1 LAMMPS (1Feb14): SHAKE vs. RATTLE

The SHAKE algorithm for Verlet integration [2] only guarantees that the constraints on the coordinates are satisfied at time $t + \Delta t$,

$$r_{ij}^2(t + \Delta t) \stackrel{!}{=} d_{ij}^2, \tag{1}$$

where $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ and d_{ij} is the distance to be imposed between the sites i and j. However, with velocity Verlet the velocities are integrated explicitly and the SHAKE algorithm requires modification [1]. This additional velocity correction in the RATTLE algorithm is such that the time derivative of (1) is satisfied as well:

$$\phi_{ij}^{n+1} := 2\mathbf{r}_{ij}(t + \Delta t) \cdot \mathbf{v}_{ij}(t + \Delta t) \stackrel{!}{=} 0. \tag{2}$$

With other words, there should be no velocity component along the bonds. In order to test, whether the current SHAKE implementation satisfies (2), I ran short simulations (1000 timesteps) of 108 water molecules and monitored

$$\phi := \max_{n,i,j} |\phi_{ij}^{n+1}|, \tag{3}$$

which is the largest absolut deviation from condition (2). Of course the maximum over i, j in (3) is restricted to pairs (i, j) with fixed bonds. Both ϕ and ϕ_r were monitored in a modified fix (FixHeat::end_of_step(), but the original code was commented out and the heat flux set to zero). The SHAKE constraints, (1), were perfectly satisfied up to a tolerance of $\approx 10^{-12}$ throughout the run. The results are shown in Fig. 1 and one can clearly see that the maximum error ϕ scales as $\mathcal{O}(\Delta t^2)$. This is exactly what one would expect, since the Lagrange parameters λ_{ij} are of $\mathcal{O}(\Delta t)$ [1].

References

[1] HC Andersen. RATTLE: A Velocity version of the SHAKE algorithm for molecular dynamics calculations. *Journal of Computational Physics*, pages 24–34, 1983.

[2] JP Ryckaert, G Ciccotti, and HJC Berendsen. Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes. *Journal of Computational Physics*, 341, 1977.

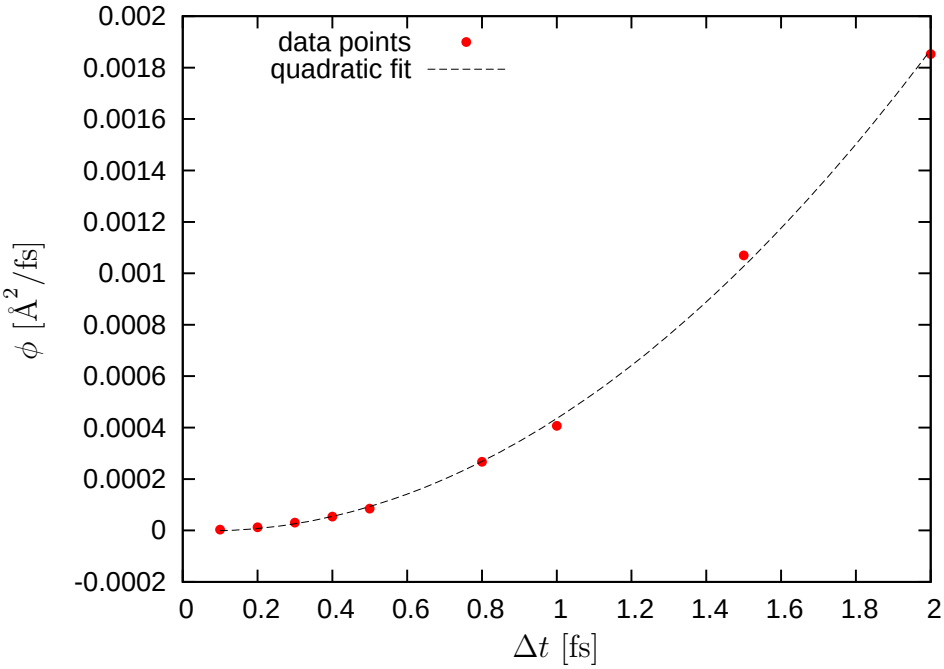

Figure 1: Each value of ϕ (red dots) was calculated at a different timestep Δt. Each run was 1000 timesteps long and the temperature was approximately 298 K. All runs started from the same, previously equilibrated binary restart file. The SHAKE contraints, (1), were satisfied with an absolute tolerance of less than 10^{-12} throughout the simulation.