

Efficient Implementation of Constant pH Molecular Dynamics on Modern Graphics Processors

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Content

Table SI-1. Computer specifications used to benchmark the new GPU-enabled CPHMD algorithm.

part	description	notes
main processor	2 x Intel Xeon E5-2620	2.0GHz, 6 cores each, 12 cores total
GPU	GeForce GTX 780 Ti	875 MHz, 2880 cores, 3.1 GB memory
motherboard	ATX Server Motherboard Dual LGA 2011	DDR3 1600 MHz
power supply	CORSAIR AX1200i	1200W
RAM	8 x 4GB Ripjaws Z Series DDR3	240-Pin, 1600 MHz, 32GB total
hard drive	Crucial M500 480GB SATA	480GB of storage
heatsink	2 x Supermicro SNK-P0050AP4	

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