NAMD Serial and Parallel Performance

Jim Phillips
Theoretical Biophysics Group
Beckman Institute, UIUC

Serial performance basics

- Main factors affecting serial performance:
  - Molecular system size and composition.
  - Cutoff distance and cycle length.
  - Full electrostatics (PME) parameters.
  - Processor architecture and speed.

System size and density

- Time per step scales
  - linearly with the number of atoms.
  - linearly with density (atoms per volume).
- Example: explicit H vs. united atoms
  - 1/3 the number of atoms.
  - 1/3 the density.
  - Expect 9 X the performance (for protein).

Cutoffs and frequencies

- Time per step scales cubically with cutoff.
- Steps per cycle has a much smaller effect.
- Example: 10 A vs. 14 A
  - 1000 vs. 2744
  - Expect 2.7 X the performance.

PME and grid sizes

- PME with a shorter cutoff breaks even.
- Grid spacing should be about 1 A.
- Grid sizes should be $2^i\ 3^j\ 5^k$. (2^i is best!)
- Only affects FFT (should be minor).

- Example: 47A x 31A x 39A periodic cell
  - Grid sizes: 48 32 40

Processors

- Limited dependence on memory system:
  - Small amount of data.
  - Cache friendly design.
- Performance scales
  - linearly with clock speed (for one architecture).
  - uncertainly with SPEC benchmarks.

- Example:
  - 1333 MHz Althon equals 667 MHz Alpha

Parallel performance basics

- Speedup = (serial time) / (parallel time).
- Ideal (linear) speedup is number of CPUs.
- Amdahl's law says best speedup possible is (total work) / (non-parallelizable work).
- In MD, each timestep must be parallelized.

NAMD parallel design

- Atoms are "spatially decomposed" into cubes which are distributed among CPUs.
  - Generates 25-400 cubes to distribute.
- Interactions between pairs of cubes are also distributed among CPUs.
  - Generates 300-5000 interaction groups.
- Interactions are redistributed among CPUs based on measurement of their run time.

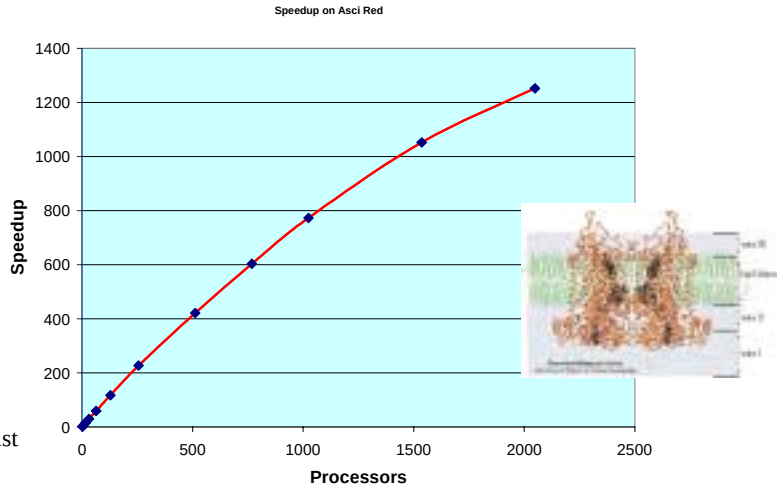
Calculating speedup

- Run 500 steps on 1,2,4,8,… CPUs.
- Final performance, ignore startup time.
- Be aware of dynamic load balancing:
  - Don’t use timing at start of simulation.
  - Don’t use timing including load balancing step.
  - Don’t use “Initial timing: …” value.
  - Best estimate is “Benchmark timing: …”.

Cutoff and system size

- Smaller cutoff may improve efficiency.
  - Data is distibuted to more CPUs.
  - But there is less work to distribute.
- A larger simulation can employ more CPUs.
  - More work to divide among CPUs.
  - More data to distribute as well.
- Length of the simulation doesn’t matter.

Best recorded scaling (cutoff)

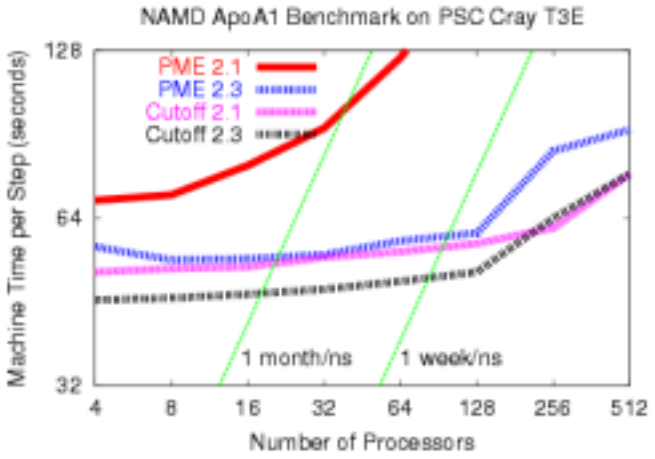


Published in SC2000: Gordon Bell Award Finalist

PME and parallel scaling

- PME is harder to parallelize:
  - More communication.
  - More stages of communication.
  - Only uses number of CPUs equal to grid size.
- But…
  - Superlinear speedup observed on T3E.

PME performance increase

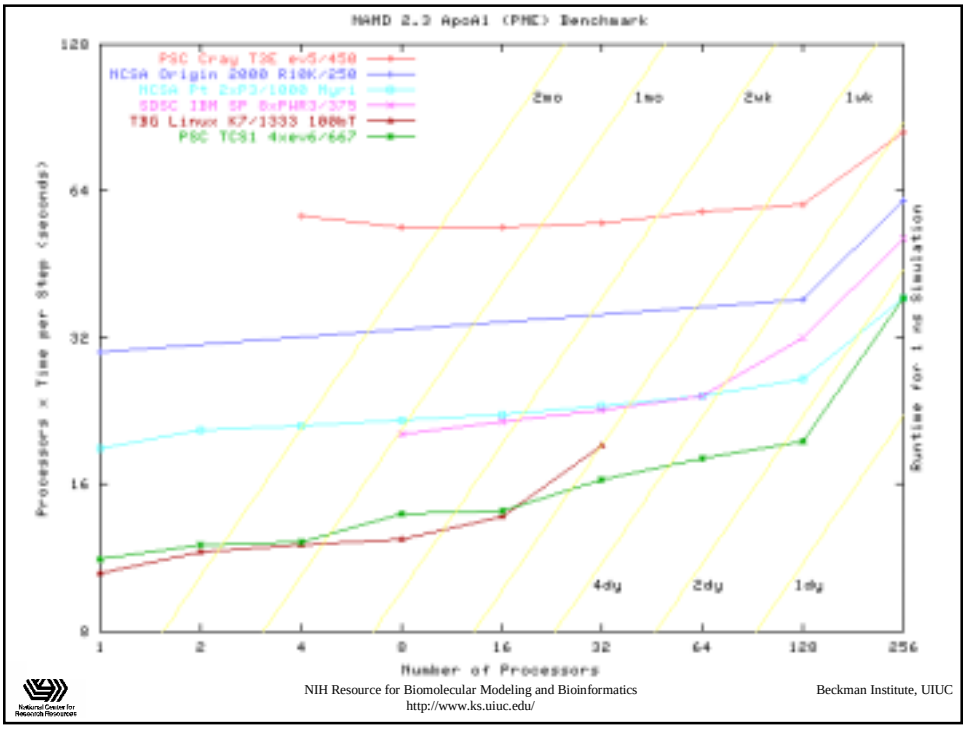


Parallel machines

- Three dimensions to machine performance:
  - Performance of the individual processors.
  - Bandwidth of the communication network.
  - Latency of the communication network.
- CPUs are improving faster than networks.
- Slow CPUs and fast networks give best speedups, but not best price/performance.

Latency tolerant design

- Some communication is necessary, but we don't want to sit idle waiting for it.
- Work is broken down into interaction sets which require different parts of the incoming data.
- Interactions are calculated as soon as required data is received, not in any particular order.



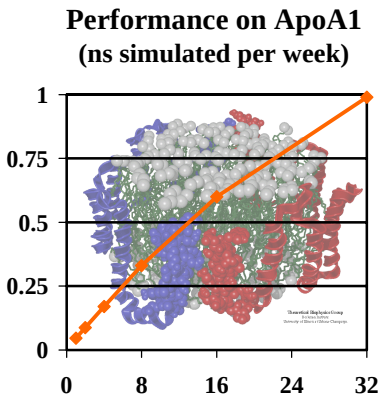
NIH Resource for Biomolecular Modeling and Bioinformatics
http://www.ks.uiuc.edu/
Beckman Institute, UIUC

Cost of large simulations

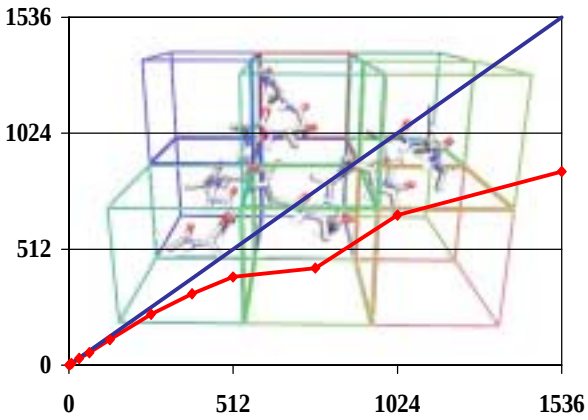
- 100,000 atom simulation with PME.
- 20s per timestep on one 1GHz CPU.
- One nanosecond of simulated time requires:
  - 5000 CPU-hours
  - 8 CPU-months
  - 1 week on 32 CPUs
- You can buy 32 processor machines but they cost $300K (or more, we don't ask).

NAMD 2.3 on Athlon cluster

- 67% efficiency on 32, *commodity hardware*.
- NAMD design is
  - latency tolerant,
  - cache friendly.
- Can simulate 100K atoms at 50 ns/year on 32 CPUs.
- Equivalent to owning a 100 CPU Cray T3E for only $32K.



NAMD: Scalable Molecular Dynamics



- Parallel simulation of biomolecular systems
- Spatial decomposition for distributed memory
- Message driven for latency tolerance
- Object-oriented and implemented in C++

Kalé *et al.,* J. Comp. Phys., **151**, 283 (1999)

NAMD
Scalable Molecular Dynamics