

Applicable Hardware and Software for MD

Jim Phillips

Theoretical Biophysics Group

Beckman Institute, UIUC

Outline

- Software
 - X-PLOR / CNS
 - AMBER
 - CHARMM
 - GROMACS
 - NWChem
 - TINKER
 - NAMD
 - Rasmol
 - VMD
- Hardware
 - NCSA Origin
 - NCSA IA32
 - NCSA IA64
 - PSC T3E
 - PSC LeMieux
 - SDSC Horizon
 - Beowulf Clusters
 - Desktop Graphics

X-PLOR / CNSsolve

- X-ray crystallography and NMR analysis.
- CHARMM 19 (united atom) force field.
- X-PLOR useful for setup, dynamics, etc. but abandoned due to commercialization.
- <http://atb.csb.yale.edu/xplor-info/>
- CNSsolve developed from scratch, without MD.
- <http://cns.csb.yale.edu/>
- Not parallelized.

AMBER

- Multiple programs for different functions.
- Varying degrees of parallelization.
- Development work in free energy perturbation, polarizable force fields, continuum solvent models.
- Force field (Cornell et al.) also available in CHARMM format.
- \$400 academic, \$20K commercial.
- <http://www.amber.ucsf.edu/amber/>

CHARMM

- Originally from Harvard.
- Similar to AMBER, but single program.
- Parallelized.
- Force field (MacKerell et al.) available.
- \$600 academic, commercial through Accelrys.
- <http://yuri.harvard.edu/>
- <http://www.accelrys.com/insight/charmm.html>
- http://www.scripps.edu/brooks/charmm_docs/charmm.html

GROMACS

- From Groningen, version 3.0 under GPL.
- Simpler, united atom force field.
- Few VDW, charges on all-atom version.
- Good performance due to assembly code.
- Apparently used for many lipid simulations.
- Parallelized.
- <http://www.gromacs.org/>

TINKER

- Serial code for method development.
- Many force fields, simulation methods.
- Freely available.
- <http://dasher.wustl.edu/tinker/>

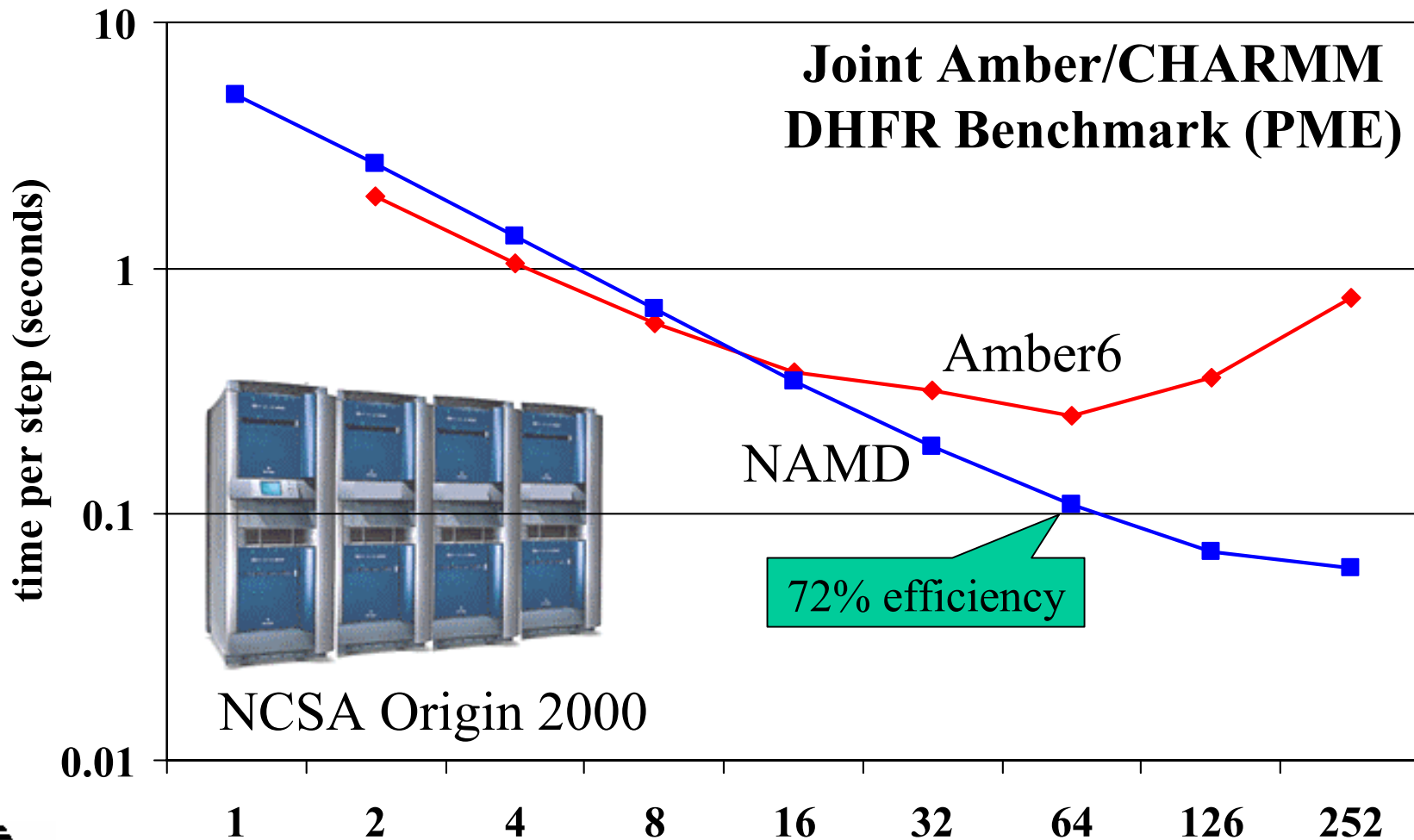
NWChem

- Complex package from PNNL.
- Many quantum methods, also has MD.
- Freely available but absolutely no support.
- Parallelized using global arrays model.
- <http://www.emsl.pnl.gov/pub/docs/nwchem/>

NAMD

- CHARMM, AMBER, GROMACS input.
- Highly parallelized (1000 CPUs).
- Doesn't provide every feature (yet).
- Developing a complete environment.
- Freely available, binaries, and support.
- Development continuing for several years.

NAMD Relative Performance



Rasmol

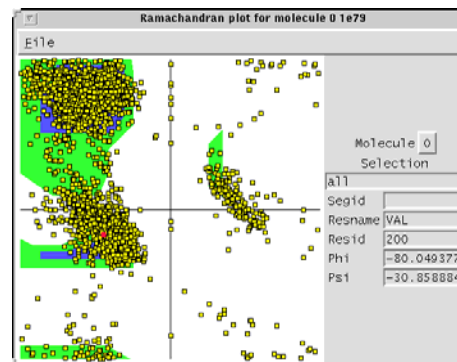
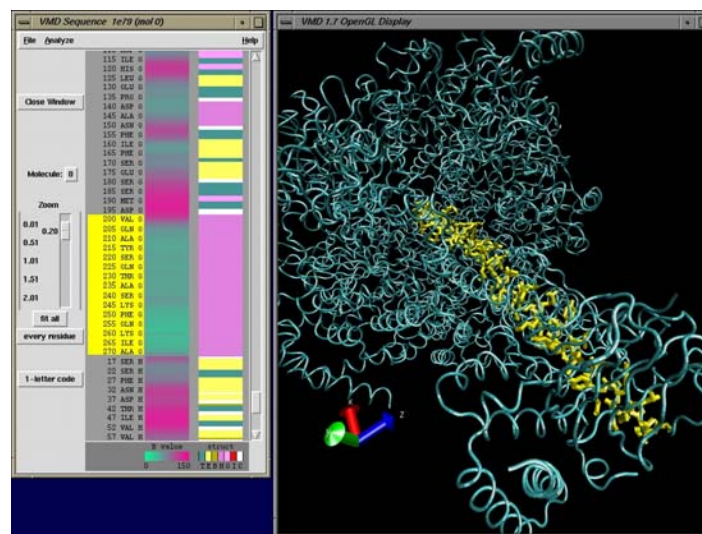
- Ubiquitous, basic molecular visualizer.
- Fast direct drawing, no acceleration.
- Free, public domain, commercialized.
- <http://www.umass.edu/microbio/rasmol/>
- There are a large number of free visualization packages available.

VMD

- Sister package to NAMD.
- Focus on trajectories and large molecules.
- OpenGL-based, uses graphics accelerators.
- Runs, somewhat slower, on other hardware.
- Freely available, binaries, and support.
- Development continuing for several years.
- <http://www.ks.uiuc.edu/Research/vmd/>

VMD Highlights

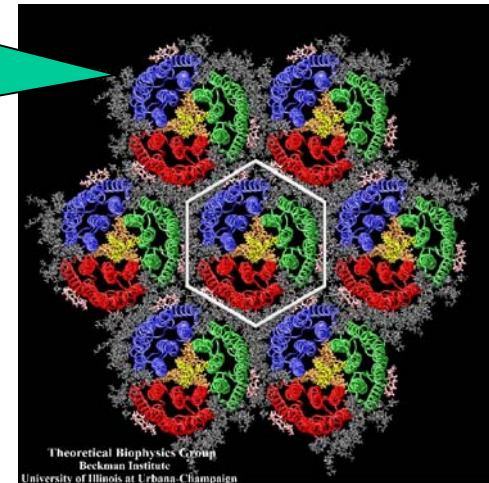
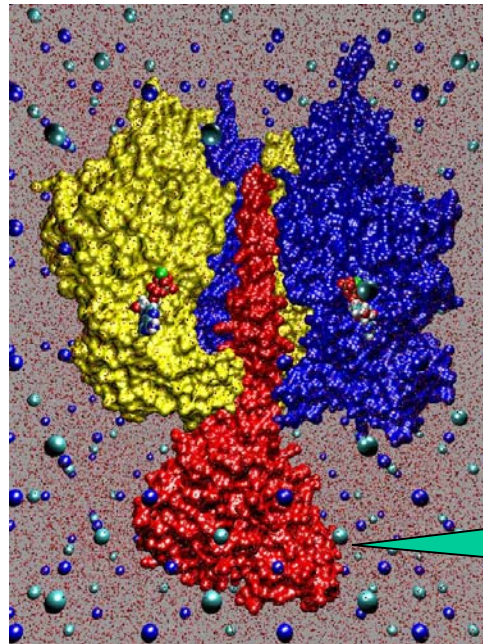
- Platforms:
 - Unix (16 builds)
 - Windows
 - MacOS X
- Display of large biomolecules and simulation trajectories
- Sequence browsing and structure highlighting
- User-extensible scripting interfaces for analysis and customization
- Interactive MD



VMD Permits Large Scale Visualization

- Large structures: 300,000 atoms and up
- Complex representations
- Long trajectories: thousands of timesteps
- Volumetric data
- Multi-gigabyte data sets break 32-bit barriers
- GlpF: each 5 ns simulation of 100K atoms produces a 12GB trajectory

Purple Membrane
150,000 Atoms



Theoretical Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign

F1 ATPase
327,000 Atoms

NCSA Origin 2000

- Non-uniform shared memory model.
- Allows OpenMP, thread parallelization.
- NCSA machines older, but only choice for shared memory programming model.
- SGI Origin 3000 sold today.
- Effective way to put many processors, disks, and graphics in a single box.

NCSA IA32 Linux Cluster

- Dual 1GHz Pentium 3 with Myrinet.
- Requires MPI message passing model.
- Straightforward, commodity solution.

NCSA IA64 Linux Cluster

- Dual 800 MHz Itanium with Myrinet.
- Similar to IA32 cluster, only IA64.
- Processor is twice as fast for NAMD.
- Performance is very compiler dependent.
- Warmup for TeraGrid McKinley clusters.

PSC Cray T3E

- 512 450 MHz Alpha ev5 processors.
- Unique 3D toroidal interconnect.
- Direct memory access SHMEM library.
- Highly scalable, low latency network.
- Processors slow by today's standards.
- Similar machines are being sold today.

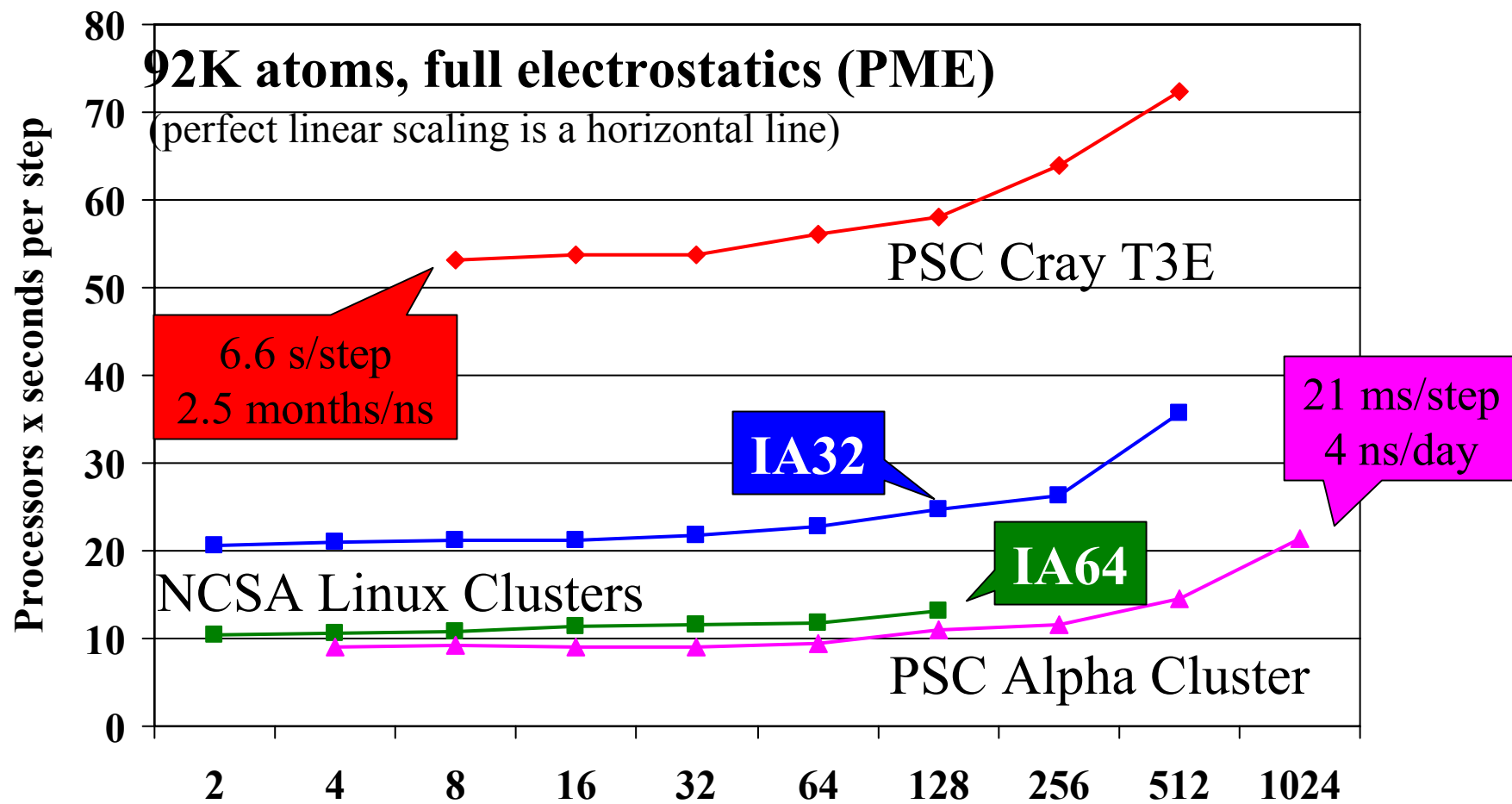
PSC LeMieux Alpha Cluster

- 3000 1GHz Alpha ev67 processors.
- 4 per box, special Quadrics interconnect.
- Very fast processors, still well balanced.
- Fastest machine for non-classified work.
- Processor being abandoned by Compaq.

SDSC Blue Horizon IBM SP

- 1000 360 MHz Power3 processors.
- 8 per box, special IBM interconnect.
- Hybrid shared memory and message passing programming model encouraged.
- Well integrated, very busy machine.
- Until recently IBM owned this market.

NAMD Performance



Beowulf Linux Clusters

- Commodity parts for lowest cost solution.
- Usually, Linux, IA32, and fast ethernet.
- Designed to run a single problem.
- Not as scalable or multi-purpose as others.
- NAMD is effective up to 32 CPUs.
- This is a whole workshop in itself!

Affordable Clusters

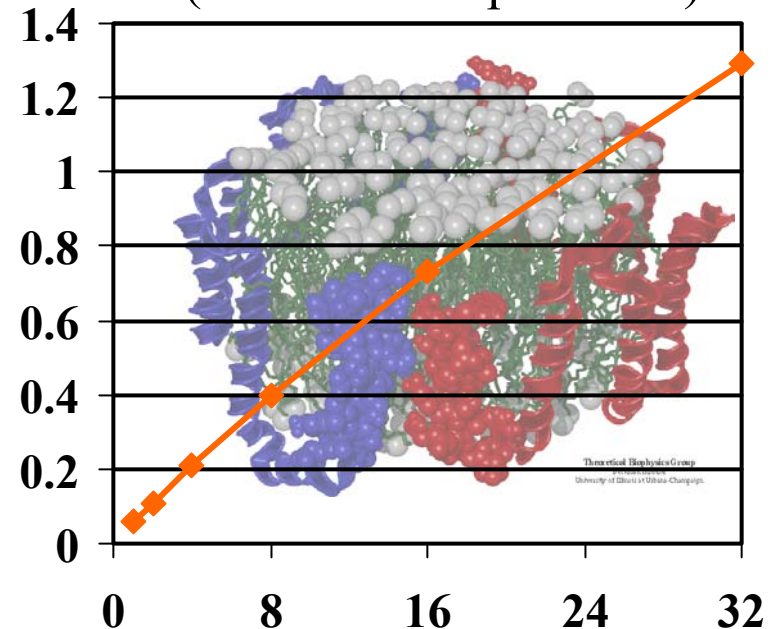
**NAMD tolerates network latency,
making commodity clusters affordable.**



**\$1000 per
processor**



92K atoms with PME
(ns simulated per week)



Desktop Graphics Hardware

- High end (\$5K to \$20K):
 - Sun Blade 100/1000/2000 workstation
 - Expert3D/Expert3D Lite/XVR-1000 graphics
 - Crystal Eyes stereo LCD glasses
- Low end (PC + \$300):
 - GeForce graphics card
 - Eye3D stereo LCD glasses

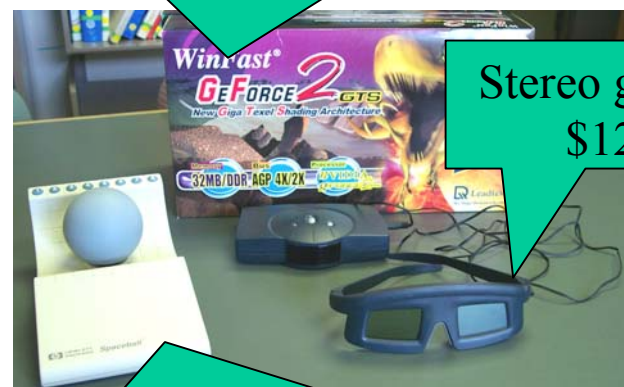
Affordable Visualization with VMD

- Hardware accelerated 3-D graphics not required for simpler molecular representations
- Inexpensive, game-oriented hardware technologies
 - 3-D graphics accelerators
 - Stereo glasses
 - Joysticks and other devices
- Most PCs can be upgraded with 3-D acceleration, stereo glasses, and input devices for about \$275



Runs on unaccelerated laptops

Midrange 3-D accelerator: \$100



Stereo glasses
\$120

Joystick, or a used Spaceball: \$50-\$100

Conclusions

- Variety of software depending on needs.
- Variety of hardware for large runs.
- Beowulf clusters affordable for local work.
- Good graphics now a commodity as well.
- Use others experiences as a guide.
- Adapt any purchases to your needs.
- Don't buy hardware until it's time to run!