Short Course on Molecular Dynamics Simulation

Lecture 3:
Integration Algorithms

Professor A. Martini
Purdue University

High Level Course Outline

1. MD Basics
2. Potential Energy Functions
3. Integration Algorithms
4. Temperature Control
5. Boundary Conditions
6. Neighbor Lists
7. Initialization and Equilibrium
8. Extracting Static Properties
9. Extracting Dynamic Properties
10. Non-Equilibrium MD

Integration Algorithms

- Potential energy (force) is a function of 3N atomic positions
- There is no analytical solution to the equations of motion which must be solved numerically

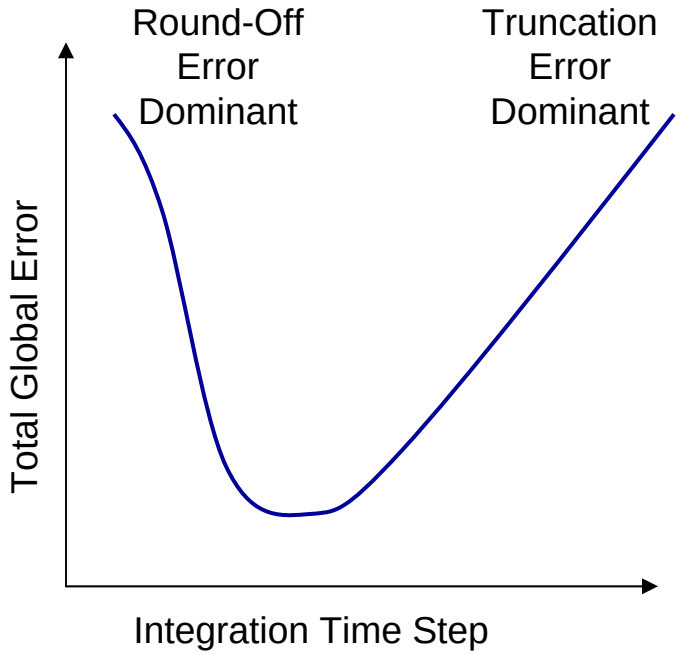
$$\vec{F}_i = m_i \vec{a}_i \qquad \vec{a}_i = \frac{d\vec{v}_i}{dt} \qquad \vec{v}_i = \frac{d\vec{r}_i}{dt}$$

Integration Algorithms

- General Rules:
  - Conservation of energy
  - Reversible
  - Computational efficient
  - Enable a “long” integration time step
  - Only one force evaluation per time step
- Commonly used integrators:
  - Verlet
  - Velocity Verlet
  - Predictor-Corrector
  - Gear Predictor-Corrector

Integration Algorithms

- Error:
  - Round off error vs. truncation
  - Local vs. global



Integration Algorithms

- Verlet Algorithm:
  - Derived from two Taylor expansions

$$r(t+\delta t) = r(t) + \frac{dr(t)}{dt}\delta t + \frac{1}{2}\frac{d^2r(t)}{dt^2}\delta t^2 + \frac{1}{3!}\frac{d^3r(t)}{dt^3}\delta t^3 + O(\delta t^4)$$

$$r(t-\delta t) = r(t) - \frac{dr(t)}{dt}\delta t + \frac{1}{2}\frac{d^2r(t)}{dt^2}\delta t^2 - \frac{1}{3!}\frac{d^3r(t)}{dt^3}\delta t^3 + O(\delta t^4)$$

  - Add together and simplify

$$r(t+\delta t) = 2r(t) - r(t-\delta t) + \frac{d^2r(t)}{dt^2}\delta t^2 + O(\delta t^4)$$

Integration Algorithms

- Notes on Verlet:
  - Velocities not explicitly solved, calculated typically from first order central difference

$$v(t) = \frac{r(t+\delta t) - r(t-\delta t)}{2\delta t}$$

  - Position vector at $t+\delta t$ requires positions previous two time steps; a two-step method; not self starting
  - Advantages: simplicity and good stability
  - Global error $O(\delta t^{2})$

Integration Algorithms

- Velocity Verlet Algorithm:
  - Improved accuracy compared to standard Verlet
  - Start with position and velocity expansions

$$r(t+\delta t) = r(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 + \ldots$$

$$v(t+\delta t) = v(t) + \frac{1}{2}\delta t[a(t) + a(t+\delta t) + \ldots$$

Integration Algorithms

- Velocity Verlet Algorithm:
  - Each integration cycle

1. Calculate velocities at mid-step $$v(t+\frac{\delta t}{2}) = v(t) + \frac{1}{2}a(t)\delta t$$

2. Calculate positions at the next step $$r(t+\delta t) = r(t) + v\left(t+\frac{\delta t}{2}\right)\delta t$$

3. Calculate accelerations at next step from the potential

4. Update the velocities $$v(t+\delta t) = v\left(t+\frac{\delta t}{2}\right) + \frac{1}{2}a(t+\delta t)\delta t$$

Integration Algorithms

- Predictor-Corrector Algorithms:
  1. Predict positions and velocities at the end of the next timestep
  2. Evaluate forces at the next time step using the predicted positions
  3. Correct the predicted positions and velocities

Integration Algorithms

- Predictor-Corrector Algorithms:
  1. Predict the system configuration at the end of the next timestep using Taylor expansion

$$r(t+\delta t) = r(t) + \ldots$$

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

$$a(t+\delta t) = a(t) + \ldots$$

$$b(t+\delta t) = b(t) + \ldots$$

Integration Algorithms

- Predictor-Corrector Algorithms:
  2. Evaluate forces at the next time step using the predicted system state; difference between the predicted and newly calculated acceleration is the error

$$\Delta a(t+\delta t) = a^c(t+\delta t) - a^p(t+\delta t)$$

Integration Algorithms

- Predictor-Corrector Algorithms:
  3. Use the error calculated in the previous step to correct all next step values

$$r^c(t+\delta t) = r^p(t+\delta t) + c_0 \Delta a(t+\delta t)$$

$$v^c(t+\delta t) = v^p(t+\delta t) + c_1 \Delta a(t+\delta t)$$

$$a^c(t+\delta t) = a^p(t+\delta t) + c_2 \Delta a(t+\delta t)$$

$$b^c(t+\delta t) = b^p(t+\delta t) + c_3 \Delta a(t+\delta t)$$

  - Coefficients maximize stability and are dependant on the specific algorithm chosen

Integration Algorithms

- Gear Predictor-Corrector Algorithms:
  - Predict using 5th order Taylor series
  - So need five derivatives of position at each timestep
  - Coefficients are tabulated for q-order predictors:
    - For example, with q=3
      - C_0=1/6
      - C_1=5/6
      - C_2=1
      - C_3=1/3
  - Error is $O(\delta t^{q+1})$

Integration Algorithms

- Choosing a time step
  - Too small → trajectory covers only a limited part of the phase space
  - Too large → numerical instability
  - Timestep should be ~ 1 order of magnitude smaller than the shortest motion time scale
  - In general:

System	Types of Motion	Time Step (s)
Atoms	Translation	10^{-14}
Rigid molecules	Translation and Rotation	$5x10^{-15}$
Flexible molecules, rigid bonds	Translation, Rotation and Torsion	$2x10^{-15}$
Flexible molecules, flexible bonds	Translation, Rotation, Torsion and Vibration	10^{-15} or $5x10^{-16}$