Mathematical Models and Computer Simulations 2010 vol.2 N1, pages 46-54

Gramm-software package for molecular dynamics on graphical processing units

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Abstract

© 2010, Pleiades Publishing, Ltd. This work describes the software package and algorithms for molecular dynamics using NVIDEA GPU G80, G84, and G92. All potentials needed for MM2 and AMBER force fields are implemented and the combination of different potentials is allowed. The performance comparison of different MD algorithms on GPU and CPU is presented. All software is available from www.gpamm.mntech.ru.

http://dx.doi.org/10.1134/S2070048210010059