

Supporting information for: Routine microsecond molecular dynamics simulations with AMBER on GPUs. 2. Explicit Solvent Particle Mesh Ewald

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The following contains a description of the supplementary material used in the development of this paper, provided for download in the accompanying zip file. We also show additional plots of energy conservation during constant energy MD simulations obtained with the CPU implementation and GPU implementation of the AMBER molecular dynamics (MD) package.

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1 Performance measurement input files

AMBER input files used for the performance tests of the PMEMD GPU implementation (DHFR, factor IX and cellulose) are contained in the subdirectory “Performance Measurement Inputs”. For each simulation this includes the AMBER MD input file “mdin”, the parameter and topology file “prmtop” and the starting coordinate file “inpcrd”.

2 Validation: Single point forces input files

AMBER input files used for the tests of the precision of the single point forces of the PMEMD GPU implementation (DHFR, factor IX, cellulose and the Satellite Tobacco Mosaic virus (STMV)) are contained in the subdirectory “Validation Single Point Forces Inputs”. For each simulation this includes the AMBER MD input file “mdin”, the parameter and topology file “prmtop” and the starting coordinate file “inpcrd”.

3 Validation: Energy conservation input files

AMBER input files used for the energy conservation tests of the PMEMD GPU implementation (DHFR, factor IX and cellulose) are contained in the subdirectory “Validation Energy Conservation Inputs” under subdirectories for each system. For each simulation this includes the AMBER MD input files “mdin”, the parameter and topology file “prmtop” and the starting coordinate file “restrt”. We are including “mdin” files for all time steps (0.5 fs and 1.0 fs without constraints and 2.0 fs using SHAKE constraints for bonds to hydrogen atoms). The “prmtop” files for time steps 0.5 fs and 1.0 fs use “spc-fw” as a water model, while 2.0 fs time step uses “tip3p”. In all cases, first an equilibration was performed followed by removal of the center of mass motion before running the constant energy validation simulations (NVE).

4 Validation: Energy conservation plots

Plots showing the total energy for the trajectories of DHFR, factor IX and cellulose for the different precision models and time steps $dt = 1.0$ fs and $dt = 2.0$ fs, are shown in Figure 1 and Figure 2.

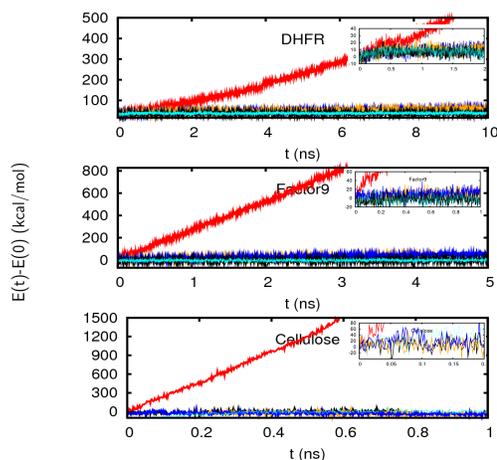


Figure 1: Total energy (kcal/mol) along constant energy trajectories using a time step of 1.0 fs without constraints. Shown are results for DHFR (top), Factor IX (center) and cellulose (bottom) for different precision models. Red SPSP, dark blue SPFP, orange SPDP, black DPDP and light blue CPU.

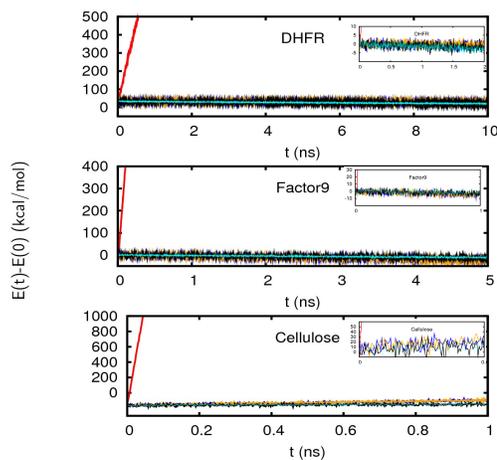


Figure 2: Total energy (kcal/mol) along constant energy trajectories using a time step of 2.0 fs with SHAKE. Shown are results for DHFR (top), Factor IX (center) and cellulose (bottom) for different precision models. Red SPSP, dark blue SPFP, orange SPDP, black DPDP and light blue CPU.

5 Validation: Structural Properties input files

AMBER input files used for the analysis of structural properties of ubiquitin are contained in the subdirectory “Validation Structural Properties Inputs/ubiquitin”. This includes the AMBER MD input file “mdin”, the parameter and topology file “1UBQ-TIP3P.prmtop”, and 60 restart files “restrt.removeCOM” in subdirectories “p1” to “p60” inside the directory “60structs”. These starting files were obtained by extracting the coordinates from three long trajectories, 200 ns each. These coordinate extractions were followed by assignment of random velocities and short heating. The “mdin.prod_NVT-ntt1” file is for NVT simulations with a time step of 2.0 fs using SHAKE constraints for bonds to hydrogen atoms at 300 K using the Berendsen thermostat with a time constant $\tau_T = 10\text{ps}$ for the heat bath coupling.