HPDC12
Seattle
Structured Data and the Grid
Access and Integration
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Outline

- What is e-Science?
  - Structured Data at its Foundation
  - Key Uses of Distributed Data Resources
  - Data-intensive Challenges

- Data Access & Integration
  - DAIS-WG
  - OGSA-DAI: Progress and Dreams

- Unanswered Architectural Questions
Foundation for e-Science

- e-Science methodologies will rapidly transform science, engineering, medicine and business
  - Driven by exponential growth (×1000/decade)
  - Enabling and requiring a whole-system approach

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
Database-mediated Communication

Experimentation Communities

Simulation Communities

Curated & Shared Databases

Analysis & Theory Communities

Discoveries

global in-flight engine diagnostics

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

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

EMBL Database Growth

PDB Content Growth

Bases 39,856,567,747

Distributed Structured Data

- Key to Integration of Scientific Methods
- Key to Large-scale Collaboration
- Growing Number of Growing Data Resources
  - Independently managed
  - Geographically distributed
- Key to Discovery and Decisions!
  - Extracting nuggets from multiple sources
  - Combing them using sophisticated models
  - Analysis on scales required by statistics
- Repeated Processes
Tera → Peta Bytes

- RAM time to move
  - 15 minutes
- 1Gb WAN move time
  - 10 hours ($1000)
- Disk Cost
- Disk Weight
  - 5.6 Kg
- Disk Footprint
  - Inside machine
- RAM time to move
  - 2 months
- 1Gb WAN move time
  - 14 months
  - Cost:
    - 900 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, ...
- Distributed collaborating communities
  - Expertise in curation, simulation & analysis
    - Can’t collocated data in a few places
- Distributed & diverse data collections
  - Discovery depends on insights
    - Unpredictable sophisticated application code
  - Tested by combining data from many sources
Dynamically

Move computation to the data

- Assumption: code size << data size
  - Code needs to be well behaved
- 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

Data Access & Integration
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

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
Conceptual Model
External Universe

External data resource manager
External data resource
External data set

Conceptual Model
DAI Service Classes

Data resource manager
Data resource
Data activity session
Data request
Data set
$5 million, 20 months, started February 2002
Additional 24 months, starts October 2003
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
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

Future DAI Services

1a. Request to Registry for sources of data about “x” & “y”
1b. Registry responds with Factory handle
2b. Factory creates GridDataService to manage access
2c. Factory returns handle of GDS to client
2d. Factory creates GridDataService network
3a. Client submits sequence of scripts each has a set of queries to GDS with XPath, SQL, etc
3c. Sequences of result sets returned to analyst as formatted binary described in a standard XML notation

SOAP/HTTP  
service creation  
API interactions
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?

Comments & Questions Please

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Scientific Data

- **Opportunities**
  - Global Production of Published Data
  - Volume $\uparrow$ Diversity $\uparrow$
  - Combination $\Rightarrow$ Analysis $\Rightarrow$ 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