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Reconfigurable Molecular Dynamics Simulator

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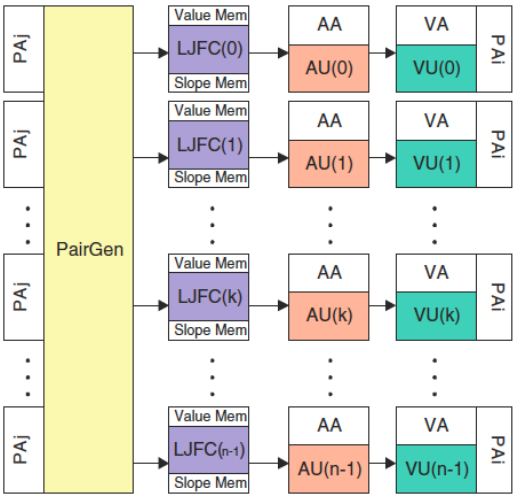

Molecular dynamics (MD) involves the computer simulation of Newtonian mechanics as applied to a system of atoms or molecules. Since its discovery in 1957, it has become one of the most widely used tools for studying molecular behaviour and, due to its large computational requirements, one of the most demanding problems for supercomputers. MD simulations have practical applications in materials design, thermodynamics, protein folding/unfolding and drug discovery. This paper was the first of many using MD to demonstrate the feasibility of applying FPGA-based field-programmable custom computing machines to large-scale problems.

Several techniques were employed to maximise performance: spatial parallelism, pipelining, input/output optimisation, and precision optimisation. Spatial parallelism was applied so that operations without dependencies are processed in parallel computational units. Pipelining allowed the system to execute stages in parallel, resulting in higher clock rates. Memory accesses were carefully optimised to ensure that the maximum available bandwidth was utilised, and the data were kept on the acceleration hardware to minimise host to accelerator communications. Previous application-specific integrated circuit implementations of MD simulations used floating-point arithmetic. This was avoided here since its implementation is both resource hungry and slow. Instead, computations were done in fixed-point arithmetic and a careful precision analysis was made to ensure accuracy.

The ultimate bottleneck in the described Transmogrifier 3 implementation was memory bandwidth. Performance could be further increased with an improved memory system and the paper also detailed how this could be achieved.

The employed techniques can be applied to many applications beyond molecular dynamics and this work represents a good example of a state-of-the-art reconfigurable computing application in 2004.

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