Step 3: Lennard-Jones experiments

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January 18, 2019

The following plot is for the minimum distance against time with parameters 100 1e4 5e-9 0 0 0 0 0 39.948 0 0 0 1e-12 0 0 39.948. Different time steps were tested: $10^{-1}, 10^{-2}, 10^{-3}, ..., 10^{-6}$. For the distance, explicit Euler was used for their computation truncated after the first order derivative (the velocity is the first derivative of the distance) resulting in error of $O(h^2)$. Actual Distance expression:

$$x(t+\delta t) = x(t) + \delta t v(t) + \delta t^2 a(t)/2 + ...$$

Expression used:

$$x(t+\delta t) = x(t) + \delta t v(t)$$

Resulting error will be the accumulation of the higher order derivatives, in other words $O(h^2)$. The convergence order is of order 1, $O(h)$. The following plots and table below confirms this result. As the time step is divided by 10, the error is reduced by a factor of 10 as well.

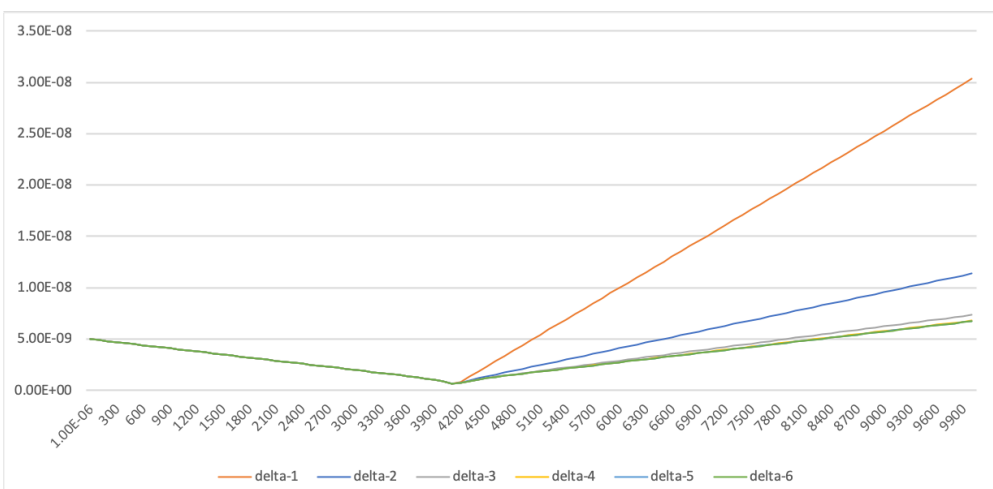


Figure 1: Minimum distance until t=1e4

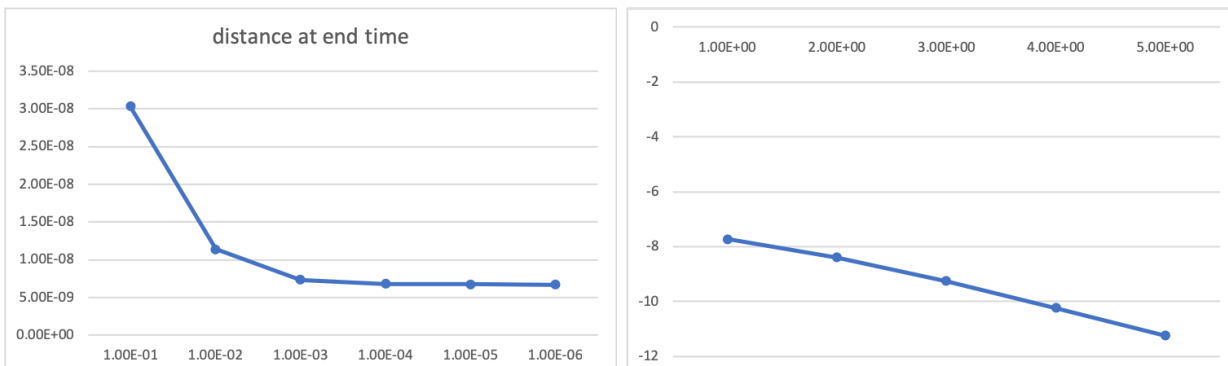
As the exact solution is not known an iterative approach was taken to compute the convergence, table-1. To approximate C_i, the following expression was used:

$$|y^{i+1} - y^i| \leq C_i |y^i - y^{i-1}|^p$$

Minimum Distance	δt	error ($\lvert y^{i+1} - y^i \rvert$)	approximate C_i
3.03E-08	1e-1	1.9e-8	
1.14E-08	1e-2	4.04e-9	2.13E-01
7.34E-09	1e-3	5.45e-10	1.35E-01
6.79E-09	1e-4	5.72e-11	1.05E-01
6.73E-09	1e-5	5.75e-12	1.00E-01
6.73E-09	1e-6		

Table 1: Results at t=1e4 with Lennard-Jones to compute the force for p=1

Below are the plots for table-1:



(a) Minimum distance at t=1$e4$ (b) Error for each δt (both axis were taken at log_{10})

Figure 2: convergence order for distance evaluation

It is evident from plot-2b that C is indeed 0.1 and is constant when p=1, so the convergence order is 1.