Parallelization and Improvements of the Generalized Born Model with a Simple sWitching Function for Modern Graphics Processers: Supporting Information

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Content

Enclosed are supporting figures and one table for the Parallelization and Improvements of the Generalized Born Model with a Simple sWitching Function for Modern Graphics Processers manuscript. Several cutoffs in the algorithmic implementation of GBSW on graphics processing units were required to achieve a high degree of efficiency in the calculation, and we explain those here.

Figure SI1. Different lookup table sizes were explored by setting a maximum limit to the number of resident atoms per voxel. The effects were measured as a change in forces and energies of each atom: A) magnitude of energy, B) magnitude of force, and C) angle of force. We see that setting a maximum limit of 25 atoms per voxel had barely any effect on the GBSW forcefield.

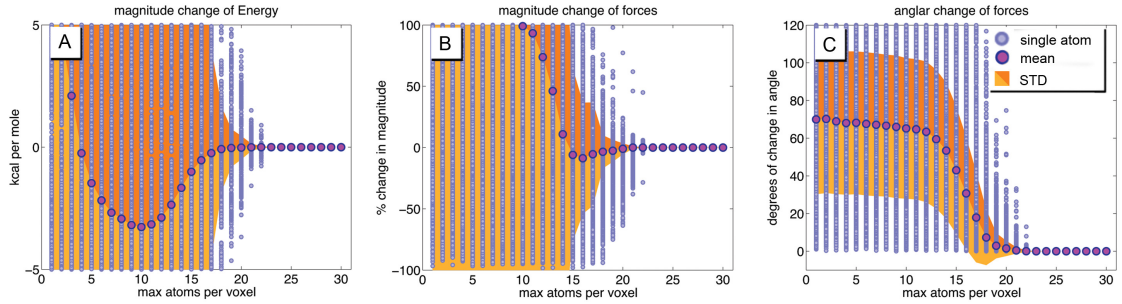

Figure SI2. The volume exclusion function V_{solute} for the quadrature points was pre-integrated to determine which points were most influential at producing the forces and energies for each atom of the 4,107-atom system. For quadrature points near atomic centers we tested for $V_{solute}(r)=1$, and for points far from atom center we tested for $V_{solute}(r)=0$. Deviations in forces and energies indicate that quadrature points at a particular radius are important to the GBSW forcefield. We found that for non-hydrogen heavy atoms (A-C) integrating beyond the 14th Gaussian-Legendre radius or closer than the 7th radius had little effect on the forces and energies. Since hydrogen atoms have a smaller atomic radius, more radii closer to the atomic centers were needed (D-F).

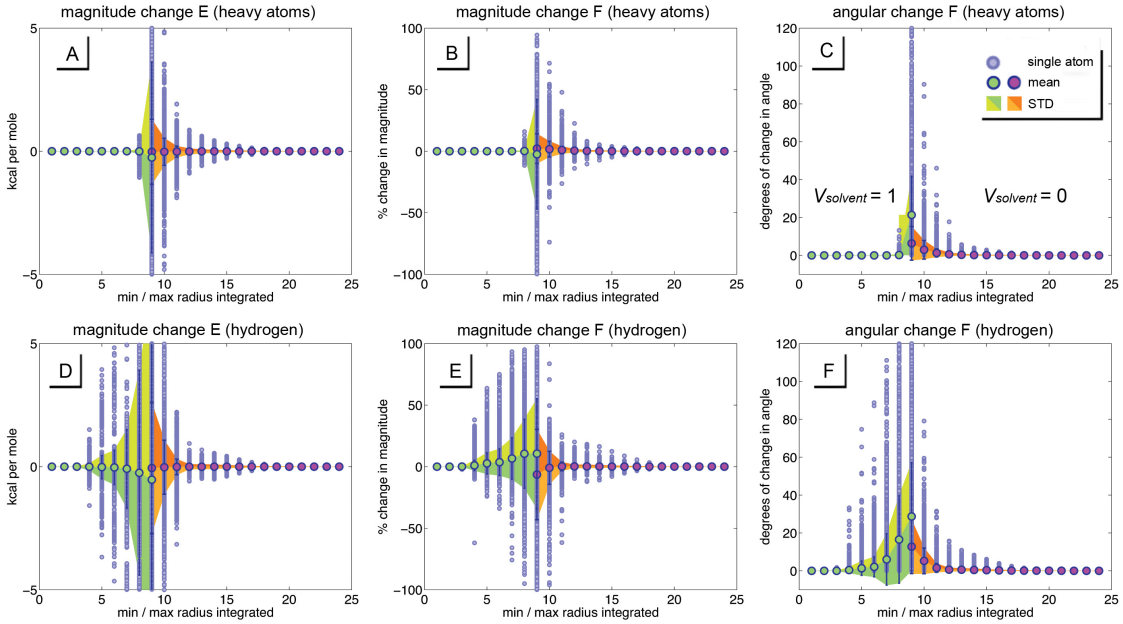

Figure SI3. The final exploratory measure for imposing array sizes and limits is trying to quantify the number of quadrature points needed per atom in order to calculate the gradient of the Born radius with respect to atom position $\partial R^{Born} / \partial \mathbf{r}$: The distribution of gradient quadrature points for each atom shown in C), and the effect on force angles A) and magnitudes B) by setting a maximum number of points per atom. 256 was found to be a reasonable maximum.

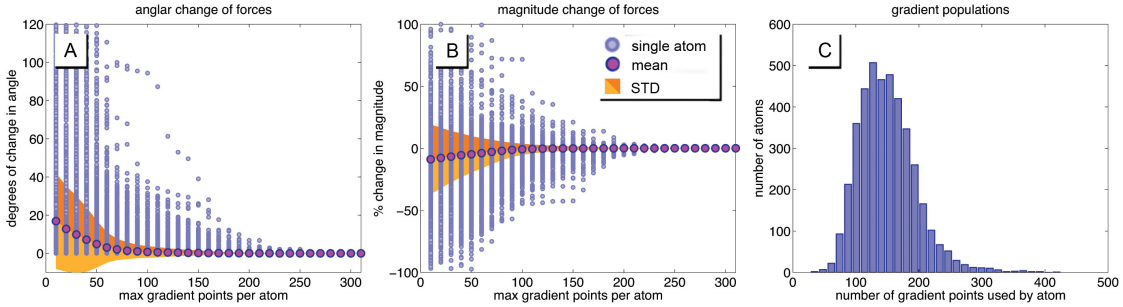

Table SI1. This is the computer parts list used for benchmarking and testing the CUDA-GBSW algorithm.

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	