An Investigation on New Numerical Methods for Molecular Dynamics Simulation

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What is Molecular Dynamics?

- A way to simulate materials
- First, specify
  - Initial positions
  - Initial velocities
  - Mass of particles
  - The way in which the particles interact
- The system evolves in time
- Keys to accuracy
  - Force Field
  - Method of phase space propagation
What is Molecular Dynamics?

Click to play movie

Click to play movie
What are the applications of MD?

- As a counterpart to observation
  - Parameters available
    - Temperature
    - Pressure
    - Volume
  - Measurements possible
    - Thermodynamics properties
    - Transport coefficients
    - Space-time correlation functions
- As a means of developing new materials
  - Following the paradigm of virtual prototyping
    - Test for desirable properties
    - Modify the design
    - Retest to see if improvement was made
What are the major challenges in MD?

- Accurate Force Fields
  - Functional form
  - Parameterization

- Long simulation times
  - Evaluating interactions between particles, $O(N^2)$
  - Short time steps means performing many force evaluations per unit of real time simulated

\[
F_{ij} = \left(\frac{48\varepsilon}{\sigma^2}\right)\left[\left(\frac{\sigma}{r_{ij}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma}{r_{ij}}\right)^8\right]r_{ij}
\]
What is the current standard for phase space propagation?

- Implicit versus explicit integrators
  - Explicit Euler
    \[ r_{n+1} = r_n + v_n \Delta t \]
  - Implicit Euler
    \[ r_{n+1} = r_n + v_{n+1} \Delta t \]
- Velocity Verlet
  \[ v_{n+1/2} = v_n + \frac{f_n \Delta t}{2m} \]
  \[ r_{n+1} = r_n + v_{n+1/2} \Delta t \]
  \[ v_{n+1} = v_{n+1/2} + \frac{f_{n+1} \Delta t}{2m} \]
What is our proposed alternative?

- HHT family of integrators

\[
Ma_{n+1} = (1 + \alpha)F_{n+1} - \alpha F_n
\]
\[
v_{n+1} = v_n + \Delta t((1 - \gamma)a_n + \gamma a_{n+1})
\]
\[
r_{n+1} = r_n + \Delta tv_n + \frac{\Delta t^2}{2}((1 - 2\beta)a_n + 2\beta a_{n+1})
\]
What are the advantages of our method?

- Able to take longer time steps
  - Implicit methods have been shown to be stable and accurate for longer time steps than explicit integrators
  - A tenfold increase in time step length means, roughly, a tenfold speedup in simulation time
- Tunable numerical damping
  - Spurious high frequency modes can be damped
  - Large conformational motions are preserved
What are the disadvantages of our method?

- More difficult implementation
  - Implicit methods require more storage, testing and debugging
- More computationally complex
  - When done naively, implicit methods are much more computationally intensive per time step
  - Energy drift (dissipation) due to numerical damping can cause unphysical measurements
What are the results, so far?

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Full Jacobian – 6.2fs time step

Total energy conserved
What are the results, so far?

Click to play movie

Mass matrix only – 2.6fs time step

Total energy conserved
What are the results, so far?

Click to play movie

Full Jacobian – 8.6fs time step

Total energy NOT conserved
What are the plans for future research?

- Reduced Jacobian evaluation
  - Mass matrix
  - Full Jacobian with infrequent evaluations
- Stiff ODE methods
- Variational integrators
- Code optimization
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