (MD).

Keywords: high-performance computing; particle methods; fast neighbor lists; cell list; Verlet list; GPU

AMS Classification: 76M28, 65M70

References

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