Supporting Collaborative Product Design in Industry

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Case studies: IT infrastructure for inter-enterprise collaboration
Grid Computing Now, Web seminar
February 15th 2007
Contents

• SIMDAT Project Overview
• Pharmaceutical Case Study
• SIMDAT Grid Solution Portfolio
• Conclusions

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Four sectors of international economic importance:
- Automotive
- Pharmaceutical
- Aerospace
- Meteorology

Seven Grid-technology development areas:
- Grid infrastructure
- Distributed Data Access
- VO Administration
- Workflows
- Ontologies
- Analysis Services
- Knowledge Services
Who are the SIMDAT Partners?

End Users
- GSK
- Renault
- Audi
- EUMETSAT
- EADS
- Met Office
- IDestyle

Capability Providers
- MSC Software
- ESI Group
- LMS
- Inpharmatica
- Ontoprise
- InforSense
- University of Southampton

Grid Technologists
- IT innovation
- NEC
- IBM
- FhG
- Universität Karlsruhe (TH)
- Oracle

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Demanding Application Drivers

- Integration of the product design process chain (CAE/CAD/CAT) including external engineering companies, developers and suppliers
- Multi-disciplinary collaborative configuration design of complex aerospace products
- Drug discovery environment managing the distribution of both public and commercial bioinformatics data and analysis services
- Virtual Global Information System Centre supporting the distribution and integration of large scale meteorology data data providers

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The Drug Discovery Pipeline

• Drug discovery is big business
• Top eight spend $30 billion annually on new product R&D (2004)
• 20% of the $150 billion of product sales
Challenges for the Drug Discovery Pipeline

• The health of a company's pipeline is a key performance measure
• Bottlenecks or gaps indicate a potential down turn
• Massive advances in technology and biological information have not translated into more drugs
  – too much information
  – only just beginning to understand how to process information meaningfully
• Companies are adopting new approaches and technologies for information processing
  – distribution, integration, discovery, analysis, visualisation, annotation and validation
Powering the Pipeline

- Pharmacogenetics
- Bioinformatics
- Cheminformatics
- High Throughput Screening
- Performance Based Innovation
- Co-development Partnerships
- Outsourcing
- Specialisation

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Powering the Pipeline

Pharmacogenetics
Bioinformatics
Cheminformatics
High Throughput Screening
Performance Based Innovation
Co-development Partnerships
Outsourcing
Specialisation

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Collaborative Drug Discovery Test case

- B2B and B2A collaborative drug discovery
- Focusing on the target identification
  - data distribution
  - gene lists
  - structural domains
  - functional assignment/druggability
- Bioinformatics data and analysis capabilities shared between organisations
- Distributed Bioinformatics workflows and data management over the Internet
B2B/B2A Partnerships

Academic Service Provider

Industrial Service Provider

Academic Consumer

Internet
Characteristics of Business Grids

- Customers control which services they consume, how much they are used, and by whom
- Service providers operate independently and compete to provide service
- Service providers operate within the terms of relevant application software licenses
- Services are subject to Service Level Agreements
- Security to commercial standards
- Heterogeneous infrastructures
- Maintenance should be cost-effective
The SIMDAT Grid Solution Portfolio

• The SIMDAT architecture is a framework for delivering interoperable business Grid technologies — today
  – based on service oriented architecture (SOA) principles and web service specifications
  – used to build domain-specific Grid solutions
  – used to communicate SIMDAT ideas, structure and results to application communities within and beyond SIMDAT
The SIMDAT Architecture

- Problem Solving Environments
  - Simulation Portals
  - Project Management
  - Workflow Administration
  - Process Management & Automation
  - Knowledge Management
  - Data Management
  - Application Integration

- Workflow

- Information

- Data

- Execution Management

- Security

- Service Management

- Core

- Analysis Services
  - CAE Analysis Methods
  - Design Optimisation
  - Parametric Geometry
  - Bioinformatics Analysis Methods
  - Metadata- and Knowledge Extraction Services

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Pharmaceutical Domain Solution

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GRIA: A Grid for business

- Open Source Grid middleware for supporting B2B collaborations based on a service-oriented architecture
- Easy to use yet powerful functionality
  - business-to-business accounting and service level agreements
  - dynamic trust and security
  - distributed file transfer, storage and processing
  - distributed database access using OGSA-DAI
  - distributed inter-domain workflow composition, enactment and publication using Taverna/Freefluo
  - cross-platform, running on Windows XP and various Linux distributions
  - developers kit for new managed application services
- Available free and open source from http://www.gria.org
Operational Scenarios

- **Client Management**
  - Project Manager
  - Engineer

- **Service Level Agreement**

- **Usage Constraints**

- **Basic Application Services**
  - Data Storage
  - Data Processing
  - Applications

- **Service Provider Management**

- **Access Constraints**

- **Client Organisation**
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- **Service Provider**
I want to use high-end applications, but I don't have enough processing power.
I want to provide applications and data services and specify terms and conditions for using them.
I want to manage my organisation’s relationships, and decide who in my team (and partners teams) can access my resources.
Managing Relationships

Client Organisation A

Project A
Client Mgmt Service

Trade Acc 1
Trade Account Service

Trade Acc 2

Project Manager A
Administrator A

Client Organisation B

Project B
Client Mgmt Service

Trade Acc 3
Trade Account Service

Trade Acc 4

Project Manager B
Administrator B

Service Provider A

Service Provider B
Application Service Management

- Trade Account Service
- SLA Management Service
- Capacity
- SLA Templates
- Notify Usage Reports
- Administrator
- Propose SLA
- Check SLA
- Manage Applications
- Basic Application Services
- OGSA-DAI Service
- Bespoke Application Service

Client Management
Client
Project Manager
Engineer
I generate usage metrics (CPU time, number of active application license, number of jobs, transaction time, data storage, etc)
I define my overall capacity model and SLA templates using metric constraints plus pricing terms.
Application Service Management

I record and constrain metric usage against SLA terms and service provider capacity

Propose SLA

Check SLA

Notify Usage Reports

Manage Applications

Capacity

SLA Templates
Conclusions

• SIMDAT is delivering business Grid middleware for inter-enterprise collaboration...today
• The Grid solution portfolio developments are driven by industrial requirements
• GRIA middleware satisfies the core requirements for relationships management
  – dynamic trust and security using commercial best-practice
  – SLA based monitoring, management and billing
  – accounting
• Key technologies are undergoing accreditation procedures by industrial partners
For more information

- www.simdat.eu
- www.gria.org