An introduction to clusters and high performance computing

Andreas Engelbredt Dalsgaard

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What is a Cluster Anyway

- It is NOT something that does any of the following:
 - Use magic
 - Automatically make your program run faster
 - Provide a single virtual OS image of all resources
 - Always makes your software faster
- Then what is it?

Terminology

Cluster

- A set of closely connected computers
- Usually homogeneous
- Connectivity: GB Ethernet, Infiniband
- They usually run some form of *nix
- High Performance Computing (HPC)¹
 - "above a teraflop ... floating-point operations per second"
 - "near the currently highest operational rate for computers"
 - "use custom-made components"
 - Usually use Infiniband as connectivity

¹http://searchenterpriselinux.techtarget.com/definition/high-performancecomputing

Terminology

• Grid Computing

- Virtual Supercomputer
 - Composed of several clusters
- Distributed within organisation or globally
- High-energy Physics E.g. CERN
- Cloud Computing
 - Software as a service
 - On demand resources
 - Cloud storage
 - Commodity hardware components
 - Usually virtual access to resources

So what is a cluster used for and by whom

Purpose

- To solve problems faster than on a single machine
- To solve problems that cannot be solved on a single machine
- Performance is everything
 - $\bullet~$ Users want the last 10%
 - Think about how the cache is used
 - Think about memory organisation
 - Consider communication overhead
- Users
 - Scientific researchers
 - Engineers
 - Academic institutions
 - Government agencies E.g. military

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What does it look like





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Cluster Overview



Compute nodes

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Cluster Overview(2)



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How are clusters used

- A LRMS: Local Resource Management System
- Also called batch systems
 - Tasks are split into jobs
 - Jobs are executed by the batch system
 - Order of execution depend on scheduler
 - A job gets a set of nodes/CPUs (exclusively)
- How are most LRMS used
 - Make a job description
 - Submit it to the LRMS
 - The LRMS will decide when to run the job
- Torque/PBS, SLURM, LoadLeveler, Condor
 - Some are open source, some are proprietary

What Runs a Cluster

- OpenSSH is used intensively
- Admin node
 - A LRMS server
 - OpenLdap server(user directory service)
 - Application file server (/pack)
 - $\bullet\,$ Compilers, Gnu and Intel c,c++ and fortran
 - Libraries, E.g. openmpi
 - Firewall
 - Dhcp, tftp, email, mailinglist, monitoring, monitoring and monitoring
- Frontend node
 - LRMS client
 - Mount application filesystem
 - Firewall

What Runs a Cluster(2)

Compute nodes

- LRMS client
- Mount application filesystem
- /scratch partition
- Everything else is read only
- Storage
 - User data
 - Automounted on all nodes
 - Battery backed RAM, SSD, disks
 - No guaranties, use backup

A Little About Hardware

- For common jobs
- 84 IBM blade computers in 6 bladecenters.(killing1-84) 672 cores, 1,3 Tb
 - With two Xeon E5345 quad core 2.33 GHz CPUs, 16 GB RAM, a 53 GB scratch partition, Gbit ethernet and Infiniband interconnect.
- 24 HP computers (lion1-24) 288 cores, 3,5 Tb RAM
 - With two Xeon X5650 six core 2.66 GHz CPUs, 145 Gb RAM, a 53GB scratch partition, Gbit ethernet and Infiniband interconnect.
- Multi-core CPUs is the norm
- This is why this course is important

A Little About Hardware(2)

- Test jobs
- 5 SUN computers (sister1-5)
 - With a Xeon X3220 quad core 2.40GHz CPU, 8GB RAM, a 66 GB scratch partition, Gbit ethernet interconnect
- Interactive jobs
- 4 SUN computers (tiger1-4)
 - With two Xeon X5570 quad core 2.93GHz CPU with hyperthreading(HT) enabled, 68GB RAM, Gbit ethernet interconnect.
- GPU jobs
- 10 Colfax computers (cub1-10)
 - With two Xeon X5570 quad core 2.93GHz CPU with HT enabled, 48GB RAM, Gbit ethernet and Infiniband interconnect, 3xTesla C2070 or Tesla C1050(soon GTX 580)

A Little About Hardware(3)

- Trends
 - GPU used for calculations
 - Massive parallelism
 - 10 gbit ethernet
 - This is why this course is important!



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What people use a cluster for

- Scout
 - Analysis of integrated circuits
 - Continues systems
 - E.g. Noise Analysis in integrated circuits
 - Mobile communication
- Fyrkat
 - Continues systems
 - Simulate an antennas behaviour
 - Antenna near field simulation using Finite-difference time-domain method
 - Acoustic simulations
 - Grid computing



PART 2

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What I do

- Development
 - Resources trading project
 - Irmsurgen
 - Scripting
 - MultiAdm
 - Torque Power Management
- User management
 - More than 100 users
 - Many new user request
 - Verifying need for resources
 - Automate as much as possible

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What I do(2)

- Mails back and forth
- Run adduser script
- Add user to groups
- Send sms with password
- Add user to scheduling groups
- Add user to /etc/aliases
- Add user to mailinglist
- Add user to shared google doc document
- Send mail with link to wiki

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What I do(3)

- Automate as much as possible
- Standardise as much as possible
- Make tools to assist in common tasks



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Why don't people use clusters

- Getting parallel program to perform well is immensely difficult
 - But challenges are fun!
 - The need for skilled multi-core programmers is raising
 - Apps using multi-core is becoming the norm
 - Not just in clusters
 - Also in desktops and smart phones

How people use clusters

Parameter sweeps

- Serial code run in parallel
- Distributed jobs
 - Programs are made explicitly parallel
 - This is hard work
 - OpenMP, Pthreads, MPI
 - MPI is the hard part
 - Usually it is more of a rewrite than a port
 - Many MPI solutions for different interconnect types

Considerations when using a cluster

• Task generation

- Static task generation
 - Matrix-multiplication
 - Parameter sweeps
 - State-space exploration E.g. 15-puzzle
- Dynamic task generation
 - Ray tracing
 - State-space exploration E.g. 15-puzzle
- Task size
 - Uniform versus non-uniform
- Size of Data Associated with Tasks

How to get an account

https://fyrkat.grid.aau.dk/useraccount

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PART 3

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Fyrkat

- ssh fyrkat.grid.aau.dk
 - Pretty easy to get access to Talk to your supervisor and use:
 - https://fyrkat.grid.aau.dk/useraccount



Scout

- ssh scout.es.aau.dk
 - Hard to get access to Talk to Torben Larsen or Josva Kleist







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Demonstration