Implementation of an Effective Non-Bonded Interactions Kernel for Biomolecular Simulations on the Cell Processor

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In biomolecular simulations intensive computations are spent in non-bonded interactions kernels, i.e., electrostatic interactions. Therefore this part can be considered as a bottleneck, and its optimization permits biomolecular simulation methods to deal with more complex systems or to simulate longer time scales. Using novel computational architectures, i.e., the Cell processor, and programming it adequately in parallel, can considerably improve the performance of biomolecular simulation methods. Programming the Cell processor is difficult, but we show a strategy, using the metacompiler Cellsuperscalar. We obtain sustained speedups of around 150 times.