Workflow and Parallelism Session Summary

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Outline

- **Reduce latency!**
  - Tools, optimization, workflow, parallelism

Francesco Giacomini	The gLite Workload Management System	Tools
Cécile Germain-Renaud	Towards a statistical model of EGEE load	Optimization
Jeremy Coles	Extension of DIRAC to enable distributed computing using Windows resources	Parallelism
Maximilian Berger	Optimizing a Grid workflow for the EGEE infrastructure: The case of Wien2k	Workflow
Lim Mei Kuan	Execution Time Prediction of Imperative Paradigm Tasks for Grid Scheduling Optimization	Optimization
Branislav Simo	Interactive Workflow Management in int.eu.grid	Tools
Boro Jakimovski	GRid-aware Optimal data Warehouse design (GROW)	Workflow
Mariusz Sterzel	Parallel Execution of Chemical Software on EGEE Grid	Parallelism
Kiril Dichev	MPI Support on the Grid	Tools
Fabio Bellavia	Non-parametric parallel GRID Harris-affine detector	Parallelism

Tools

- **gLite (Francesco Giacomini)**

- **Collections and parametric jobs**
  - Bulk submission, matchmaking
- **MPI Support**
  - “Normal” job with multiple CPUs
  - More flexibility for users and system administrators
- **Directed Acyclic Graph (DAG)**
  - Allows collection of jobs with dependencies
  - Access to job output of previous stages
- **Workflow engines**
  - Web service interface! Using taverna, moteur, … simplified!
  - Want interoperability with different languages, engines

Tools

- **MPI support (Kiril Dichev)**
  - mpi-start:
    - § backbone of MPI support in EGEE
    - § modular support for MPI flavors, batch systems, tools
  - Marmot: MPI checking and debugging tool
  - PACX-MPI
    - § cross-site MPI support
    - § requires cross-broker and modified CE

- **Interactive workflow (Branislav Simos)**
  - Adapt analysis interactively based on partial results
  - Mix of MPI, agent scheduling, interactive access

Optimization

- **Grid Observatory (Cécile Germain-Renaud)**
  - Understand grid use via L&B and Real Time Monitor information
  - Attempt to model load, bursts, scheduling, etc.
  - Useful for alarms, improving decision making, etc.
  - Improve contact between comp. scientists and prod. grids

- **Job duration prediction (Lim Mei Kuan)**
  - Improve estimates of job duration to improve efficiency
  - Static analysis of R! scripts to predict running time
  - On 60 R! scripts, prototype successfully predicted run times
  - Benefits to grid scheduling if extended

Parallelism/Workflow

- **DIRAC: Agent scheduling (Jeremy Coles)**
  - Mature implementation of agent scheduling system
  - Windows port to increase available resources
  - Proof of multi-platform support, but requires significant effort

- **Comp. Chem. software (Mariusz Sterzel)**
  - Gaussian, Turbomole, … exist in seq. and parallel versions.
  - Important assumptions: OpenMP, nodes have same topology.
  - Solutions can always be found with cooperation.
  - Need more flexible specification of MPI resource constraints.
  - Longer waits for OpenMP than for normal MPI.

Workflow/Parallelism

- **Image feature extraction (Fabio Bellavia)**
  - Use “farm” allocated via MPI.
  - Use clever, adaptive algorithm to split the work dynamically.
- **GROW (Boro Jakimovski)**
  - Genetic algorithms used to optimize database design.
  - Views and indexes are the genetic components.
  - Expensive if large number of islands, epochs, … used.
  - Uses workflow/parallelism for faster results.
- **Wien2k (Maximilian Berger)**
  - Control and data dependencies may be different.
  - Latencies for both are important.
  - Efficient grid workflow may be very different from efficient application workflow.

Conclusions

- **All scientific analyses are complex!**
  - Multiple codes with data or execution dependencies
  - Large numbers of jobs
  - Branch points within analysis

- **Nonetheless, scientists want their results ASAP.**
  - Reduce latencies via optimization, workflow, parallelism
  - Improved middleware functionality, capturing common patterns
  - Better understanding of grid and its use

- **Grid technology is maturing.**
  - Scientists asking for complete analysis to run on the grid.
  - Asking for differing qualities of service.