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

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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.

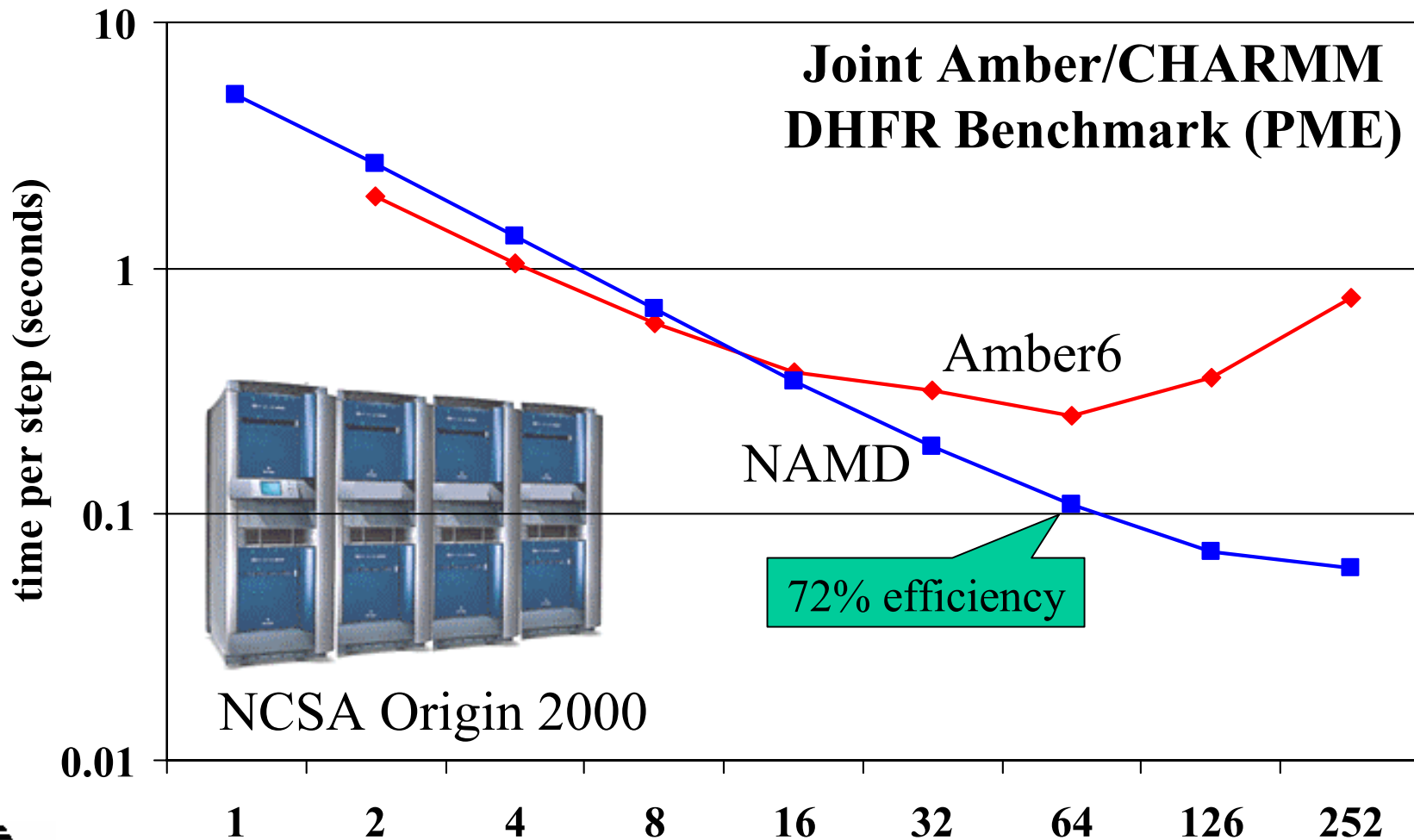- http://dasher.wustl.edu/tinker/

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.

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NAMD Relative Performance

Joint Amber/CHARMM DHFR Benchmark (PME)

time per step (seconds)

10

1

0.1

0.01

Amber6

NAMD

72% efficiency

NCSA Origin 2000

1   2   4   8   16   32   64   126   252

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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
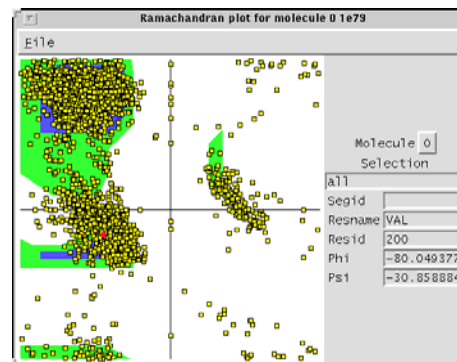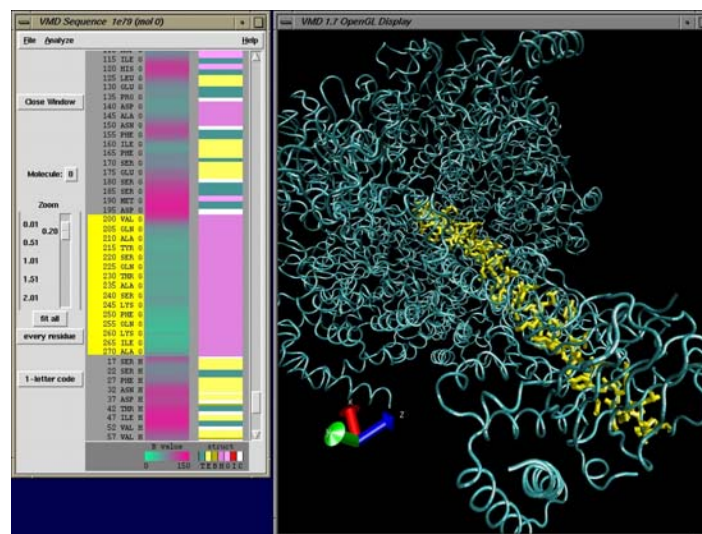
VMD Permits Large Scale Visualization

- 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
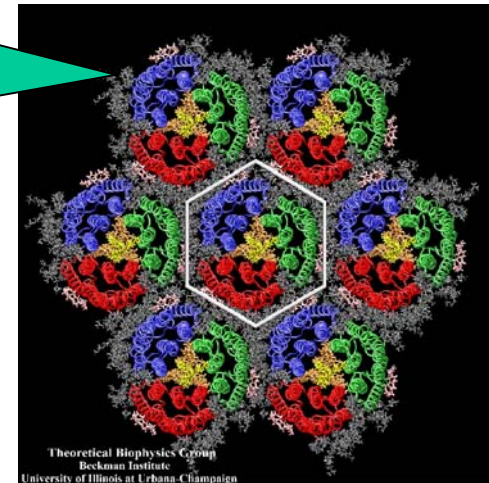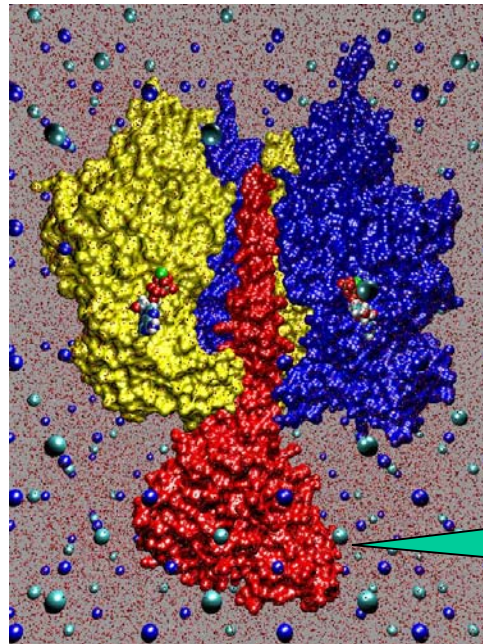
F1 ATPase 327,000 Atoms

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 todays standards.

- Similar machines are being sold today.

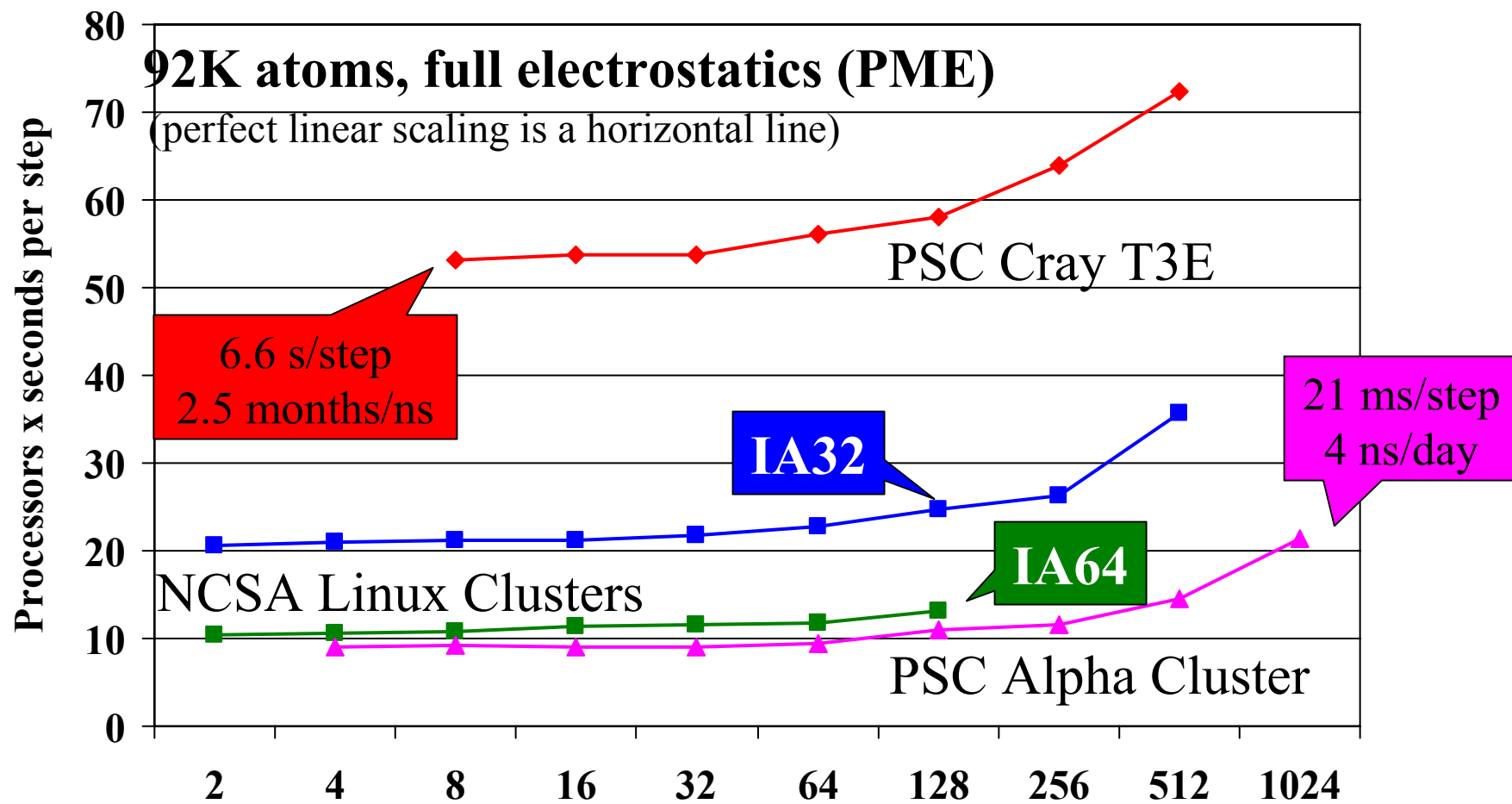National Center for
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PSC LeMieux Alpha Cluster

- 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.

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NAMD Performance

92K atoms, full electrostatics (PME)
(perfect linear scaling is a horizontal line)

PSC Cray T3E

6.6 s/step
2.5 months/ns

21 ms/step
4 ns/day

IA32

IA64

NCSA Linux Clusters

PSC Alpha Cluster

Processors x seconds per step

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

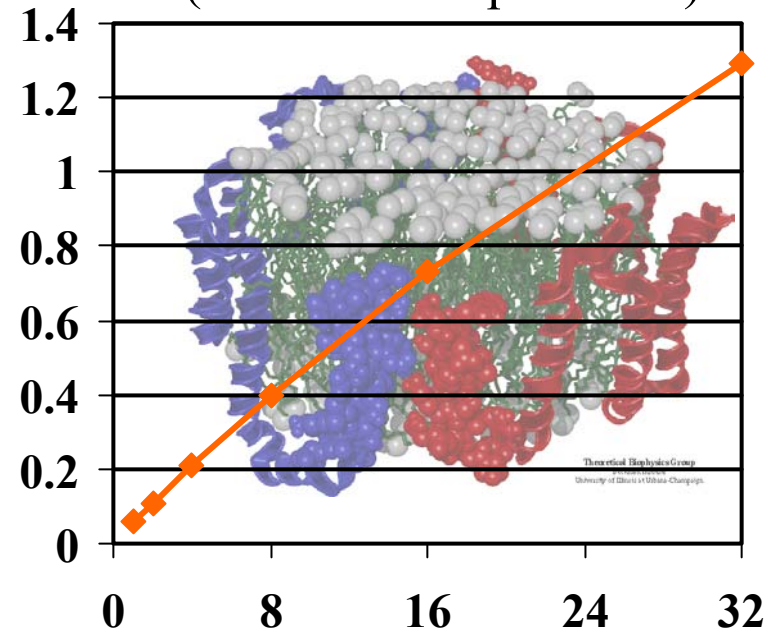**NAMD tolerates network latency, making commodity clusters affordable.**

$1000 per processor

Easy to manage

92K atoms with PME
(ns simulated per week)

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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
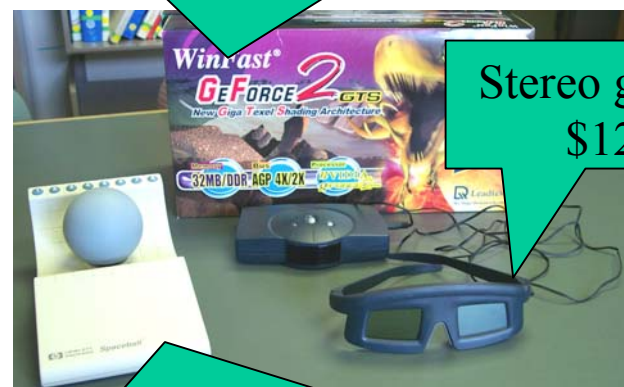
Stereo glasses $120

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!

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