Demo and Poster Session

Erwin Laure
KTH
10 Demos

- Laboratory for Virtual Experimentation in Virology and Bioinformatics
  ACC CYFRONET AGH
- Grid Development Tools
  University of Marburg
- The Planck Process Coordinator workflow engine on the Grid
  Leibniz Supercomputer Centre
- Support for cooperative experiments in VL-e: from scientific workflows to knowledge sharing
  University of Amsterdam
- Interactive Simulations on the Grid
  Leibniz Supercomputer Centre
- UNICORE 6 - A European Grid Technology
  Juelich Supercomputing Centre
- Scientific Workflows in the UNICORE Rich Client
  Juelich Supercomputing Centre
- Jawari - A Grid Benchmarking and Monitoring Service for Grid Assessment
  Fraunhofer Institut ITWM
- DORII - Deployment of Remote Instrumentation Infrastructure
  Ludwig-Maximilians-Universität München
- The C3-Grid Project: Seamless Volume-optimized Access to Federated Climate Data
  Technische Universität Dortmund
ViroLab virtual laboratory

- Distributed and collaborative e-research platform
- Integrates various data sources and computational resources
- Enables to build and execute experiments
- Facilitates knowledge sharing
- Dedicated to support virologists, epidemiologists and clinicians, but is also applicable in other domains

*In silico experiment*

- Mirrors an experiment in real world
- Defines input data and operations that need to be performed to obtain result
- Include experiment logic
- Expressed as a Ruby script
Scientific aspects and solution

Scientific issues

– Heterogeneous computational and data resources
– Expressiveness vs simplicity
– Provenance of results and result reuse
– Collaboration (share data, knowledge and resources but preserve security)

```
require 'cyfronet/gridspace/goi/core/g_obj'
drs = GObj.create('org.virolab.DrugRankingSystem2')
mut = 'P1M I2L S3T P4Q E6G V10N K11F'.split(' ')
ranking = drs.drs('ANRS', 'rt', mut)
puts ranking
```

Applications

– Virtual Patient Experiment Pilot ViroLab application
– Early Protein Folding
– Computational chemistry apps
– Data mining with WEKA

Links to remember

Grid Development Tools
http://mage.uni-marburg.de

- Grid Service Development
- Certificate Management
- Grid Browser
- Workflow Orchestration
- Workflow Execution
- Workflow Monitoring

Kay Dörnemann, Tim Dörnemann, Ernst Juhnke
and Prof. Dr. Bernd Freisleben
Kay Dörnemann
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Full-time research assistant
Research interests:
• Grid Computing in combination with P2P-Computing
• Grid Tools, responsible: Grid Service Development, Certificate Management, Grid Management

Tim Dörnemann
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Full-time research and teaching assistant
Research interests:
• BPEL-based Workflow Modeling and Execution in Grid and Cloud Environments

Ernst Juhnke
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Full-time research assistant
Research interests:
• BPEL-based Workflow Modeling and Execution in Grid and Cloud Environments

Staff Developers:
• Kay Dörnemann
• Tim Dörnemann
• Ernst Juhnke
• Roland Schwarzkopf
• Thomas Friese
• Matthew Smith
• Steffen Heinzl
• Markus Mathes
• Dominik Seiler

Students
• Marian Harbach
• Fabian Schwarzer
• Stanimir Dimitrov
• Sebastian Kirch
Today’s Demonstration

- Tool Support for the Entire Grid Software Development and Execution Lifecycle

- Live demonstration of selected tools
  - Grid Service Development (Service Generator)
  - Workflow Orchestration
  - Workflow Execution
  - Workflow Monitoring
  - Certificate Management
  - Grid Browser

Visual Grid Service Orchestration (BPEL) and BPEL Workflow Engine
The Planck Process Coordinator workflow engine on the Grid

LRZ: Arthur Carlson, Ilya Saverchenko, Jarno Laitinen, ...
MPA (ProC): Torsten Enßlin, Wolfgang Hovest, Thomas Riller, ...
AEI (GAT): Alexander Beck-Ratzka, ...
each point in parameter space configures a simulation workflow

each workflow is sent to a different computing host on the Grid

ProC & GAT hide Grid complexity from scientist
Cooperative experiments in VL-e: from scientific workflows to knowledge sharing

S.Koulouzis(1) Z.Zhao (1) V. Guevara(1) A. Wibisono(1) A. Belloum(1) M. Bubak(1,2) B. Hertzberger(1)

(1) Informatics Institute, University of Amsterdam, The Netherlands
(2) Institute of Computer Science
Complex Scientific experiments model

Problem investigation:
- Look for relevant problems
- Browse available tools
- Define the goal
- Decompose into steps

Experiment Prototyping:
- Design experiment workflows
- Develop necessary components

Results Publication:
- Annotate data
- Publish data

Shared repositories

Experiment execution:
- Execute experiment processes
- Control the execution
- Collect and analysis data
Tools to support Cooperative experiments in VL-e

• Virtual resource Browser
  http://staff.science.uva.nl/~ptdeboer/vl-

• WSRF Grid-enabled workflow system
  http://staff.science.uva.nl/~gvlam/wsvlam/

• A WfBus for interoperability of scientific workflows.
  http://staff.science.uva.nl/~zhiming/workflowbu/

• Hybrid-bAseed Match-Maker for Resources
From myexperiment to the Grid

SigWin-detector: is a grid-enabled workflow application that takes a sequence of numbers and a series of window sizes as input and detects all significant windows for each window size using a moving median false discovery rate (mmFDR) procedure.

A significant window is a window in the input sequence for which the median value is significantly higher than expected, if assumed that the ordering of the numbers in the input sequence is random.

The results of a SigWin-detector analysis are summarized in a graph called SigWin-map. In the special case that the input sequence is a transcriptome map, the significant windows are called RIDGES and the output graph is called a RIDGEOGRAM.

SigWin-detector runs under the WS-VLAM workflow management system.

DNA curvature of the Escherichia Coli chromosome

WS-VLAM composer

Human transcriptome map

discovered RIDGE

myexperiment web site

More details: http://staff.science.uva.nl/~inda/SigWin-detector.html
DEMO: Interactive Simulations on the GRID

Dr. Helmut Satzger
Dr. Ferdinand Jamitzky
Remote Visualisation:
- Connect to remote server
- Utilise remote CPU power
- Utilise remote GPU power
  (only send screenshots to client)
Example: Interactive Simulations

- **HLRB II**
  - Massive Parallel Simulation
  - NAMD

- **RVS1**
  - Visualisation
  - VMD

- Client Display
  - `vglrun`

- 1,000,000 atoms
- 2000 cores compute
- 20 iterations/second

- Bandwidths:
  - ~1 GByte/s
  - ~800 KByte/s
UNICORE 6
A European Grid Technology

http://www.unicore.eu

Jason Milad Daivandy
j.daivandy@fz-juelich.de

Jülich Supercomputing Centre (JSC)
A few facts

- **UNiform Interface to COmputing Resources**
  - seamless, secure, and intuitive Grid middleware

- In continuous development since 2002 in several EU projects

- Open Source community development since Summer 2004
  - BSD license
  - hosted on SourceForge

http://www.unicore.eu
UNICORE 6

Guiding Principles, Implementation Strategies

- **Standards-based**: OGSA-conform, WS-RF 1.2 compliant
- Open, extensible **Service-Oriented Architecture** (SOA)
- Mature **Security**: X.509, proxy and VO support
- Tightly integrated **workflow** support, highly extensible by different workflow languages and engines
- **Application integration** mechanisms on the client, services and resource level
- Variety of **clients**: graphical, command-line, API, portal, etc.
- Quick and **simple installation** and configuration
- Support for many operating and batch systems
- Implemented in **Java** to achieve platform-independence

http://www.unicore.eu
UNICORE Rich Client (URC)
UCC – Commandline Client

>ucc -h
UCC version 1.2-SNAPSHOT
Usage: ucc <command> [OPTIONS] <args>
The following commands are available:
Data management:
   ls               - list a storage
   copy-file-status - check status of a copy-file
   get-file         - get remote files
   find             - find files on storages
   resolve          - resolve remote location
   copy-file        - copy remote files
   c9m-get-file     - get remote files
   put-file         - puts a local file to a remote server
General:
   connect          - connect to UNICORE
   list-applications - lists applications on target systems
   list-jobs        - list your jobs
   list-sites       - list remote sites
   c9m-system-info  - Checks the availability of services.
Job execution:
   run              - run a job through UNICORE &
   get-status       - get job status
   abort-job        - abort a job
   batch            - run ucc on a set of files
   get-output       - get output files
Other:
   shell            - Starts an interactive UCC session
   loadtest         - load tests services
   issue-delegation - Allows to issue a trust delegation assertion
   warf             - perform a WSRF operation
   run-groovy       - run a Groovy script
Workflow:
   c9m-submit       - submit a workflow to Chemomentum
   c9m-trace        - trace info on a workflow in Chemomentum
   c9m-control      - control a workflow in Chemomentum
   c9m-workflow-info - lists info on workflows in Chemomentum
Enter 'ucc <command> -h' for help on a particular command.
BCF (bio concentration factor) prediction predicts the concentration of chemical compounds in organic tissue.
UNICORE in use – some examples

- Supercomputing
  - DEISA (EU)
  - Clinical Supercomputing (USA)
  - SKIF-GRID (Russia, Belarus)
- National Grids (Germany)
  - D-Grid
  - AeroGrid
  - BIS-Grid
- Commercial
  - T-Systems SfR
  - 52° North

http://www.unicore.eu
UNICORE

software, source code, documentation, tutorials, mailing lists, community links, and more:

http://www.unicore.eu
Goal
Support for Quality of Service Assessment and Assurance in Grids

Components
- Benchmarking and Monitoring Service
- Performance Prediction Tools

Characteristics
- Open Source
- Free of Charge
- Extensible
- Multiplatform
- Focused on Grid Services
- In production for 3 years
- Simple to use
- Mimics an End-user
How it works

User

Software

Web Portal
Command Line Tools
Web Service
Portlets

Web Service

Notifications

Web Service

Scorer

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Repository

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Deployment of Remote Instrumentation Infrastructure
Remote Instrumentation Infrastructure

**Applications**: Oceanographic-, Earthquake-, Experimental-Science, Coastal-Observation

**Middleware**: adding Instrument Element support, basing on gLite, User/Developer support: VCR and g-Eclipse

**Resources**: Gilders, Floaters, Earthquake-Sensors, Cameras, Synchrotron, CEs, SEs, ...

**Network**: GEANT, Internet, Iridium, ...
The C3-Grid Project
Seamless Volume-optimized Access to Federated Climate Data

B. Fritzsch, S. Kindermann, A. Papaspyrou, and the C3-Team
Grid Computing in Climate Research

• Earth System Science Applications
  – short term weather forecast
  – subsystem modelling
  – stormtrack analysis

• Current Situation
  – no coherent working environment
  – manual staging and transportation of relevant data
  – problem of heterogeneous resources, distributed data and different access policies

• Identified requirements for C3Grid
  – fairly typical Grid Use Cases
  – but: some special characteristics
    • comprehensive metadata support
    • special structure of data
Scientific Workflow

Collaborative Climate Community Data and Processing Grid (C3Grid):

Huge sets/archives containing structured climate data from simulation and measurements

Different (cut out) input data

Analysis need only subsets of these data

Analysis/Simulation

Results:
- storm track analysis
- chemical forecast

Put results to archives
C3-Grid Architecture

General: Service Oriented Architecture (SOA)

Portal Layer:
- interface for Grid user
- programming interface

Middleware Layer:
- distributed Grid infrastructure
- information and data related services

Abstraction Layer:
- data provider abstraction
- compute provider abstraction

Portal / API
- find data sources
- query resource state
- negotiate data acquisition
- harvest ISO metadata
- stage/preprocess data
- trigger computation
- publish/accumulate state

IS

DMS

WSS

Virtual Workspace

Data Provider Abstraction

Compute Provider Abstraction

Alexander Papaspyrou
GES 2007
5 Posters

- Maintaining Reference Graphs of Globally Accessible Objects in Fully Decentralized Distributed Systems
  Bjoern Saballus, Thomas Fuhrmann

- Adaptive Run-time Prediction in Heterogeneous Environments
  Christian Glasner, Jens Volkert

- Performance Prediction Based on Hierarchy Parallel Features Captured in Multi-Processing System
  Jiaxin Li, Feng Shi, Ning Deng

- CLOUDLET: Towards MapReduce Implementation on Virtual Machines
  Shadi Ibrahim, Hai Jin, Bin Cheng, Song Wu, Haijun Cao, Li Qi

- Investigating Software Transactional Memory on big SMP machines
  Ruibo Wang