

THE BUILDING BLOCKS OF CALCULUS

Classical derivative has additive deviations in function values due to additive changes in function arguments. May not always be interested in additive changes [1,2].

The geometric derivative f^* considers multiplicative changes in function values.

The bigeometric derivative f^π additionally scales the argument.

Linear approximations are inherent in classical calculus. Generalised calculi may be better suited:

1. Generalised tangents as seen in geometric and bigeometric Runge-Kutta schemes [3]
2. Geometric integral naturally arises when considering capacitor discharge over a time-dependent resistance

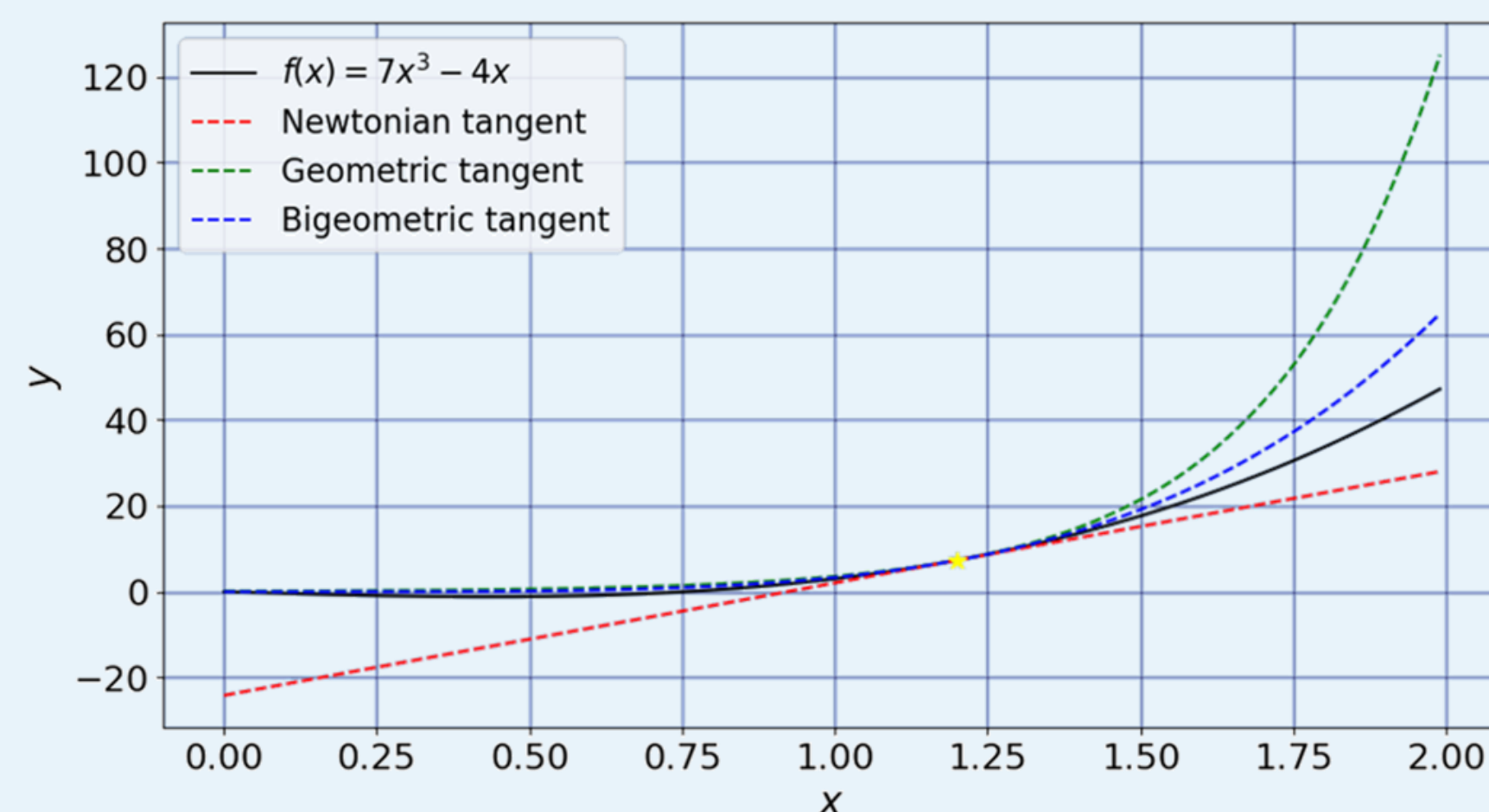


Figure 1: Newtonian, geometric and bigeometric tangents at $x = 1.2$.

AIMS AND OBJECTIVES

1. Construct and implement general Verlet integrators
2. Analyse the effectiveness of these integrators
3. Explore other areas where non-Newtonian calculi naturally arise

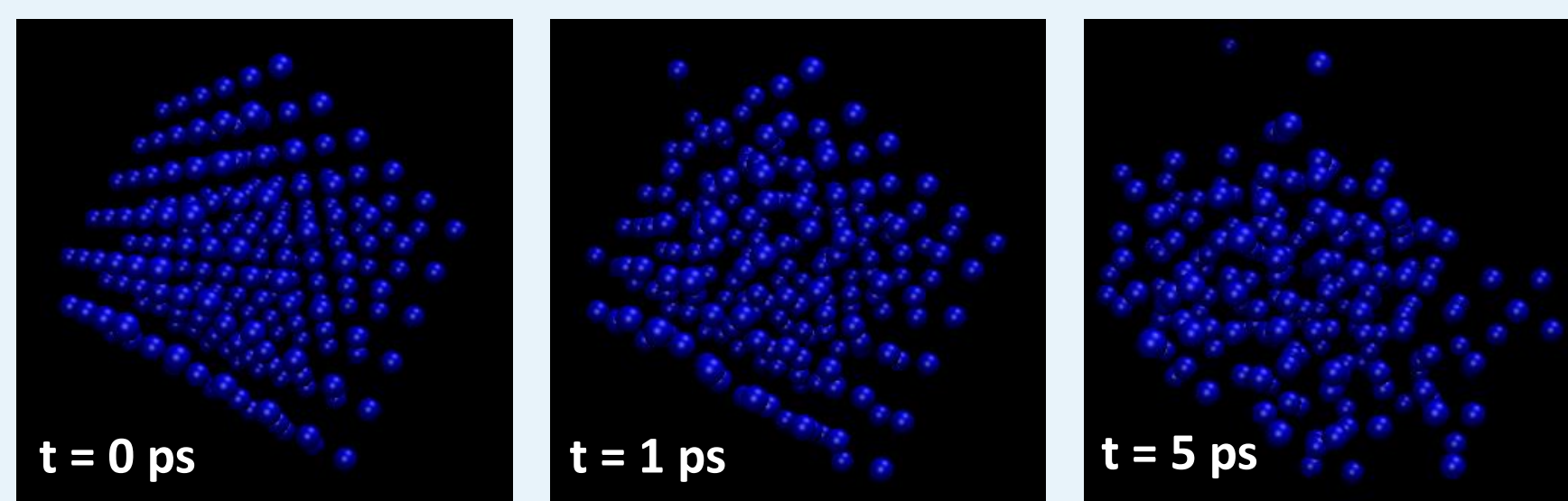


Figure 2: Visualisation simulating 25 argon atoms using molecular visualisation program VMD.

IMPLEMENTATION IN MOLECULAR DYNAMICS

We considered Newtonian, geometric and bigeometric Verlet integrators.

Accurate trajectories are beneficial, but energy conservation is a more important feature for a molecular dynamics (MD) integrator.

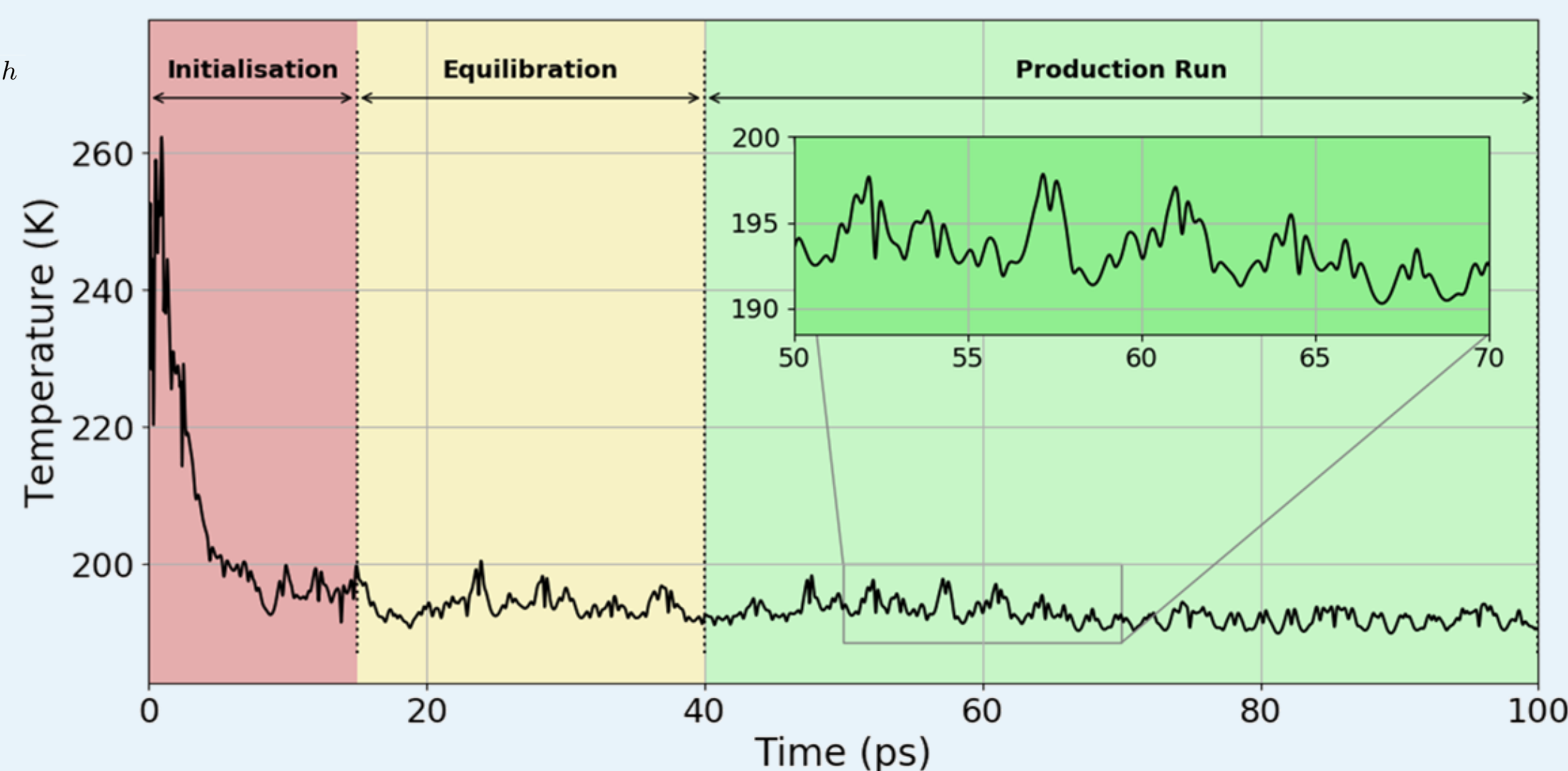


Figure 3: The three stages of an MD simulation.

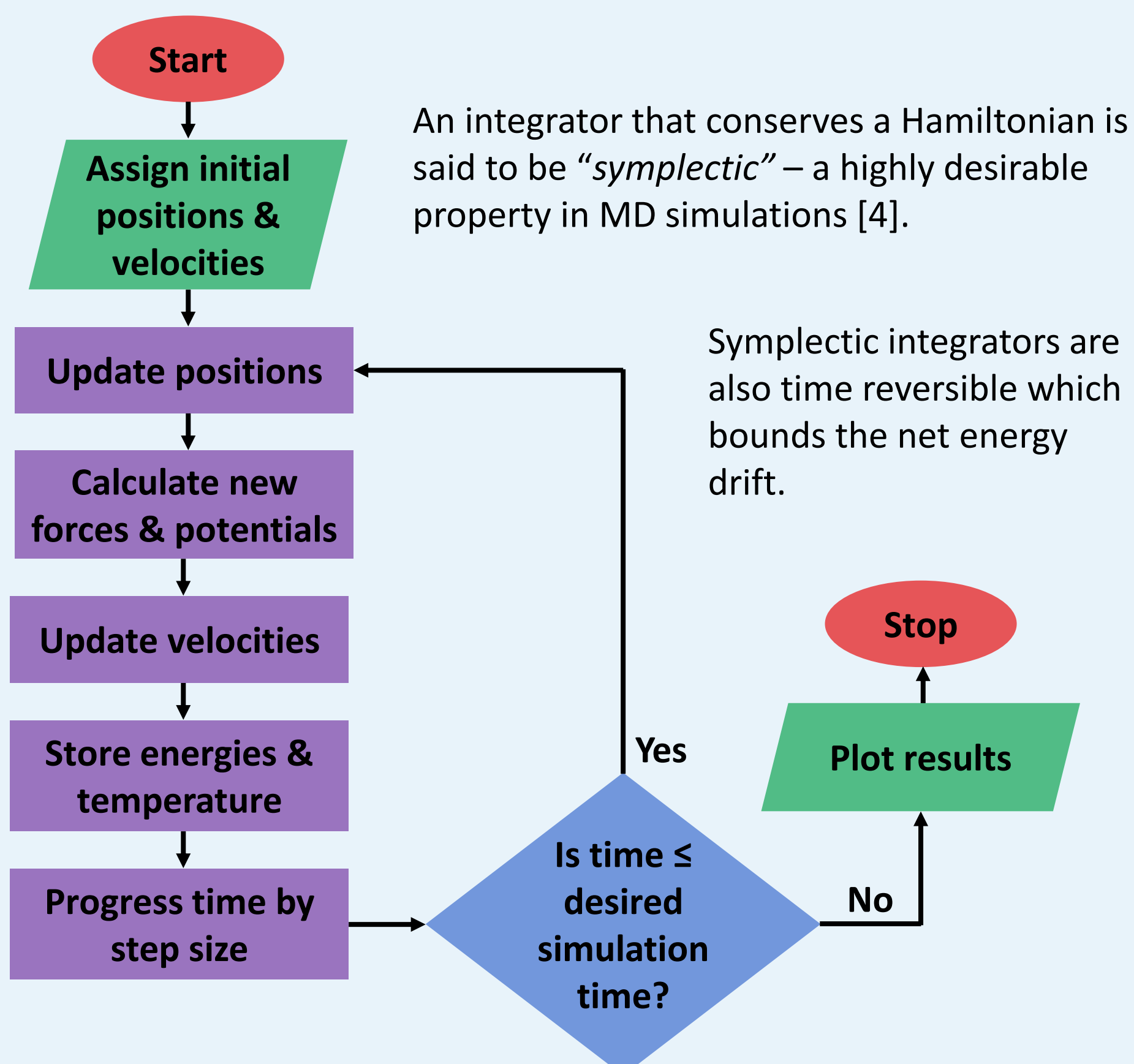


Figure 4: Flowchart of Verlet integrator scheme

RESULTS

For the geometric and bigeometric integrators, energy conservation becomes worse for small timesteps, possibly due to terms like $1/dt$.

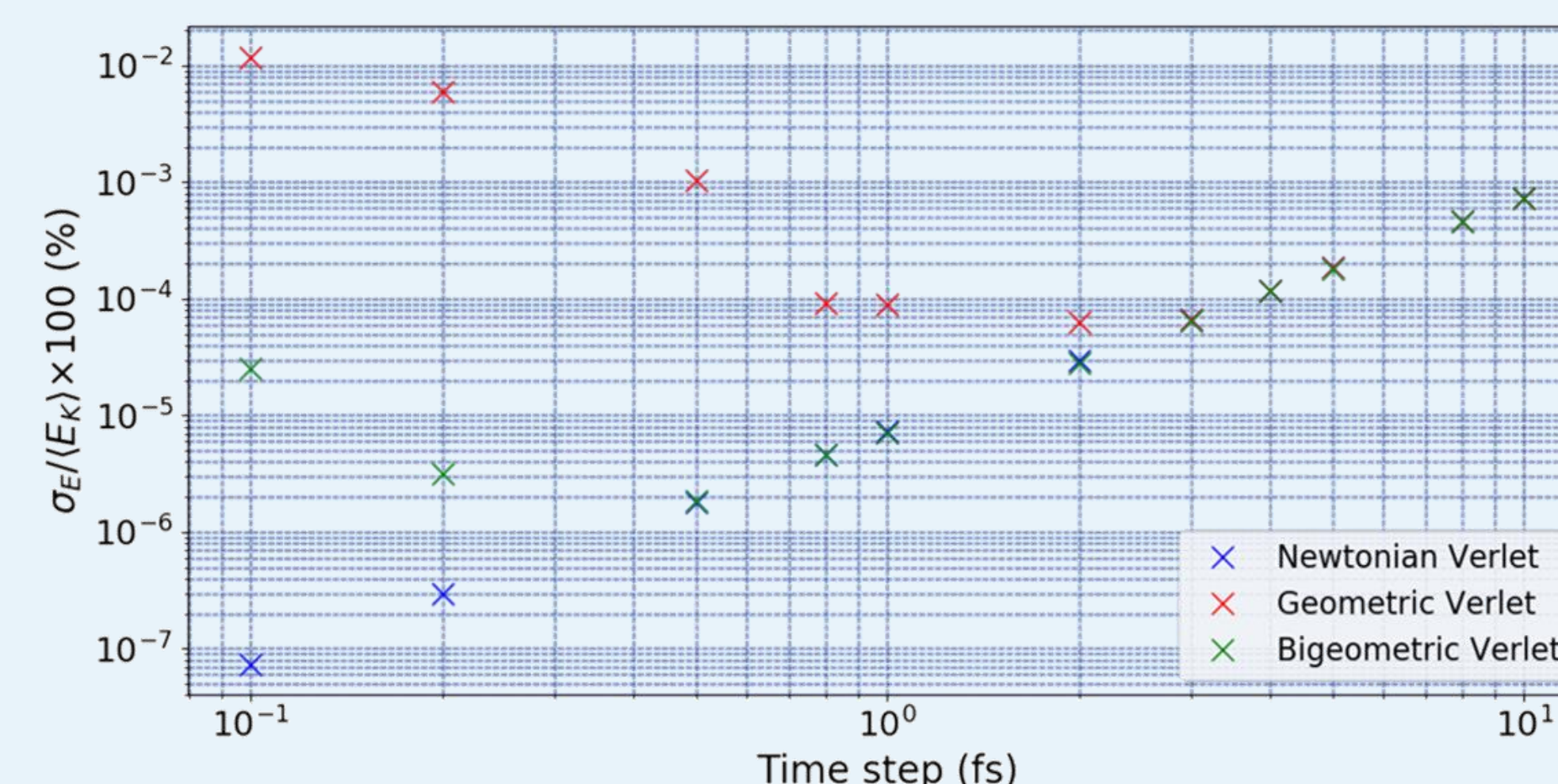


Figure 5: How standard deviation in energy as a percentage of mean kinetic energy varies with timestep.

Systematic drift in the bigeometric Verlet causes its energy to increase overtime.

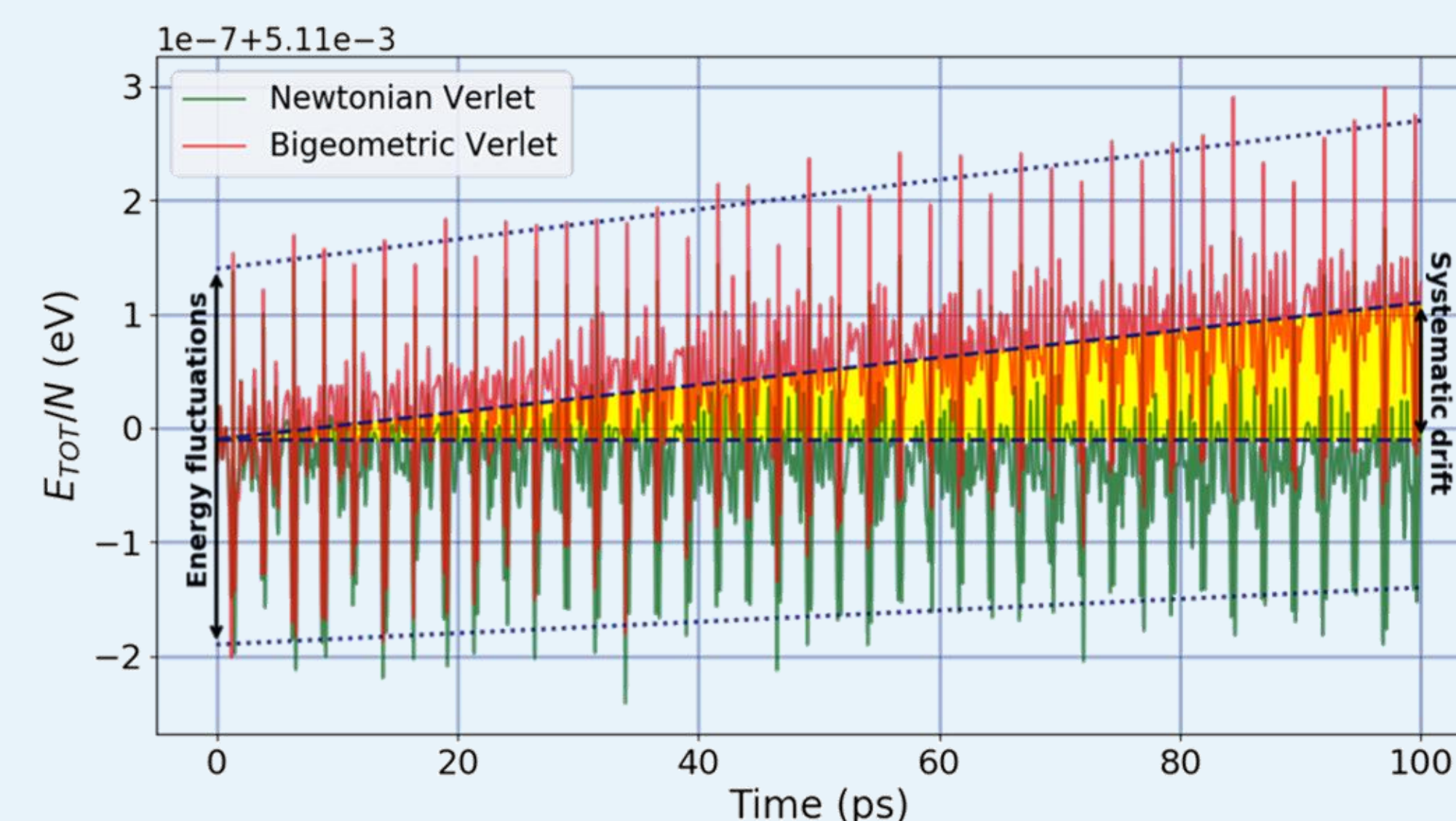


Figure 6: Total energy per particle plotted for a system of 25 argon atoms. Energy fluctuations and drift are both apparent.

CONCLUSIONS

The geometric and bigeometric Verlet algorithm have inherent flaws:

1. Origin dependence in terms like $1/r$
2. Square roots restricting the usage of each algorithm
3. Energy drift which accumulates over time