

OpenCL Implementation of the Analytical Method for the Computation of the Accessible Surface Area and Excluded Volume of Overlapping Spheres

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The aim of the paper is to present an OpenCL (Open Computing Language) implementation of the analytical method for the computation of the accessible surface area and excluded volume of a system of overlapping spheres, which can be used in macromolecular modelling. The algorithm of this method, based on the stereographic projection of spheres has been published formerly. This implementation allows to run the same program on all devices supporting OpenCL standard (both CPU and GPU). We will present an idea of modifications needed to the original algorithm in order to utilize the parallelization possibilities of OpenCL and show comparison of performance of original implementation of analytical method (written in FORTRAN) with OpenCL implementation running on different platforms (AMD Opteron, NVIDIA GeForce GTX285, NVIDIA Tesla C1060). We will show that computing the accessible surface area and excluded volume on GPU is efficient.