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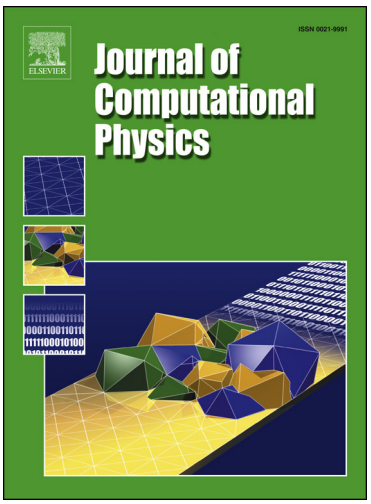

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A Fast Band–Krylov Eigensolver for Macromolecular Functional Motion Simulation on Multicore Architectures and Graphics Processors

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Abstract

We introduce a new iterative Krylov subspace-based eigensolver for the simulation of macromolecular motions on desktop multithreaded platforms equipped with multicore processors and, possibly, a graphics accelerator (GPU). The method consists of two stages, with the original problem first reduced into a simpler band-structured form by means of a high-performance compute-intensive procedure. This is followed by a memory-intensive but low-cost Krylov iteration, which is off-loaded to be computed on the GPU by means of an efficient data-parallel kernel.

The experimental results reveal the performance of the new eigensolver. Concretely, when applied to the simulation of macromolecules with a few thousands degrees of freedom and the number of eigenpairs to be computed is small to moderate, the new solver outperforms other methods implemented as part of high-performance numerical linear algebra packages for multithreaded architectures.

Keywords: Computational biology, macromolecular machines, eigenvalue problems, Krylov subspace methods, multicore processors, graphics processors