ProtoMol is an object-oriented component based framework for molecular dynamics simulations. It is designed for high flexibility, easy extendibility and maintenance, and high performance demands, including parallelization. It supports multiple time-stepping intergration to improve long-term efficiency, and fast electrostatic force evaluation algorithms like plain Ewald, Particle-Mesh-Ewald, and Multigrid summation to improve performance.

## Performance: Sequential

| Case | Boundary | # of atoms | ProtoMol | NAMD2 |
|---|---|---|---|---|
| Water | Vacuum | 423 | 0.01082 | 0.01215 |
| | Periodic | | 0.01558 | 0.01488 |
| BPTI | Vacuum | 14281 | 0.7826 | 0.889 |
| | Periodic | | 1.3855 | 1.216 |
| apoa1 | Vacuum | 92224 | 5.6221 | 6.537 |
| | Periodic | | 9.2586 | 10.056 |

Sequential comparison ProtoMol vs NAMD2 for one time step in average [s], using cutoff of 10Å on a Pentium III, 1.26 GHz running Linux RedHat.

## Performance: Parallel

| Nodes | Static [s] | Speedup | Dynamic [s] | Speedup |
|---|---|---|---|---|
| 1 | 677.2 | 1 | 677.2 | 1 |
| 2 | 337.4 | 2.0 | 343.2 | 1.97 |
| 4 | 181.6 | 3.73 | 175.2 | 3.87 |
| 8 | 98.85 | 6.85 | 89.51 | 7.57 |
| 16 | 53.48 | 12.7 | 47.91 | 14.1 |
| 32 | 30.83 | 22.0 | 28.16 | 24.0 |

ApoA, 92224 atoms, vacuum, simulating 10 fs with a cutoff of 12 Å on an Origin2000, 195MHz R10000. Left column shows the scaling using static load balancing, and the right column shows the scaling using a master-slave load balance.