Designing a Cluster for a Small Research Group

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Outline

- Why and why not clusters?
- Consider your…
  - Users
  - Application
  - Budget
  - Environment
  - Hardware
  - System Software
- Case study: local NAMD clusters

Why Clusters?

- Cheap alternative to “big iron”
- Local development platform for “big iron” code
- Built to task (buy only what you need)
- Built from COTS components
- Runs COTS software (Linux/MPI)
- Lower yearly maintenance costs
- Re-deploy as desktops or “throw away”

Why Not Clusters?

- Non-parallelizable or tightly coupled application
- Cost of porting large existing codebase too high
- No source code for application
- No local expertise (don't know Unix)
- No vendor hand holding
- Massive I/O or memory requirements

Know Your Users

- Who are you building the cluster for?
  - Yourself and two grad students?
  - Yourself and twenty grad students?
  - Your entire department or university?
- Are they clueless, competitive, or malicious?
- How will you to allocate resources among them?
- Will they expect an existing infrastructure?
- How well will they tolerate system downtimes?

Your Users' Goals

- Do you want increased throughput?
  - Large number of queued serial jobs.
  - Standard applications, no changes needed.
- Or decreased turnaround time?
  - Small number of highly parallel jobs.
  - Parallelized applications, changes required.

Your Application

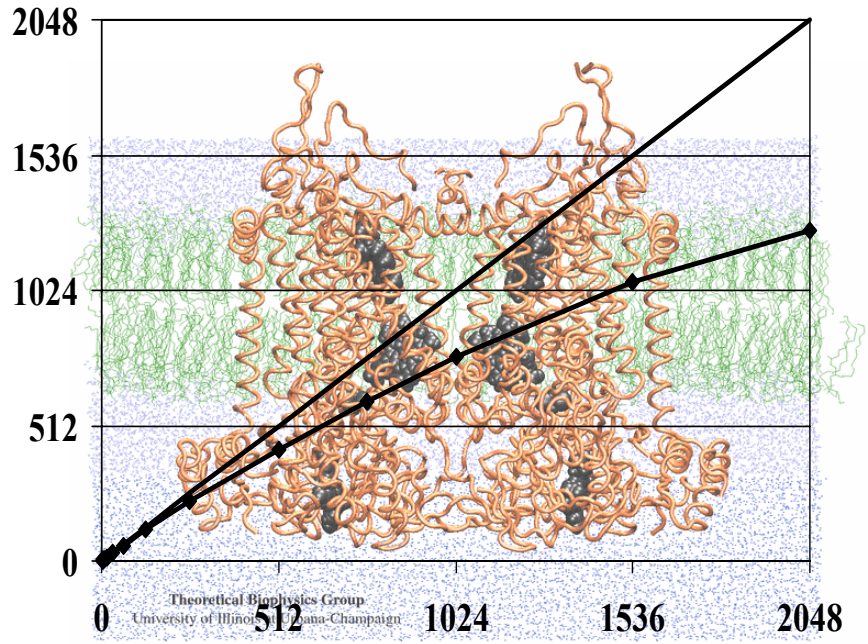
- The best benchmark for making decisions is your application running your dataset.
- Designing a cluster is about trade-offs.
  - Your application determines your choices.
  - No supercomputer runs everything well either.
- Never buy hardware until the application is parallelized, ported, tested, and debugged.

Your Application: Serial Performance

- How much memory do you need?
- Have you tried profiling and tuning?
- What does the program spend time doing?
  - Floating point or integer and logic operations?
  - Using data in cache or from main memory?
  - Many or few operations per memory access?
- Run benchmarks on many platforms.

Your Application: Parallel Performance

- How much memory per node?
- How would it scale on an ideal machine?
- How is scaling affected by:
  - Latency (time needed for small messages)?
  - Bandwidth (time per byte for large messages)?
  - Multiprocessor nodes?
- How fast do you need to run?



NAMD
Scalable Molecular Dynamics

Budget

- Figure out how much money you have to spend.
- Don’t spend money on problems you won’t have.
  - Design the system to just run your application.
- Never solve problems you can’t afford to have.
  - Fast network on 20 nodes or slower on 100?
- Don’t buy the hardware until…
  - The application is ported, tested, and debugged.
  - The science is ready to run.

Environment

- The cluster needs somewhere to live.
  - You won't want it in your office, not even a grad student's office.
- Cluster needs:
  - Space (keep the fire martial happy)
  - Power
  - Cooling

Environment: Space

- Rack or shelve systems to save space
  - 36” x 18” shelves (~$180) will hold 16 PCs with typical cases
    - Wheels are nice and don’t cost much more
    - Watch for tipping!
  - Multiprocessor systems may save space
  - Rack mount cases are smaller but expensive

Environment: Power

- Make sure you have enough power.
  - 1.3Ghz Athlon draws 1.6A at 110 Volts = 176 Watts
    - Newer systems draw more; measure for yourself!
  - Wall circuits typically supply about 20 Amps
    - Around 12 PCs @ 176W max (8-10 for safety)

Environment: Uninterruptable Power Systems

- 5kVA UPS ($3,000)
  - Will need to work out building power to them
  - Holds 24 PCs @176W (safely)
  - Larger/smaller UPS systems are available
  - May not need UPS for all systems, just root node

Environment: Cooling

- Building AC will only get you so far – large clusters require dedicated cooling.
- Make sure you have enough cooling.
  - One PC @176W puts out ~600 BTU of heat.
  - 1 ton of AC = 12,000 BTUs = ~3500 Watts
  - Can run ~50 PCs per ton of AC (30-40 safely)

Hardware

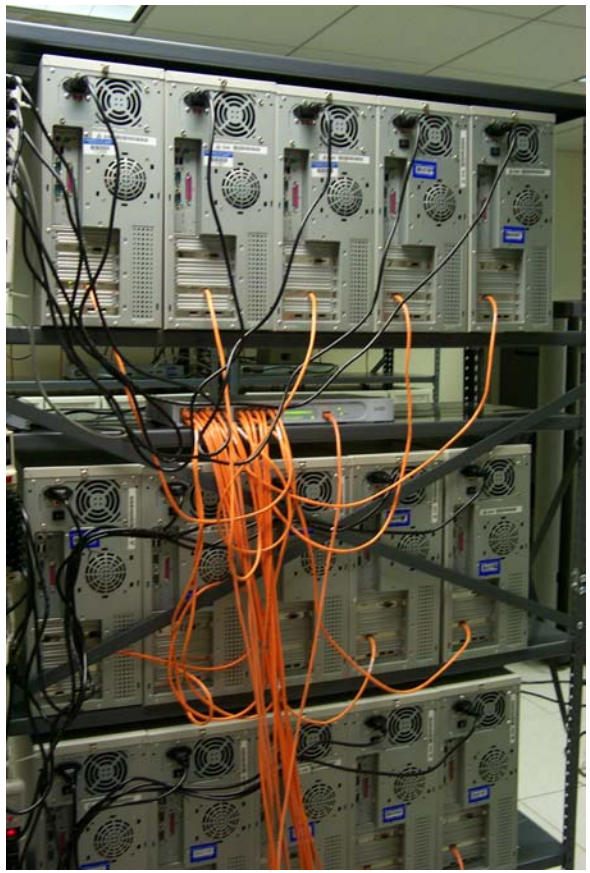
- Many important decisions to make
- Keep application performance, users, environment, local expertise, and budget in mind
- An exercise in systems integration, making many separate components work well as a unit
- A reliable but slightly slower cluster is better than a fast but non-functioning cluster

Hardware: Computers

- Benchmark a “demo” system first!
- Buy identical computers
- Can be recycled as desktops
  - CD-ROMs and hard drives may still be a good idea.
  - Don’t bother with a good video card; by the time you recycle them you’ll want something better anyway.

Hardware: Networking (1)

- Latency
- Bandwidth
- Bisection bandwidth of finished cluster
- SMP performance and compatibility?



Hardware: Networking (2)

- Three main options:
  - 100Mbps Ethernet – very cheap ($50/node), universally supported, good for low-bandwidth requirements.
  - Gigabit Ethernet – moderate ($200-300/node), well supported, fewer choices for good cards, cheap commodity switches only up to 24 ports.
  - Special interconnects:
    - Myrinet – very expensive ($2500/node), very low latency, logarithmic cost model for very large clusters.

Hardware: Gigabit Ethernet (1)

- The only choice for low-cost clusters up to 48 processors.
- 24-port switch allows:
  - 24 single nodes with 32-bit 33 MHz cards
  - 24 dual nodes with 64-bit 66 MHz cards

Hardware: Gigabit Ethernet (2)

- Jumbo frames:
  - Extend standard ethernet maximum transmit unit (MTU) from 1500 to 9000
  - More data per packet, fewer packets, lowers CPU load.
  - Requires managed switch to transmit packets.
  - All communicating nodes must use Jumbo frames, if enabled
  - Atypical usage patterns not as well optimized.

Hardware: Gigabit Ethernet (3)

- Sample prices (June 2003 from cdwg.com)
  - 24-port switches
    - D-Link DGS-1024T unmanaged: $1,655.41
    - HP Procurve 2724 unmanaged: $1,715.24
    - SMC TigerSwitch managed (w/ jumbo frames): $2,792.08
  - Network cards
    - Intel PRO/1000 MT Desktop (32-bit 33 MHz): $41.89
    - Intel PRO/1000 MT Server (64-bit 133 MHz): $121.14

Hardware: Other Components

- Filtered Power (Isobar, Data Shield, etc)
- Network Cables: buy good ones, you'll save debugging time later
- *If a cable is at all questionable, throw it away!*
- Power Cables
- Monitor
- Video/Keyboard Cables

System Software

- More choices: operating system, message passing libraries, numerical libraries, compilers, batch queueing, etc.
- Performance
- Stability
- System security
- Existing infrastructure considerations

System Software: Operating System (1)

- Clusters have special needs, use something appropriate for the application, hardware, and that is easily clusterable
- Security on a cluster can be nightmare if not planned for at the outset
- Any annoying management or reliability issues get hugely multiplied in a cluster environment

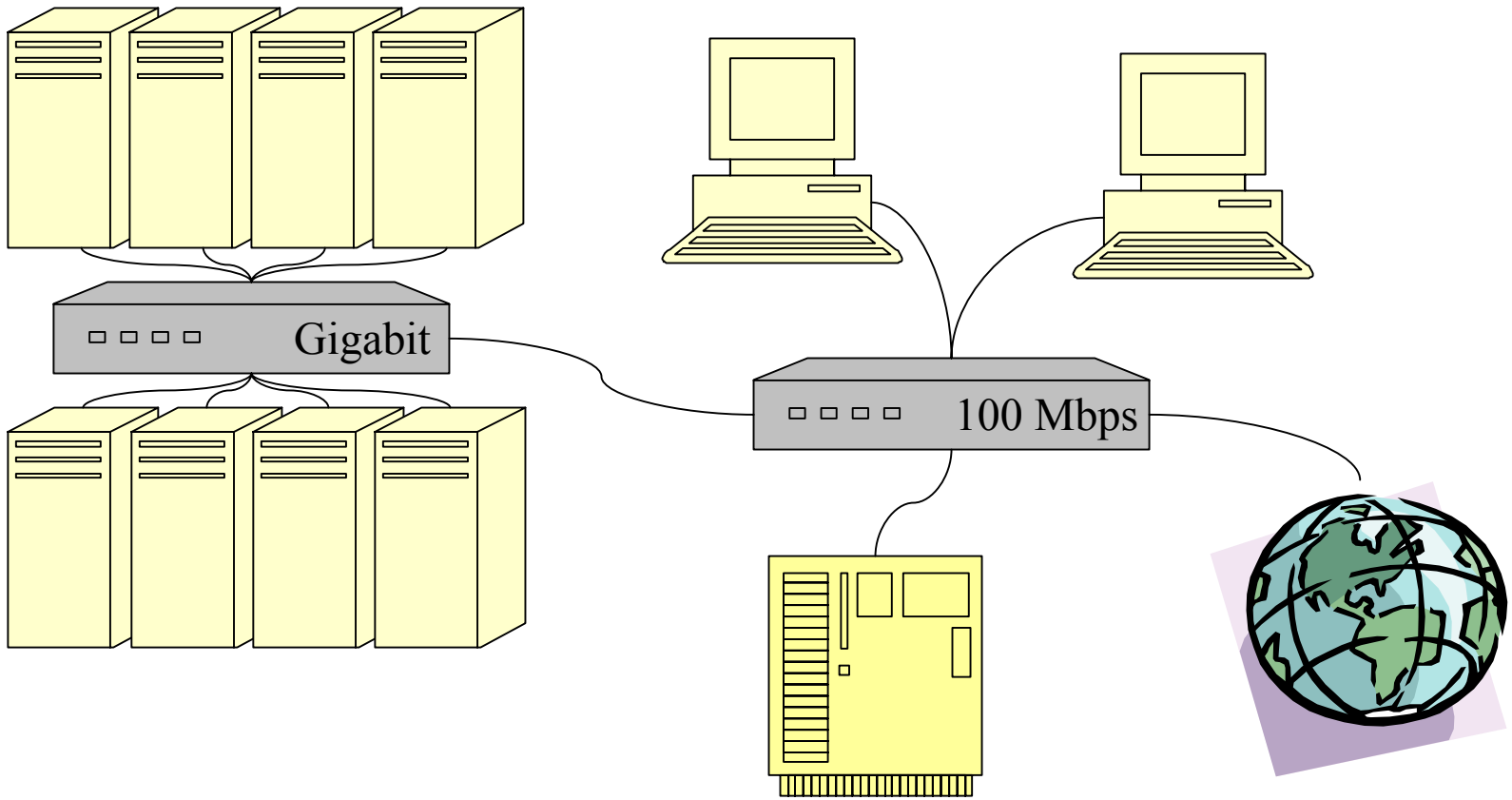
System Software: Operating System (2)

- SMP Nodes:
  - Does the kernel TCP stack scale?
  - Is the message passing system multithreaded?
  - Does the kernel scale for system calls made by your applications?
- Network Performance:
  - Optimized network drivers?
  - User-space message passing?
  - Eliminate unnecessary daemons, they destroy performance on large clusters (collective ops)

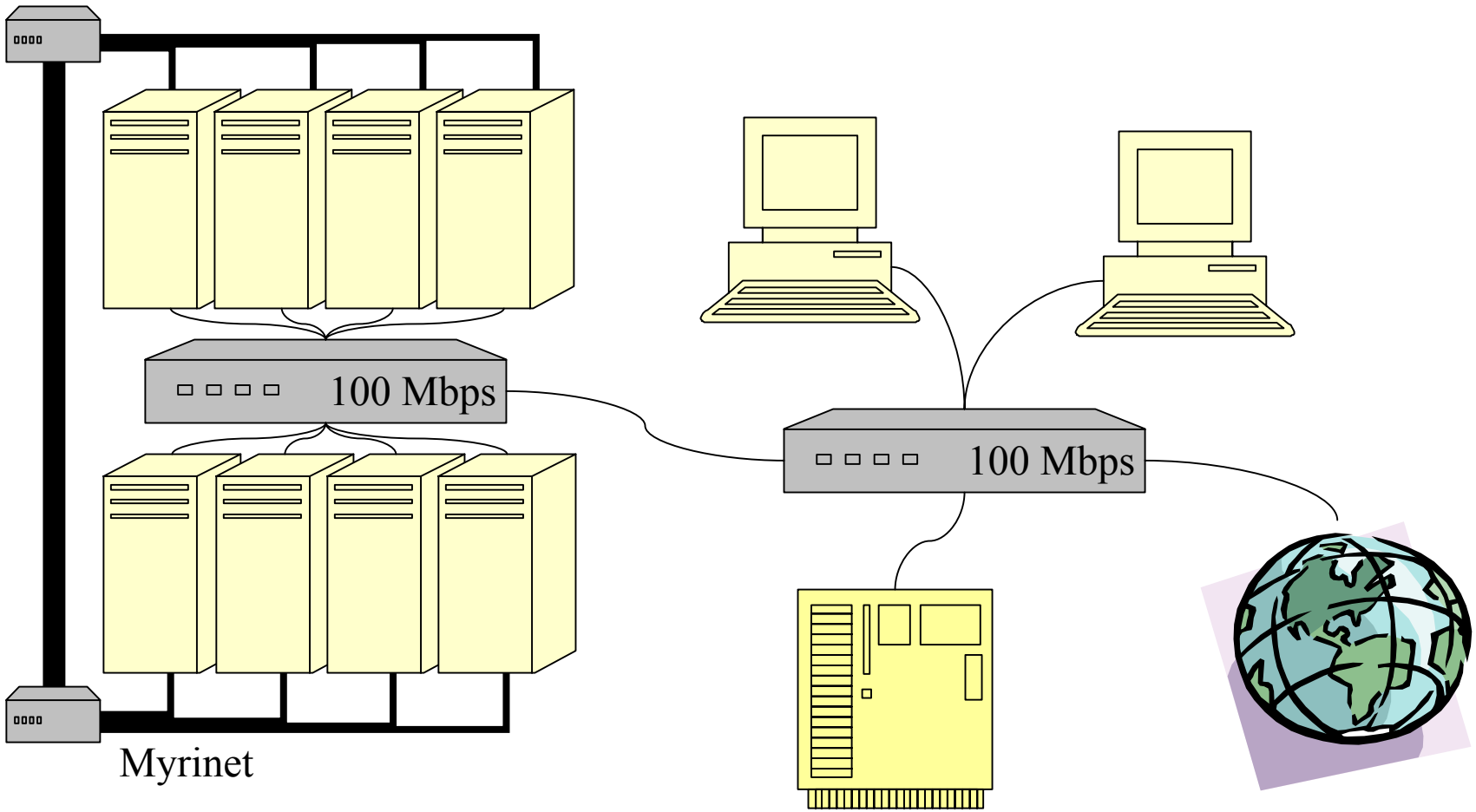
Software: Networking

- User-space message passing
  - Virtual interface architecture
  - Avoids per-message context switching between kernel mode and user mode, can reduce cache thrashing, etc.

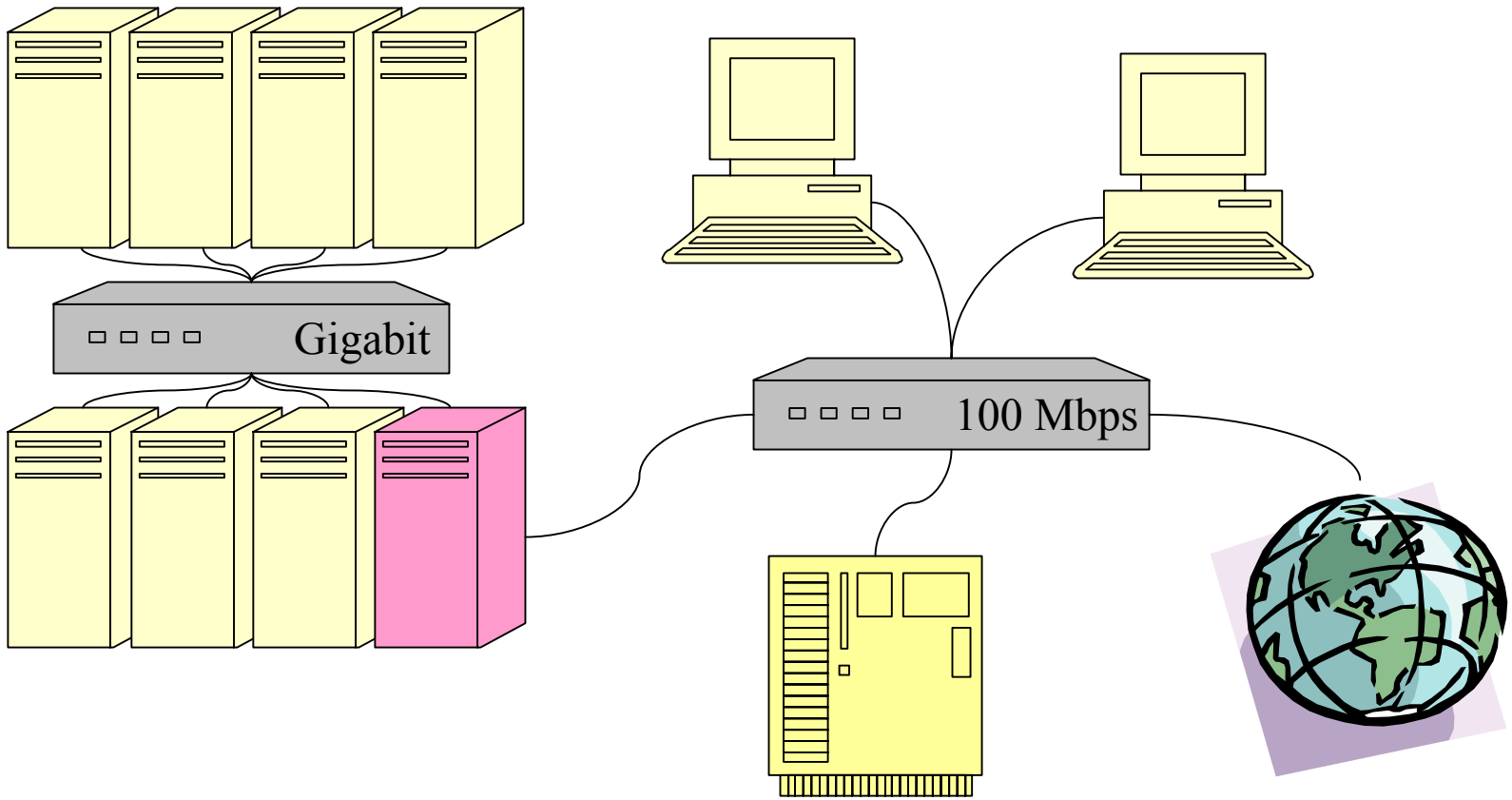
Network Architecture: Public



Network Architecture: Augmented



Network Architecture: Private



Scyld Beowulf / ClusterMatic

- Single front-end master node:
  - Fully operational normal Linux installation.
  - Bproc kernel patches incorporate slave nodes.
- Severely restricted slave nodes:
  - Minimum installation, downloaded at boot.
  - No daemons, users, logins, scripts, etc.
  - No access to NFS servers except for master.
  - Highly secure slave nodes as a result

System Software: Compilers

- No point in buying fast hardware just to run poor performing executables
- Good compilers might provide 50-150% performance improvement
- May be cheaper to buy a $2,500 compiler license than to buy more compute nodes
- Benchmark real application with compiler, get an eval compiler license if necessary

System Software: Message Passing Libraries

- Usually dictated by application code
- Choose something that will work well with hardware, OS, and application
- User-space message passing?
- MPI: industry standard, many implementations by many vendors, as well as several free implementations
- PVM: typically low performance avoid if possible
- Others: Charm++, BIP, Fast Messages

System Software: Numerical Libraries

- Can provide a huge performance boost over "Numerical Recipes" or in-house routines
- Typically hand-optimized for each platform
- When applications spend a large fraction of runtime in library code, it pays to buy a license for a highly tuned library
- Examples: BLAS, FFTW, Interval libraries

System Software: Batch Queueing

- Clusters, although cheaper than "big iron" are still expensive, so should be efficiently utilized
- The use of a batch queueing system can keep a cluster running jobs 24/7
- Things to consider:
  - Allocation of sub-clusters?
  - 1-CPU jobs on SMP nodes?
- Examples: Sun Grid Engine, PBS, Load Leveler

2001 Case Study (1)

- Users:
  - Many researchers with MD simulations
  - Need to supplement time on supercomputers
- Application: NAMD
  - Not memory-bound, runs well on IA32
  - Scales to 32 CPUs with 100Mbps Ethernet
  - Scales to 100+ CPUs with Myrinet

2001 Case Study (2)

- Budget:
  - Initially $20K, eventually grew to $100K
- Environment:
  - Full machine room, slowly clear out space
  - Under-utilized 12kVA UPS, staff electrician
  - 3 ton chilled water air conditioner (Liebert)

2001 Case Study (3)

- Hardware:
  - 1.3 GHz AMD Athon CPUs (fastest available)
  - Fast CL2 SDRAM, but not DDR
  - Switched 100Mbps Ethernet, Intel EEPro cards
- System Software:
  - Scyld clusters of 32 machines, 1 job/cluster
  - Existing DQS, NIS, NFS, etc. infrastructure

2003 Case Study (1)

- What changed since 2001:
  - 50% increase in processor speed
  - 50% increase in NAMD serial performance
  - Improved stability of SMP Linux kernel
  - Inexpensive gigabit cards and 24-port switches
  - Nearly full machine room and power supply
  - Popularity of compact form factor cases
  - Emphasis on interactive MD of small systems

2003 Case Study (2)

- Budget:
  - Initially $65K, eventually grew to ~$100K
- Environment:
  - Same general machine room environment
  - Additional space available in server room
    - Retiring obsolete HP compute servers
  - Old clusters are still useful, not obsolete
    - Need to be more space-conscious

2003 Case Study (3)

- Option #1:
  - Single processor, small form factor nodes
  - Hyperthreaded Pentium 4 processors
  - 32-bit 33 MHz gigabit network cards
  - 24 port gigabit switch (24-processor clusters)
- Problems:
  - No ECC (error correcting) memory
  - Limited network performance
  - Too small for next-generation video cards

2003 Case Study (4)

- Final decision:
  - Dual Athlon MP 2600+ in normal cases
    - No hard drive or CD-ROM in slaves
    - 64-bit 66 MHz gigabit network cards
  - 24 port gigabit switch (48-proc clusters)
  - ClusterMatic OS
    - Boot slaves from floppies, then network
- Benefits:
  - Server class hardware w/ ECC memory
  - Maximum processor count
    - Use all processors for large simulations
  - Maximum network bandwidth
    - Better scaling for 24-processor simulations

2003 Case Study (5)

- Recycled 36 old (2001) nodes as desktops
  - Added video cards, hard drive, extra RAM
    - Cost: ~$300/machine
- Remaining old nodes move to server room
  - 4x 16-node clusters
  - Used for smaller simulations (hopefully…)