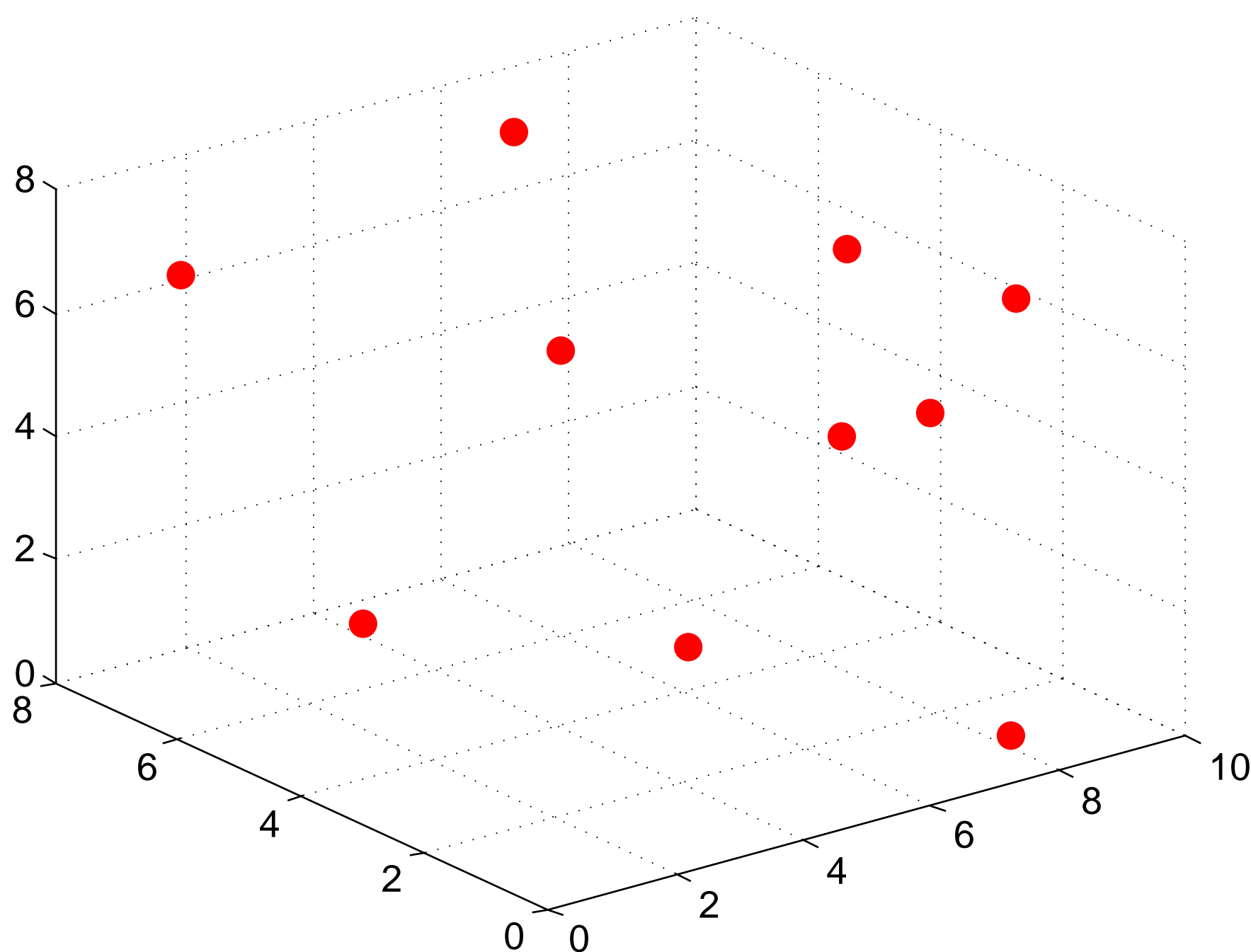


Molecular Dynamics Example

Configuration

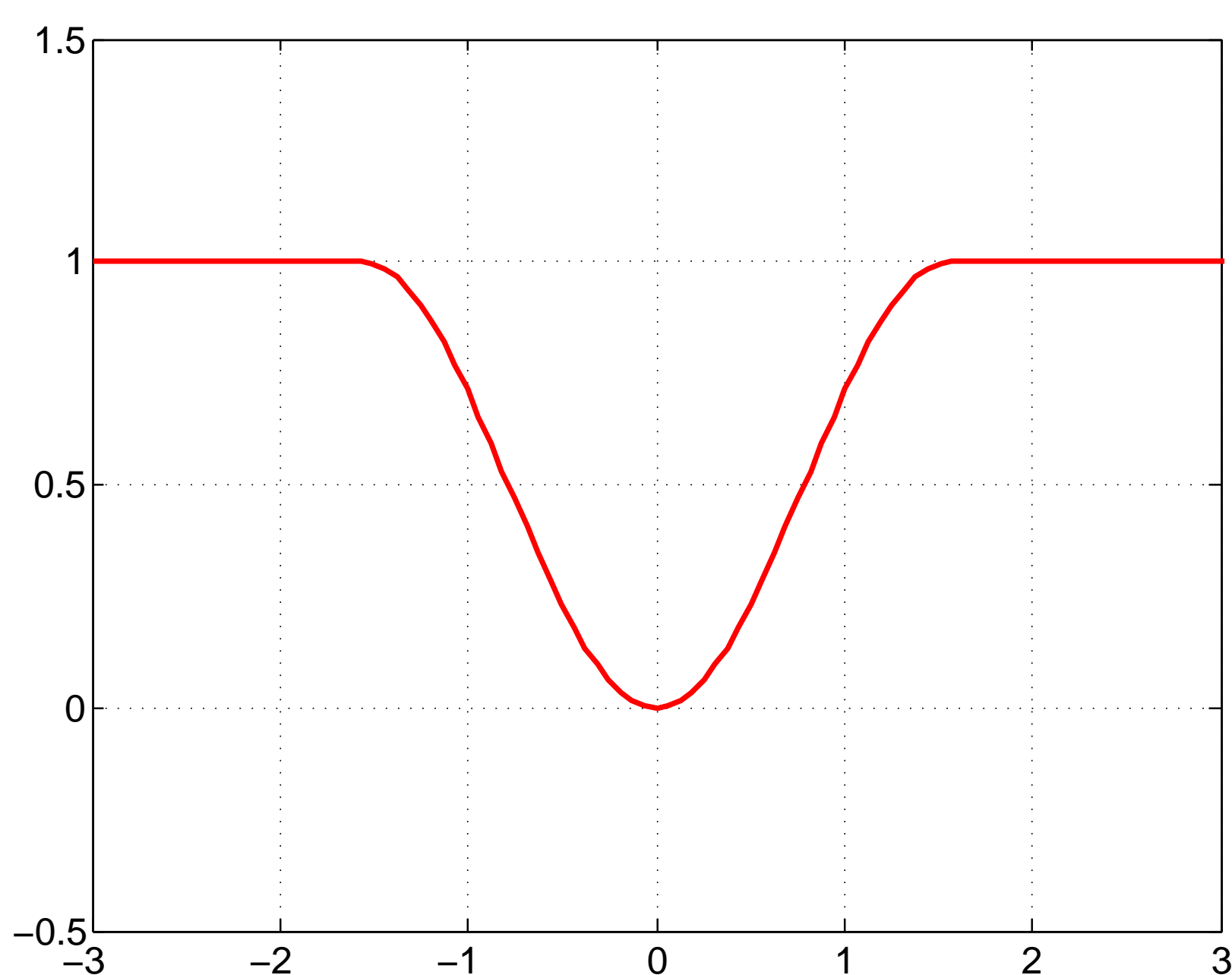


A set of NP particles move in 3D space, subject to an interparticle Lennart-Jones force.

Model Problem

Particle equations of motion

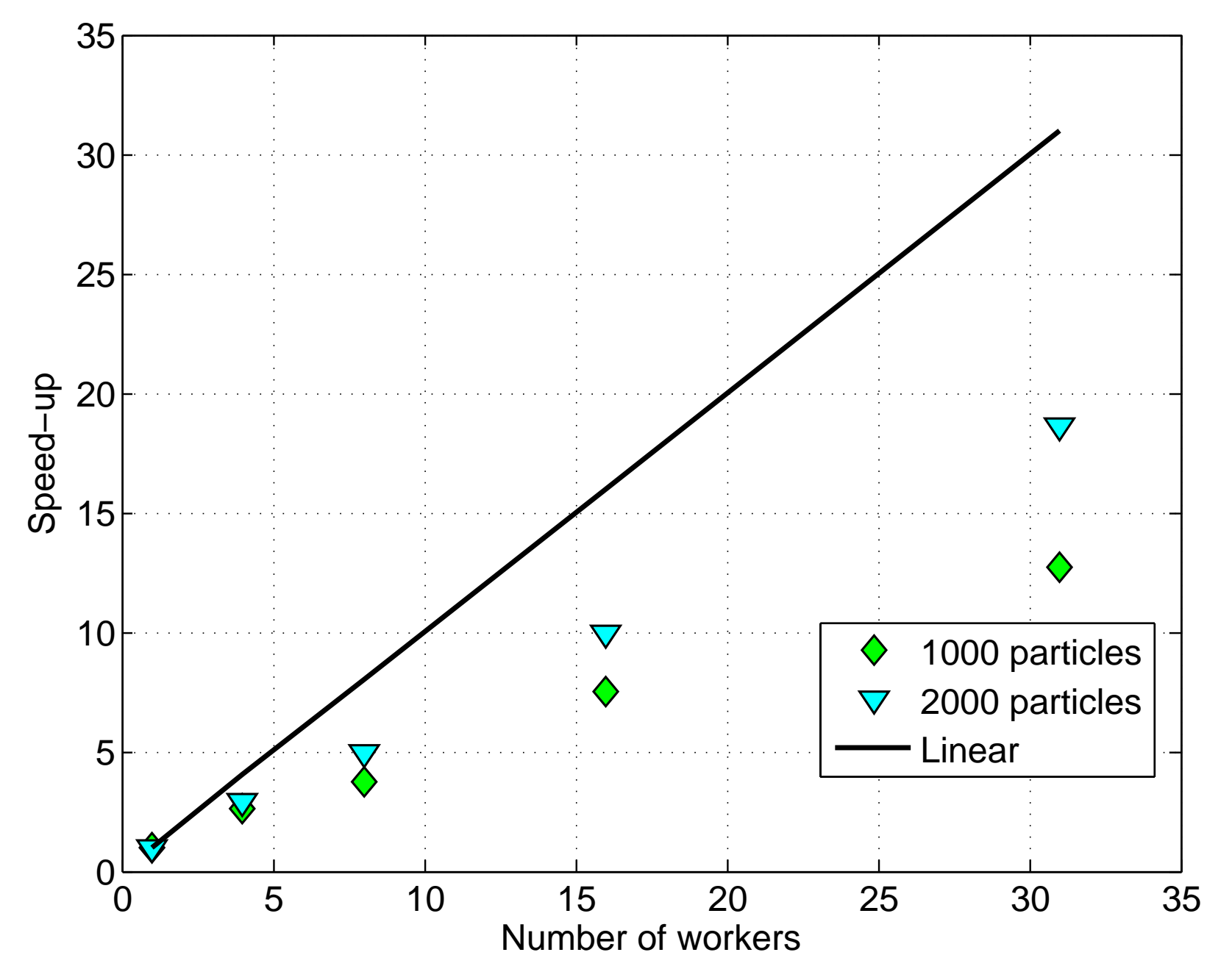
$$m\ddot{\vec{r}}_i(t) = \vec{f}_i = \sum_{j \neq i} \vec{f}_{j \rightarrow i}, = \sum_{j \neq i} \nabla V(\vec{r}_j - \vec{r}_i).$$



Code Fragment

```
parfor i = 1 : np
    Ri = pos-repmat(pos(:,i),1,np);
    D = sqrt(diag(Ri'*Ri));
    Ri = Ri(:,(D>0.0));
    D = D(D>0.0);
    D2 = D.*(D<=pi2)+pi2*(D>pi2);
    pot = pot+0.5*sum(sin(D2).^2);
    f(:,i) = Ri*(sin(2*D2)./D);
end
```

Timing



Discussion

For a relatively small problem using NP=1000 particles, the program's performance improved across the range of processors; however, the speedup was only about half the ideal improvement. When the problem size was increased to 2000 particles, the program got a much greater benefit from parallelism. This suggests that, at least over this range of processors, parallel MATLAB will be increasingly efficient as the problem size increases.

Reference

[http://people.sc.fsu.edu/~burkardt/...](http://people.sc.fsu.edu/~burkardt/)

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 Timing Results on an Intel Nehalem Cluster,*
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