M-grid Experiences Using ARC

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Slide 1(15)

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Contents

- Introduction to the Finnish Material Sciences Grid (M-grid)
- ARC installation challenges
- Resource sharing policy in M-grid
- Grid experiences
- Plans how to serve users better
- Security challenges

The Material Sciences Grid (M-grid)

- Goal: Throughput computing capacity mainly for the needs of physics and chemistry researchers
- Joint project between seven Finnish universities, Helsinki Institute of Physics and CSC
 - Partners mainly laboratories and departments, not university IT centers
- Jointly funded by the Academy of Finland and the participating universities
 - Funding application Nov 2003, deployment Oct 2004
- First large initiative to put Grid middleware into production use in Finland
- Platform: Linux based PC clusters





Hardware and CPU Distribution

• Ten clusters of varying size

- Dual AMD Opteron computing nodes (HP DL145): 1.8-2.2 GHz, 2-8 GB RAM, 80-320 GB local disk
- Front end (HP DL585): 1-2 TB shared disk
- Network 2 x Gbit Ethernet + remote administration network
- Total 778 (CSC) + 434 (universities) CPUs in the computing nodes, theoretical total computing power 5 TFlop/s.



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Operating System and Grid Middleware

NPACI Rocks Cluster Distribution

- Cluster oriented Linux distribution, main developer San Diego Supercomputing Center, U.S.A.
- Based on Red Hat Enterprise Linux, but not a Red Hat product
- http://www.rocksclusters.org
- N1 Grid Engine batch queue system
 - Local resource management in each cluster
- NorduGrid ARC Grid middleware
 - Enables shared use of the systems, the middleware selects a free resource automatically
 - http://www.nordugrid.org









Slide 5(15)

System Administration in M-grid

- Tasks divided between CSC and site administrators
- CSC administrators:
 - Maintain (remotely) the operating system, batch queue system, Grid middleware and certain libraries for all sites except Oulu
 - Separate small test cluster for testing new software releases
- Site administrators
 - Local applications and libraries, system monitoring, user support
- Regular meetings of administrators every two months, common mailing list

Grid Use and Resource Sharing

- Policy: Jobs can be submitted both to the local queue and through the grid interface
 - Priority: local jobs 80%, grid jobs 20%
- Goal is to minimize waste of resources: empty nodes are always available for use (dynamical sharing)



Installation Timeline

- Nov 2004: Systems installed and ready for local use
- Aug 2005: ARC installation, initial successful tests
- Sep 2005: ARC tutorial at CSC
- Nov 2005: New cluster sepeli connected, access opened to all CSC customers, improved ARC support for the local batch queue system
- Plans for 1H/2006: A second tutorial, configuring MPI environments for ARC, adding runtime environments, improving operational practises

Challenges Installing ARC

• 64 bit environment

- ARC was based on Globus 2.4 which didn't support a 64 bit environment
- Installed using the Globus 4.0 source distribution and ARC source rpms
- N1 Grid Engine
 - ARC support for the N1 Grid Engine (previously Sun Grid Engine) batch queueing system was buggy
 - Fixing bugs and adding a few improvements before deployment took time
- Development version of ARC required

Grid Experiences

Currently few Grid users

- Most users are still happily submitting jobs directly to the local batch queue
- Grid environment must be better than the existing one, otherwise nobody will use it!
 - The environment is still in development: MPI environments and other runtime environments need to be added
 - Long queue in the local cluster and empty resources on the Grid may be a good enough incentive
- Collaboration model in system administration has been successful: Grid projects always have other aspects than just the technology

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Obstacles to Grid Adoption

• Need to request a certificate

- Not a very big problem: we have many more certificates requested than actual active users
- Different job description syntax compared to the local batch queue system
- Need to list the input files in the job description
 - There is no obvious way to specify a whole directory
- Getting the groups to make their software available as runtime environments
- Higher failure rate and less determined execution times require job management tools



Plans to Serve Users Better

• Concentrate first on a few selected popular applications

- Create runtime environments with detailed usage instructions and examples
- Validate with real world test cases including parallel MPI runs
- More tutorials and articles
 - Migration guide from local jobs to grid jobs
- Provide job management tools and examples
- Present M-grid more clearly on CSC web pages as one of the available computing platforms
- Improve system level monitoring to detect failures



Grid Collaboration and Security



Security Challenges in the Grid

• Grid goes beyond organizational borders

=> Mutual trust is a key requirement!

 Potential to do widespread damage with a compromised account

=> Need to consider operational security when opening access to large user groups

- Getting all the relevant parties involved
 - Computing centers, university IT departments, local admins, CERTs and also users
 - International collaboration
- Data protection and privacy

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More information

- M-grid homepage: http://www.csc.fi/proj/mgrid/
- NorduGrid homepage: http://www.nordugrid.org
- Contact people:
 - Arto Teräs <arto.teras@csc.fi>
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- Thank you! Questions?