Non-Newtonian Calculus for Molecular Dynamics

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Goals

In a molecular dynamics (MD) simulation there are 2 parts:

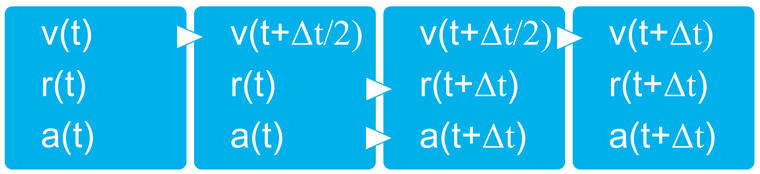
- A method for calculating the force on each particle
- An integrator which progresses the system in time

To increase the amount of data generated one must either optimize the force calculation or improve the integrator. We choose to focus on optimizing the integrator as there is more physics involved in choosing an efficient integrator (one which allows for a large timestep).

Velocity-Verlet

Traditionally, the velocity-Verlet has been used in MD simulations. It is defined as:

$$r(t+\Delta t) = r(t) + v(t)\Delta t + a(t)\Delta t^2/2$$
$$v(t+\Delta t) = v(t) + (a(t) + a(t+\Delta t))\Delta t/2$$



As you can see in the diagram, the linear velocity-Verlet involves updating velocity by a half timestep, position by a full timestep, and then velocity by another half timestep. The velocity-Verlet is perhaps the most common integrator due to a number of beneficial properties:

- It is self-starting, i.e. it relies only on properties at time t.
- It is time reversible, causing it to conserve energy
- It is stable, errors are of the order Δt^3

To optimize the velocity-Verlet for MD simulations we look to increase Δt while maintaining a similar error term. For the linear Verlet, error is a result of the potential deviating from the linear approximation made when only considering acceleration. Non-Newtonian Calculus is a natural method for approximating a function geometrically.

Non-Newtonian Calculus

Non-Newtonian calculus (NNC) was first formalized in the 1970s by Michael Grossman and Robert Katz. NNCs share key properties such as having a Fundamental theorem of calculus, but differ in the type of change they consider.

Geometric Calculus

The geometric derivative:

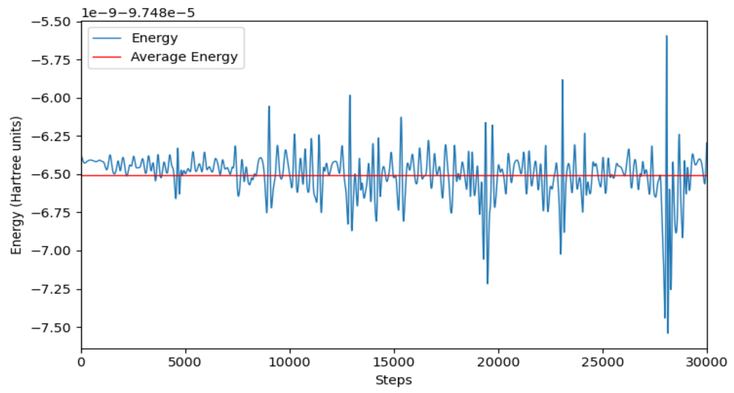
$$f^*(x) = \lim_{h\to 0}\left(\frac{f(x+h)}{f(x)}\right)^{1/h}$$

Geometric calculus deals with a function's fractional change in response to an additive change to it's argument. This leads to the property which has made geometric calculus the most used NNC:

$$\int^* f(x)\cdot g(x) = \int^* f(x)\cdot\int^* g(x)$$

The integral of a product is the product of the integrals.

So can we form a geometric calculus based velocity-Verlet? Yes, but it has been shown to be only a marginal improvement over the linear velocity-Verlet and only for specific values of r(t). These values are determined by regions in which a geometric approximation well characterizes the potential.



A graph demonstrating energy conservation over time for the velocity-Verlet. Fluctuations in energy can be made arbitrarily small by decreasing step size.

Bigeometric Calculus

Bigeometric calculus considers a fractional change in both a function's value and its argument.

$$f^{\pi}(x) = \lim_{h\to 0}\left(\frac{f(x(1+h))}{f(x)}\right)^{1/h}$$

Bigeometric calculus is inherently scale free.

A geometric progression in time is not useful for MD, so we consider varying Δt and consider $\Delta r(\Delta t)$

This yields:

$$\Delta r^{\pi}(\Delta t) = \exp\left(\frac{1}{1-\gamma}\right), \qquad \gamma = \frac{a(t)\Delta t}{2(v(t)+a(t)\Delta t)}$$

While its already known that rescaling Δt (with constraints) can maintain energy conservation and improve accuracy, little is quantitively understood about this improvement.

Summary of Results

- MD simulation framework with 25 particles in the Lennard-Jones potential.
- Demonstrated the velocity-Verlet's energy conservation.
- Measured energy fluctuation as a function of timestep for the linear velocity-Verlet.
- Derived the geometric velocity-Verlet.
- Derived basic results for a bigeometrically informed velocity-Verlet.

Current Work

- Quantitively verifying the performance of the geometric Verlet in 1D. This involves investigating energy fluctuations as a function of step size and taking 1D data for the linear velocity-Verlet.
- Euler-Lagrange equations in bigeometric calculus.
- Predicting performance for a variable timestep Verlet.
- Developing an intuitive understanding for what the bigeometric derivative represents.
- Developing a method to choose each timestep which does not break time reversibility.