Molecular Dynamics Example

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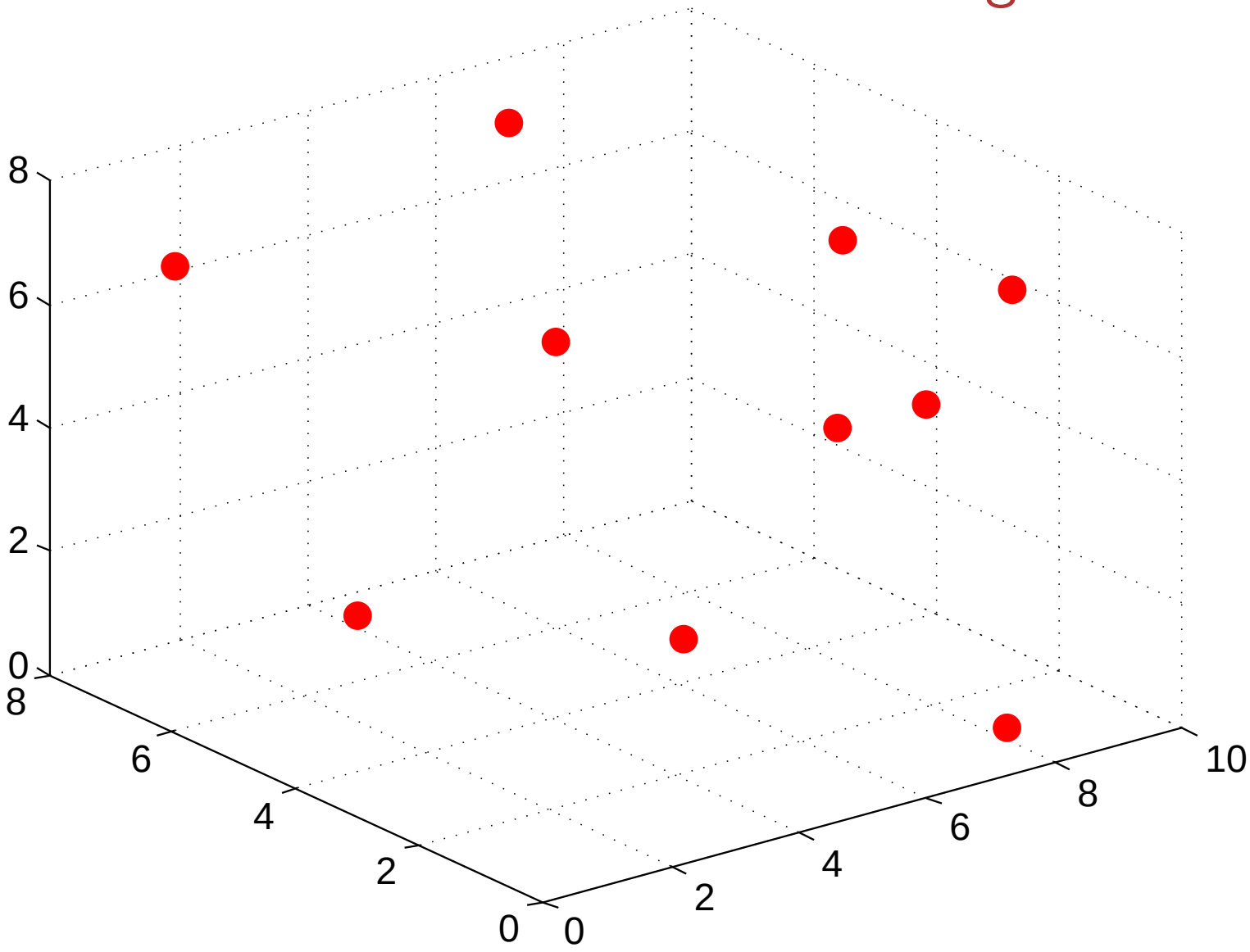
Configuration

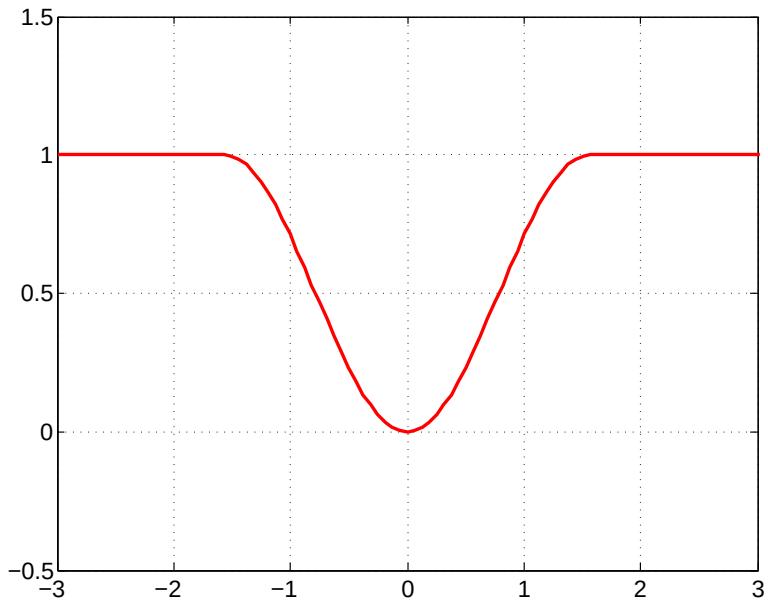


A set of NP particles move in 3D space, subject to an interparticle Lennart-Jones force.

Model Problem

Particle equations of motion

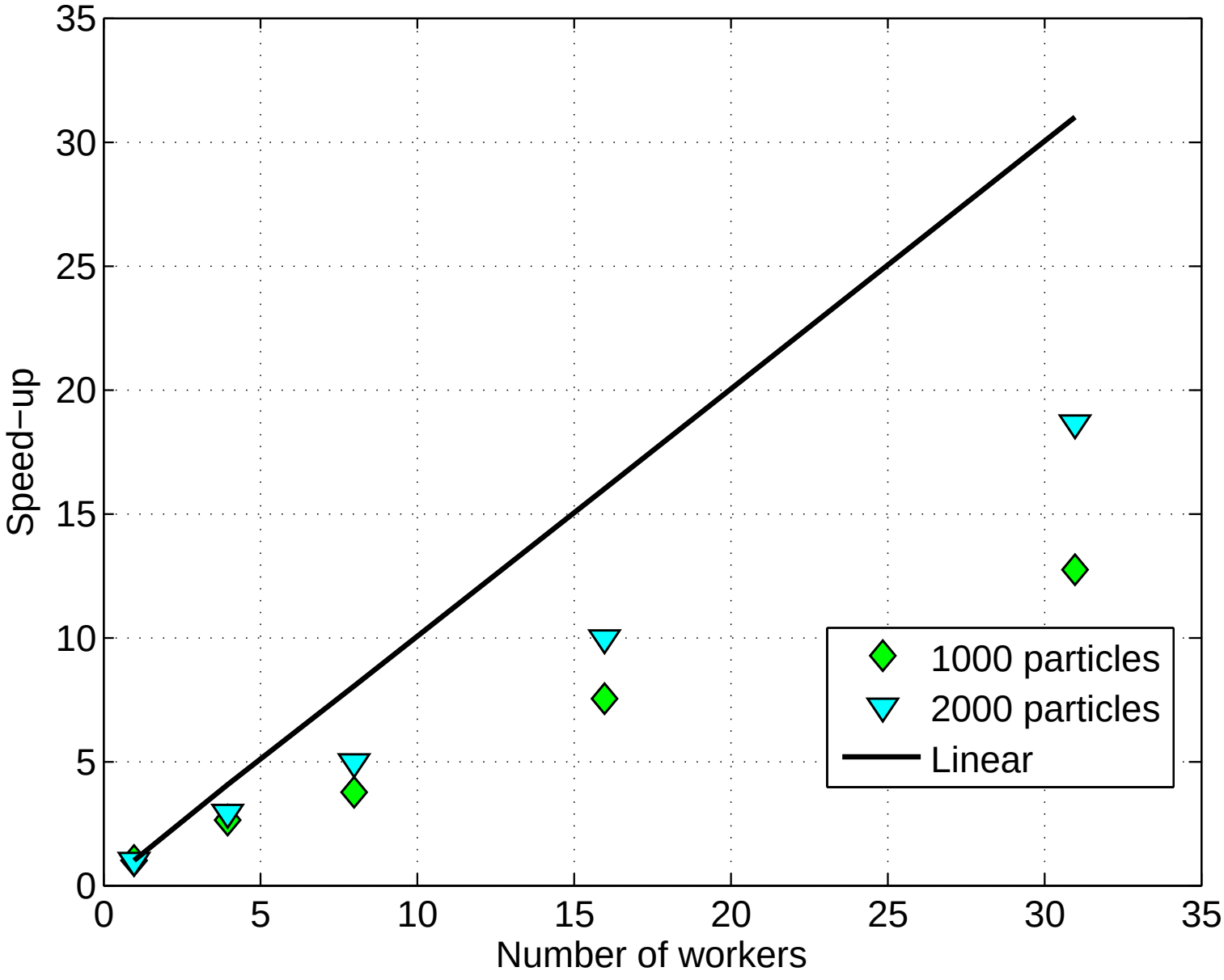
$$m\,\ddot{\vec{r}}_i(t) = \vec{f}_i = \sum_{j \neq i} \vec{f}_{j \to i} \ , \quad \text{where} \quad \vec{f}_{j \to i} = \nabla V(\vec{r}_j - \vec{r}_i) \ .$$



Code Fragment

```
parfor i = 1 : np

  Ri = pos - repmat ( pos( :, i ), 1, np );  %'i->j' vecs

  D = sqrt ( diag ( Ri' * Ri ) );            % distances

  Ri = Ri( :, ( D > 0.0 ) );

  D = D( D > 0.0 );                          % pos.

  D2 = D .* ( D <= pi2 ) + pi2 * ( D > pi2 );% truncate

  pot = pot + 0.5 * sum ( sin ( D2 ).^2 );   % accumulate

  f( :, i) = Ri * ( sin( 2*D2 ) ./ D );      % force 'i'

end
```

Timing Results: Intel Nehalem



References

Report:

- Burkardt, Cliff, Snow,
  MATLAB Parallel Programming:
  Some Timing Results on an Intel Nehalem Cluster,
  http://people.sc.fsu.edu/~burkardt/pdf/nehalem_matlab.pdf.

Source code:

- http://people.sc.fsu.edu/~burkardt/m_src/
  md_parallel/md_parallel.html
- http://people.sc.fsu.edu/~burkardt/m_src/
  satisfiability_parallel/satisfiability_parallel.html.