Linux Clusters for High-Performance Computing: An Introduction

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NIH Resource for Macromolecular Modeling and Bioinformatics
http://www.ks.uiuc.edu/

Beckman Institute, UIUC
Outline

• Why and why not clusters?
• Consider your…
  – Users
  – Application
  – Budget
  – Environment
  – Hardware
  – System Software
HPC vs High-Availability

• There are two major types of Linux clusters:
  – High-Performance Computing
    • Multiple computers running a single job for increased performance
  – High-Availability
    • Multiple computers running the same job for increased reliability
  – We will be talking about the former!
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
• Single failure does not take down entire facility
• 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?

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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 in your 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 from C-Stores)
    - 16 typical PC-style cases
    - 12 full-size PC cases
    - Wheels are nice and don’t cost much more
    - Watch for tipping!
  - Multiprocessor systems save space
  - Rack mount cases are smaller but expensive
Environment: Power

• Make sure you have enough power.
  – Kill-A-Watt
    • $30 at ThinkGeek
  – 1.3Ghz Athlon draws 183 VA at full load
    • Newer systems draw more; measure for yourself!
    • More efficient power supplies help
  – Wall circuits typically supply about 20 Amps
    • Around 12 PCs @ 183VA max (8-10 for safety)
Environment: Power Factor

- Always test your power under load
- More efficient power supplies do help!

<table>
<thead>
<tr>
<th>System</th>
<th>Current</th>
<th>Power</th>
<th>VA</th>
<th>PF</th>
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Environment: Uninterruptable Power Systems

- 5kVA UPS ($3,000)
  - Holds 24 PCs @183VA (safely)
  - Rackmount or stand-alone
  - Will need to work out building power to them
  - 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
- Make sure you have enough cooling.
  - One PC @183VA puts out ~600 BTU of heat.
  - 1 ton of AC = 12,000 BTUs = ~3500 Watts
  - Can run ~20 CPUs per ton of AC
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)

- Two main options:
  - Gigabit Ethernet – cheap ($100-200/node), universally supported and tested, cheap commodity switches up to 48 ports.
    - 24-port switches seem the best bang-for-buck
  - Special interconnects:
    - Myrinet – very expensive ($thousands per node), very low latency, logarithmic cost model for very large clusters.
    - Infiniband – similar, less common, not as well supported.
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, reduced overhead, lower processor utilization.
  – Requires managed switch to transmit packets.
  – Incompatible with non-jumbo traffic.
  – Probably not worth the hassle.
Hardware: Gigabit Ethernet (3)

- Sample prices (from cdwg.com)
  - 24-port switches
    - SMC EZSwitch SMCGS24 unmanaged $374.00
    - 3Com Baseline 2824 unmanaged $429.59
    - ProCurve 2724 managed $1,202.51
  - 48-port switches
    - SMC TigerSwitch SMC6752AL2 unmanaged $656.00
    - 3Com SuperStack 3848 managed $3,185.50
    - ProCurve 2848 managed $3,301.29
  - Network Cards
    - Most are built-in with current architectures
    - Can buy new cards for $25-60
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

- “Linux” is just a starting point.
  - Operating system,
  - Libraries - message passing, numerical
  - Compilers
  - Queuing Systems
- 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 kernel TCP stack scale?
  – Is message passing system multithreaded?
  – Does kernel scale for system calls made by intended set of 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

[Diagram showing network architecture with Gigabit and Myrinet connections.]
Network Architecture: Private
Scyld Beowulf / Clustermatic

• Single front-end master node:
  – Fully operational normal Linux installation.
  – Bproc 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
Oscar/ROCKS

• Each node is a full Linux install
  – Offers access to a file system.
  – Software tools help manage these large numbers of machines.
  – Still more complicated than only maintaining one “master” node.
  – Better suited for running multiple jobs on a single cluster, vs one job on the whole cluster.
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
- 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