

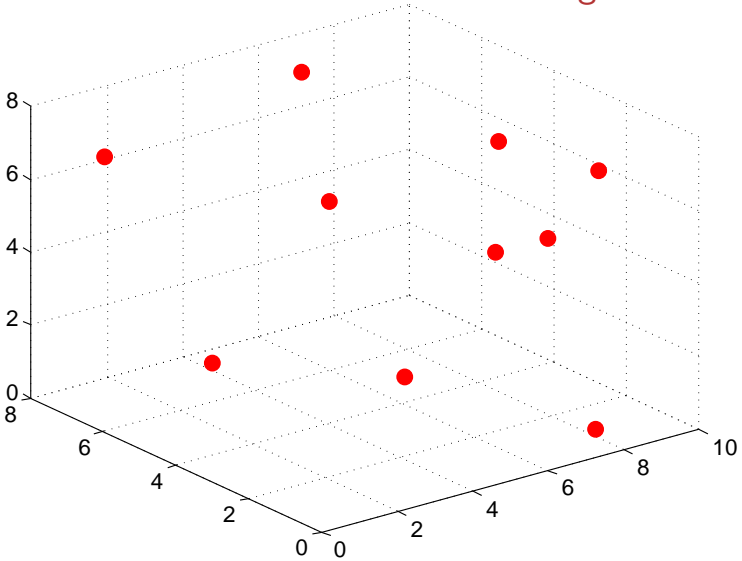
Molecular Dynamics Example

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Configuration

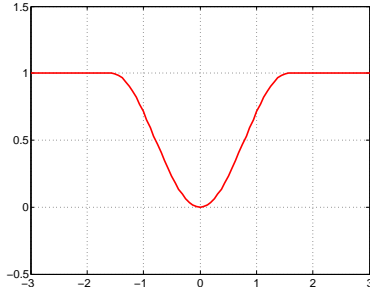


A set of NP particles move in 3D space, subject to an interparticle Lennard-Jones force

Model Problem

Particle equations of motion

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



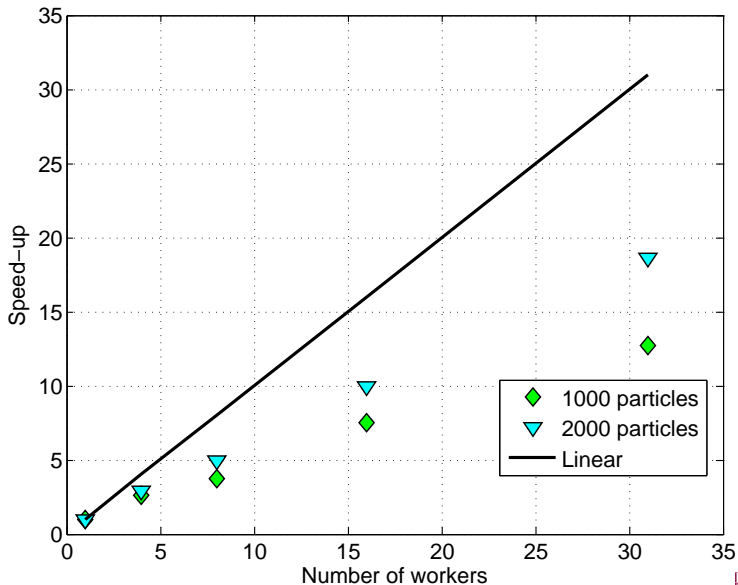
Code Fragment

```
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.