GGF International Summer School
on Grid Computing
Vico Equense (Naples), Italy

Introduction to OGSA-DAI

Prof. Malcolm Atkinson
Director
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21st July 2003
Workshop Overview
OGSA-DAI Workshop

- 08:30 – Information Grids & Introduction: Malcolm Atkinson
  - Grids and Virtual Organisations
  - Overview of the architecture
  - Typical end-to-end interaction involving configuration and perform documents – preamble to end-to-end demonstrator: Amy Krause
- 10:30 – Coffee break
- 11:00 – OGSA-DAI Architecture and Configuration: Amy Krause
- 12:15 Lab Session (installation and configuration)
- 13:00 – LUNCH
- 14:00 – Internal Structures of OGSA-DAI: Tom Sugden
  - Low-level architecture
  - Implementing Activities
  - Writing Perform Documents
- 15:00 – Lab session (configuration and perform documents)
- 16:30 – BREAK
- 17:00 – Lab Session (Writing your own perform documents)
  - Playtime with OGSA-DAI
- 18:30 – End of Lab sessions
Outline

- **What is e-Science?**
  - Grids, Collaboration, Virtual Organisations
  - Structured Data at its Foundation

- **Motivation for DAI**
  - Key Uses of Distributed Data Resources
  - Challenges

- **Introduction to DAI**
  - GGF DAIS Working Group
  - Conceptual Models
  - Architectures
  - Current OGSA-DAI components
e-Science & Grids
It’s Easy to Forget How Different 2003 is From 1993

- Enormous quantities of data: Petabytes
  - For an increasing number of communities, gating step is not collection but analysis

- Ubiquitous Internet: >100 million hosts
  - Collaboration & resource sharing the norm
  - Security and Trust are crucial issues

- Ultra-high-speed networks: >10 Gb/s
  - Global optical networks
  - Bottlenecks: last kilometre & firewalls

- Huge quantities of computing: >100 Top/s
  - Moore’s law gives us all supercomputers
  - Ubiquitous computing

- Moore’s law everywhere
  - Instruments, detectors, sensors, scanners, …

Derived from Ian Foster’s slide at ssdbM July 03
Foundation for e-Science

- e-Science methodologies will rapidly transform science, engineering, medicine and business
  - driven by exponential growth ($\times 1000$/decade)
    - enabling a whole-system approach

Diagram derived from Ian Foster’s slide
e-Science & Collaboration
Three-way Alliance

Multi-national, Multi-discipline, Computer-enabled Consortia, Cultures & Societies

Theory Models & Simulations → Shared Data

Experiment & Advanced Data Collection → Shared Data

Computing Science Systems, Notations & Formal Foundation → Process & Trust

Requires Much Engineering, Much Innovation

Changes Culture, New Mores, New Behaviours

New Opportunities, New Results, New Rewards
Biochemical Pathway Simulator

(Computing Science, Bioinformatics, Beatson Cancer Research Labs)

Closing the information loop – between lab and computational model.

DTI Bioscience Beacon Project

Harnessing Genomics Programme

Slide from Muffy Calder, Glasgow
e-Science, Virtual Organisations & Knowledge Communities
Emergence of Global Knowledge Communities

- Teams organised around common goals
  - Communities: “Virtual organisations”
  - Overlapping memberships, resources and activities
- Essential diversity is a strength & challenge
  - membership & capabilities
- Geographic and political distribution
  - No location/organisation/country possesses all required skills and resources
- Dynamic: adapt as a function of their situation
  - Adjust membership, reallocate responsibilities, renegotiate resources

Slide derived from Ian Foster’s ssdbm 03 keynote
The Emergence of Global Knowledge Communities

Slide from Ian Foster’s ssdbm 03 keynote
Global Knowledge Communities
Often Driven by Data: E.g., Astronomy

No. & sizes of data sets as of mid-2002, grouped by wavelength:

- 12 waveband coverage of large areas of the sky
- Total about 200 TB data
- Doubling every 12 months
- Largest catalogues near 1B objects

Data and images courtesy Alex Szalay, John Hopkins
Wellcome Trust: Cardiovascular Functional Genomics

Glasgow - Shared data - Edinburgh

Oxford - BRIDGES - IBM

London - Leicester - Netherlands

Public curated data
Database-mediated Communication

Experimentation Communities

Simulation Communities

Curated & Shared Databases

Data Carries knowledge

Data Carries knowledge

Analysis & Theory Communities

Discoveries
e-Science, Data Scales, Challenges & Opportunities
global in-flight engine diagnostics

100,000 engines
2-5 Gbytes/flight
5 flights/day =
2.5 petabytes/day

Distributed Aircraft Maintenance Environment: Universities of Leeds, Oxford, Sheffield & York
Database Growth

EMBL Database Growth

Bases 41,073,690,490

PDB Content Growth

Deposited structures in the year
Total available structures
Distributed Structured Data

- Key to Integration of Scientific Methods
- Key to Large-scale Collaboration
- Many Data Resources
  - Independently managed
  - Geographically distributed
  - Primary Data, Data Products, Meta Data, Administrative data, ...
- Discovery and Decisions!
  - Extracting nuggets from multiple sources
  - Combing them using sophisticated models
  - Analysis on scales required by statistics
- Repeated Processes

Petabyte of Digital Data / Hospital / Year
Tera → Peta Bytes

- RAM time to move
  - 15 minutes
- 1Gb WAN move time
  - 10 hours ($1000)
- Disk Cost
  - 7 disks = $5000 (SCSI)
- Disk Power
  - 100 Watts
- Disk Weight
  - 5.6 Kg
- Disk Footprint
  - Inside machine

- RAM time to move
  - 2 months
- 1Gb WAN move time
  - 14 months ($1 million)
- Disk Cost
  - 6800 Disks + 490 units + 32 racks = $7 million
- Disk Power
  - 100 Kilowatts
- Disk Weight
  - 33 Tonnes
- Disk Footprint
  - 60 m²

May 2003 Approximately Correct

See also Distributed Computing Economics Jim Gray, Microsoft Research, MSR-TR-2003-24
Mohammed & Mountains

- **Petabytes of Data cannot be moved**
  - It stays where it is produced or curated
    - Hospitals, observatories, European Bioinformatics Institute, ...
  - A few caches and a *small* proportion cached

- **Distributed collaborating communities**
  - Expertise in curation, simulation & analysis

- **Distributed & diverse data collections**
  - Discovery depends on insights
    - Unpredictable sophisticated application code
  - Tested by combining data from many sources
  - Using *novel* sophisticated models & algorithms

- **What can you do?**
Dynamically Move computation to the data

- Assumption: code size << data size
- Develop the database philosophy for this?
  - Queries are dynamically re-organised & bound
- Develop the storage architecture for this?
  - Compute closer to disk?
    - System on a Chip using free space in the on-disk controller
  - Data Cutter a step in this direction
- Develop the sensor & simulation architectures for this?
- Safe hosting of arbitrary computation
  - Proof-carrying code for data and compute intensive tasks + robust hosting environments
- Provision combined storage & compute resources
- Decomposition of applications
  - To ship behaviour-bounded sub-computations to data
- Co-scheduling & co-optimisation
  - Data & Code (movement), Code execution
  - Recovery and compensation

Dave Patterson
Seattle
SIGMOD 98
Scientific Data

**Opportunities**
- Global Production of Published Data
- Volume↑ Diversity↑
- Combination ⇒ Analysis ⇒ Discovery

**Challenges**
- Data Huggers
- Meagre metadata
- Ease of Use
- Optimised integration
- Dependability

**Opportunities**
- Specialised Indexing
- New Data Organisation
- New Algorithms
- Varied Replication
- Shared Annotation
- Intensive Data & Computation

**Challenges**
- Fundamental Principles
- Approximate Matching
- Multi-scale optimisation
- Autonomous Change
- Legacy structures
- Scale and Longevity
- Privacy and Mobility
- Sustained Support / Funding
The Story so Far

- Technology enables Grids, More Data & …
- Information Grids will be very important
- Collaboration is essential
  - Combining approaches
  - Combining skills
  - Sharing resources
- (Structured) Data is the language of Collaboration
  - Data Access & Integration a Ubiquitous Requirement
  - Primary data, metadata, administrative & system data
- Many hard technical challenges
  - Scale, heterogeneity, distribution, dynamic variation
- Intimate combinations of data and computation
  - With unpredictable (autonomous) development of both
Outline

- What is e-Science?
  - Grids, Collaboration, Virtual Organisations
  - Structured Data at its Foundation
- Motivation for DAI
  - Key Uses of Distributed Data Resources
  - Challenges
- Introduction to Data Access & Integration
  - DAIS-WG: Conceptual Model & Architecture
  - Data Access & Integration in OGSA
  - Introducing OGSA-DAI Services
- Looking ahead & Take-Home Messages
  - Composition of Analysis & Interpretation
Science as Workflow

- Data integration = the derivation of new data from old, via coordinated computation
- May be computationally demanding
  - The workflows used to achieve integration are often valuable artifacts in their own right

May be Data Access & Movement Demanding
- Obtaining data from files and DBs, transfer between computations, deliver to DBs and File stores

- Thus we must be concerned with how we
  - Build workflows
  - Share and reuse workflows
  - Explain workflows
  - Schedule workflows

Consider also DBs & (Autonomous) Updates
- External actions are important

Slide derived from Ian Foster’s ssdbm 03 keynote
DAIS-WG

- **Specification of Grid Data Services**
- **Chairs**
  - Norman Paton, Manchester University
  - Dave Pearson, Oracle
- **Current Spec. Draft Authors**
  - Mario Antonioletti
  - Neil P Chue Hong
  - Susan Malaika
  - Simon Laws
  - Norman W Paton
  - Malcolm Atkinson
  - Amy Krause
  - Gavin McCance
  - James Magowan
  - Greg Riccardi
Grid Database Service Specification

Status of This Memo

This memo provides information to the Grid community regarding the specification of Grid Database Services. The specification is presently a draft for discussion. It does not define any standards or technical recommendations. Distribution is unlimited.

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Abstract

Data management systems are central to many applications across multiple domains, and play a significant role in many others. Web services provide implementation neutral facilities for describing, invoking and orchestrating collections of networked resources. The Open Grid Services Architecture (OGSA) extends Web Services with consistent interfaces for creating, managing and exchanging information among Grid Services, which are dynamic computational artefacts cast as Web Services. Both Web and Grid service communities stand to benefit from the provision of consistent, agreed service interfaces to database management systems. Such interfaces must support the description and use of database systems using Web Service standards, taking account of the design conventions and mandatory features of Grid Services. This document presents a specification for a collection of Grid Database Services. The proposal is presented for discussion within the Global Grid Forum (GGF) Database Access and Integration Services (DAIS) Working Group, in the hope that it will evolve into a formal standard for Grid Database Services. There are several respects in which the current proposal is incomplete, but it is hoped that the material included is sufficient to allow an informed discussion to take place concerning both its form and substance.
Conceptual Model
External Universe

External data resource  DBMS

External data resource

DB

Data set

ResultSet
Conceptual Model
DAI Service Classes

Data resource → DBMS

Data resource → DB

Data activity session

Data request

Data set

ResultSet
Architecture of Service Interaction

- Packaging to avoid round trips
- Unit for data movement services to handle
Architecture of Service Interaction

Request
PerfomRequestDocument.xsd

<dataSet>
<performRequest>
...
</performRequest>

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Data Set

Identifiers:
- TAP
- ORS

Output:

dr

2
Architecture (2)
OGSA-DAI Project
OGSA-DAI

First steps towards a generic framework for integrating data access and computation

Using the grid to take specific classes of computation nearer to the data

Kit of parts for building tailored access and integration applications

Investigations to inform DAIS-WG

One reference implementation for DAIS

Releases publicly available NOW
OGSA-DAI Partners

$5 million, 20 months, started February 2002

Additional 24 months, starts October 2003
Infrastructure Architecture

Data Intensive X Scientists

Data Intensive Applications for Science X

Simulation, Analysis & Integration Technology for Science X

Generic Virtual Data Access and Integration Layer

Job Submission  Brokering  Workflow  Structured Data Integration

Registry  Banking  Authorisation  Structured Data Access

Data Transport  Resource Usage  Transformation

OGSI: Interface to Grid Infrastructure

Compute, Data & Storage Resources  Structured Data

Distributed

Virtual Integration Architecture
Data Access & Integration Services

1a. Request to Registry for sources of data about “x”

1b. Registry responds with Factory handle

2a. Request to Factory for access to database

2b. Factory creates GridDataService to manage access

2c. Factory returns handle of GDS to client

3a. Client queries GDS with XPath, SQL, etc

3b. GDS interacts with database

3c. Results of query returned to client as XML
Peering into the Future
Future DAI Services

1a. Request to Registry for sources of data about “x” & “y”

1b. Registry responds with factory handle

2a. Request to Factory for access and integration from resources Sx and Sy

2b. Factory creates GridDataServices network

2c. Factory returns handle of GDS to client

3a. Client submits sequence of scripts each has a set of queries to GDS with XPath, SQL, etc

3b. Client tells analyst

3c. Sequences of result sets returned to analyst as formatted binary described in a standard XML notation

Data Registry

SOAP/HTTP

service creation

API interactions

Problem Solving Environment

Semantic Meta data

Application Code

Data Access & Integration master

Data Registry

XML database

Relational database

1. Client

2. Factory

3. Client

GDS

GDS1

GDS2

GDS3

GDTS1

GDTS2

GDTS3

Sx

Sy

Application Code
A New World

- What Architecture will Enable Data & Computation Integration?
  - Common Conceptual Models
  - Common Planning & Optimisation
  - Common Enactment of Workflows
  - Common Debugging
  - ...

- What Fundamental CS is needed?
  - Trustworthy code & Trustworthy evaluators
  - Decomposition and Recomposition of Applications
  - ...

- Is there an evolutionary path?
Take Home Message

- There are plenty of Research Challenges
  - Workflow & DB integration, co-optimised
  - Distributed Queries on a global scale
  - Heterogeneity on a global scale
  - Dynamic variability
    - Authorisation, Resources, Data & Schema
    - Performance
  - Some Massive Data
  - Metadata for discovery, automation, repetition, …
  - Provenance tracking

- Grasp the theoretical & practical challenges
  - Working in Open & Dynamic systems
  - Incorporate all computation
  - Welcome “code” visiting your data
Take Home Message (2)

- **Information Grids**
  - Support for collaboration
  - Support for computation and data grids
  - Structured data fundamental
    - Relations, XML, semi-structured, files, …
  - Integrated strategies & technologies needed

- **OGSA-DAI is here now**
  - A first step
  - Try it
  - Tell us what is needed to make it better
  - Join in making better DAI services & standards
Comments & Questions Please

www.ogsadai.org.uk

www.nesc.ac.uk