

Supporting Collaborative Product Design in Industry

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IT Innovation Centre

Case studies: IT infrastructure for inter-enterprise collaboration

Grid Computing Now, Web seminar
February 15th 2007

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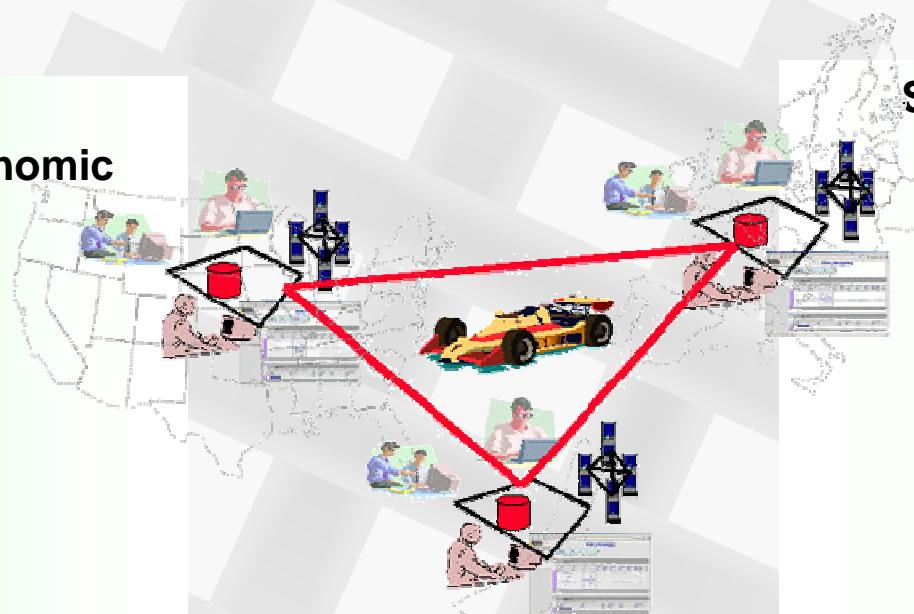
- SIMDAT Project Overview
- Pharmaceutical Case Study
- SIMDAT Grid Solution Portfolio
- Conclusions

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IST EU SIMDAT Project (Sep 2004 – Aug 2008)

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

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Who are the SIMDAT Partners?

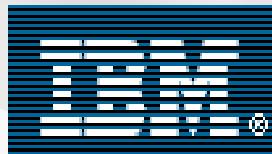
End Users



Capability Providers



Grid Technologists



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Demanding Application Drivers

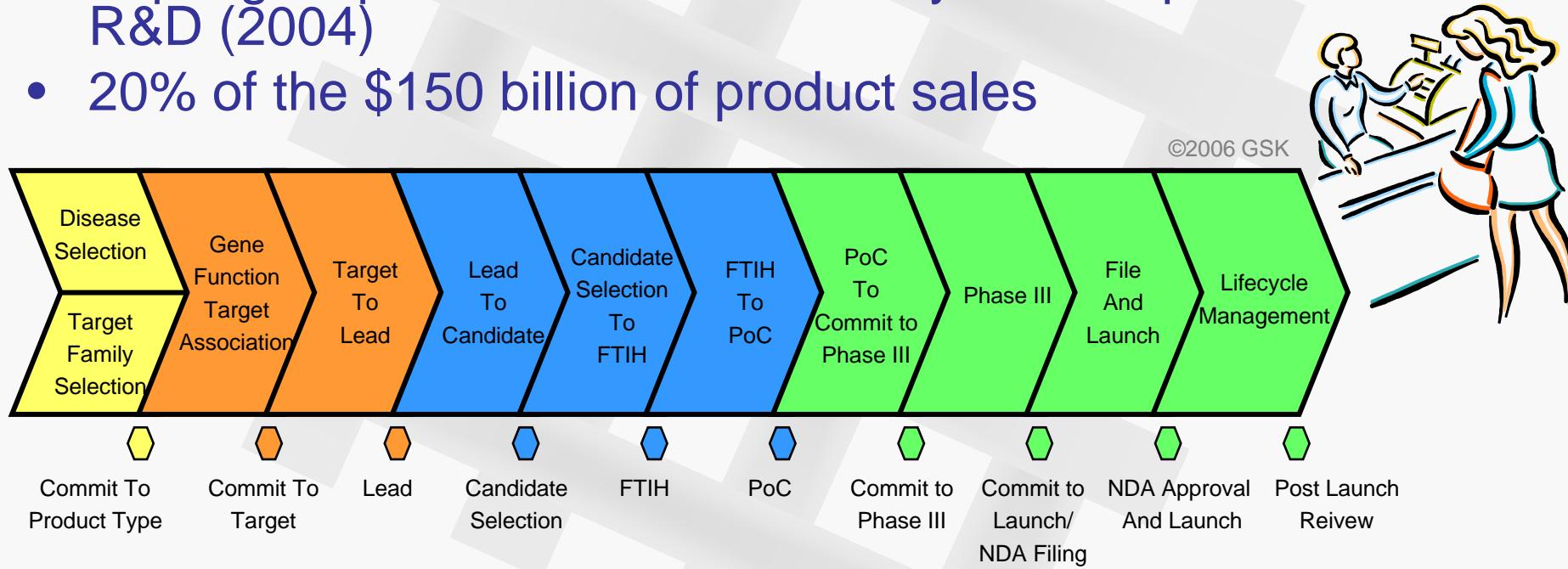


- Integration of the product design process chain (CAE/CAD/CAT) including external engineering companies, developers and suppliers
- Multi-disciplinary collaborative configuration design of complex aerospace products
- Drug discovery environment managing the distribution of both public and commercial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



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



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Challenges for the Drug Discovery Pipeline

- The health of a companies pipeline is a key performance measure
- Bottlenecks or gaps indicate a potential down turn
- Massive advances in technology and biological information has 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

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Powering the Pipeline

Bioinformatics

Pharmacogenetics

Cheminformatics

High Throughput Screening

Performance Based Innovation

Co-development Partnerships

Specialisation

Outsourcing

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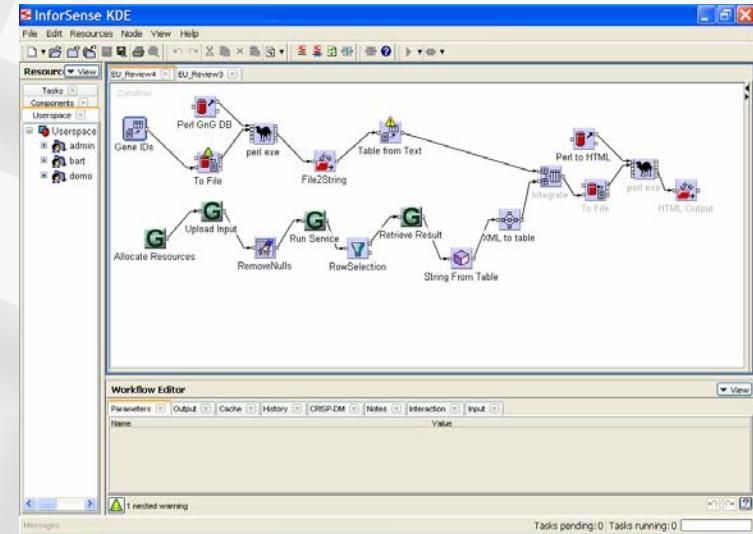
Co-development Partnerships

Specialisation

Outsourcing

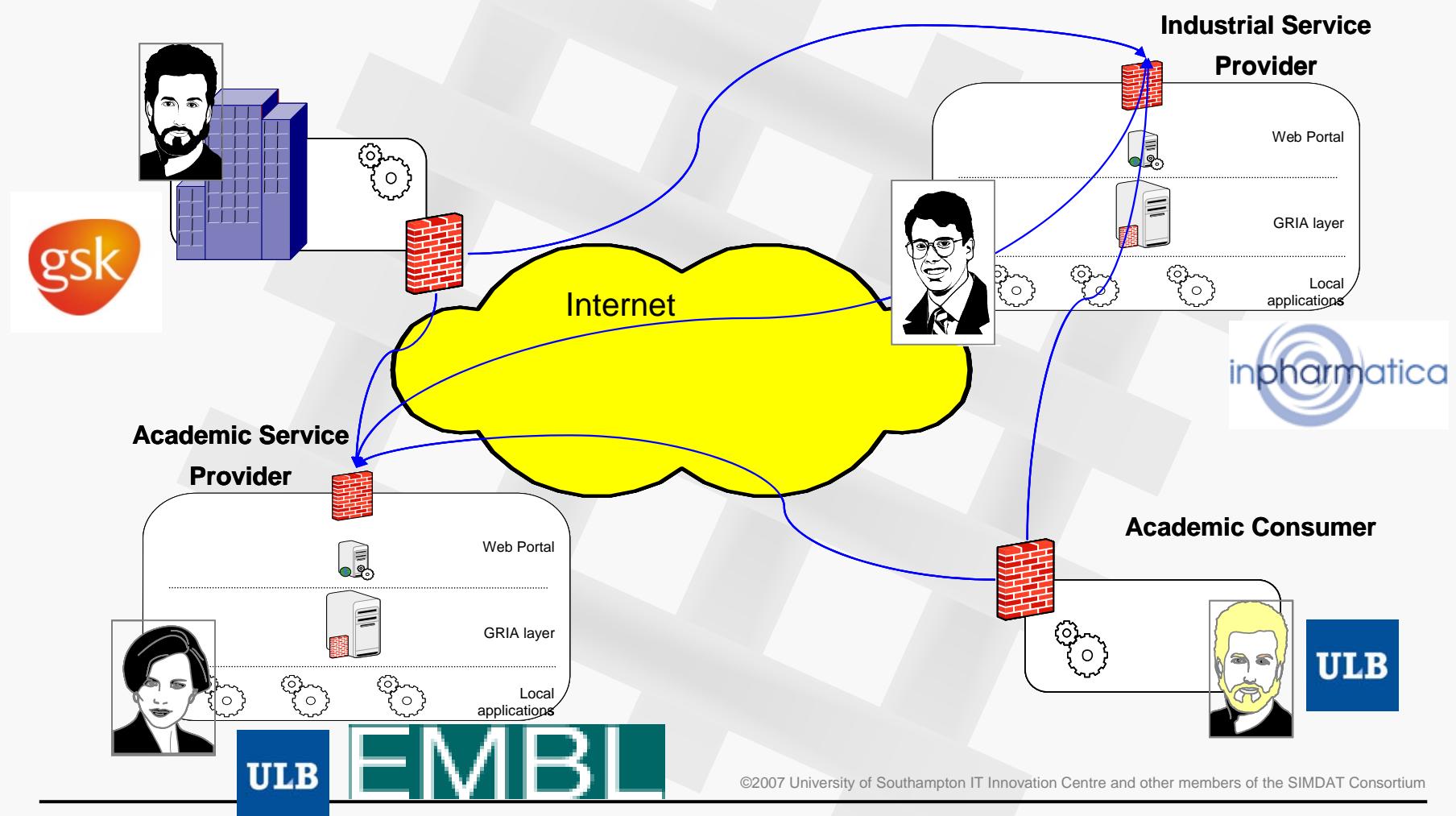
Collaborative Drug Discovery Test case

- 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



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B2B/B2A Partnerships



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

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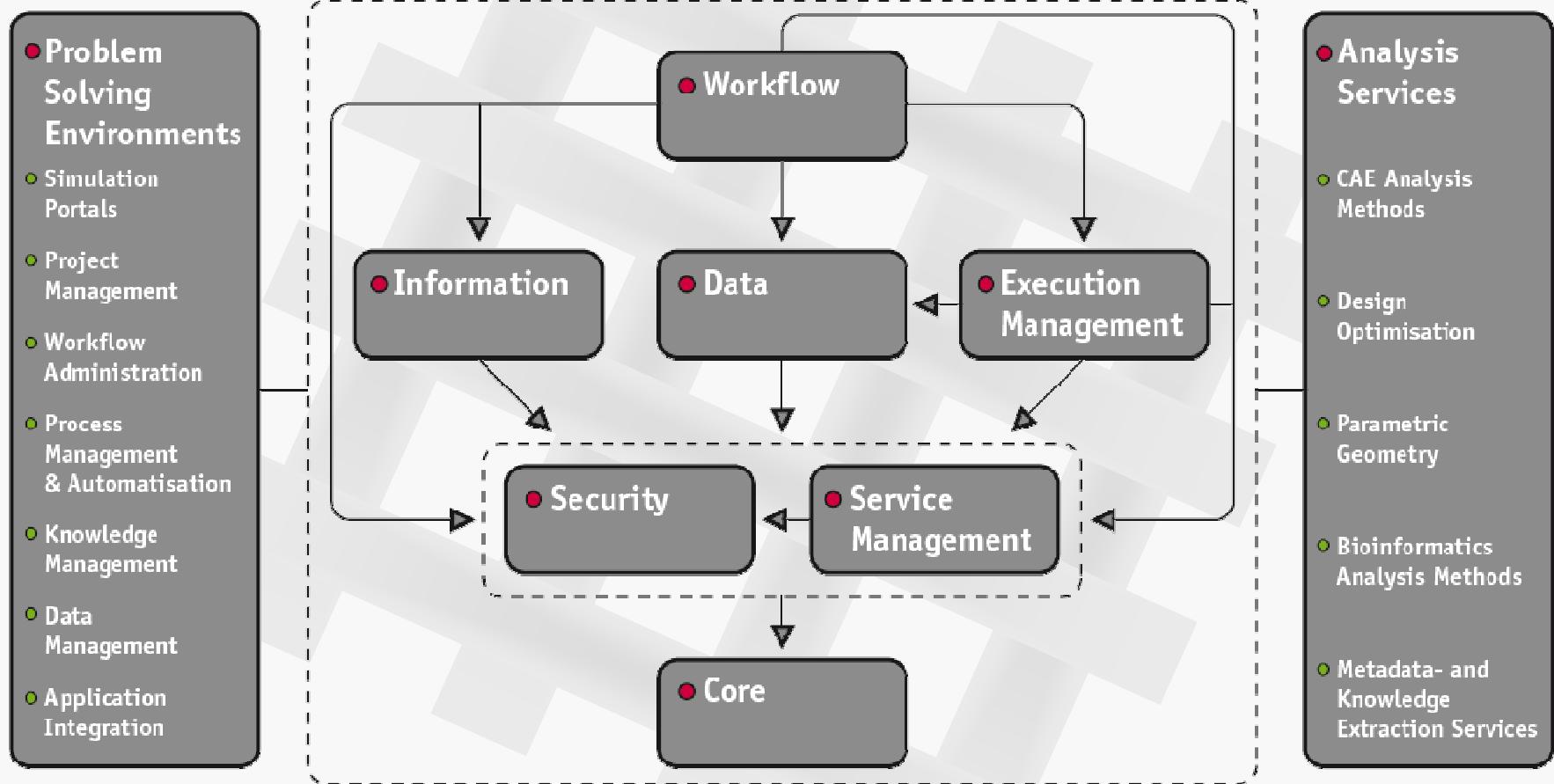
The SIMDAT Grid Solution Portfolio

- 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

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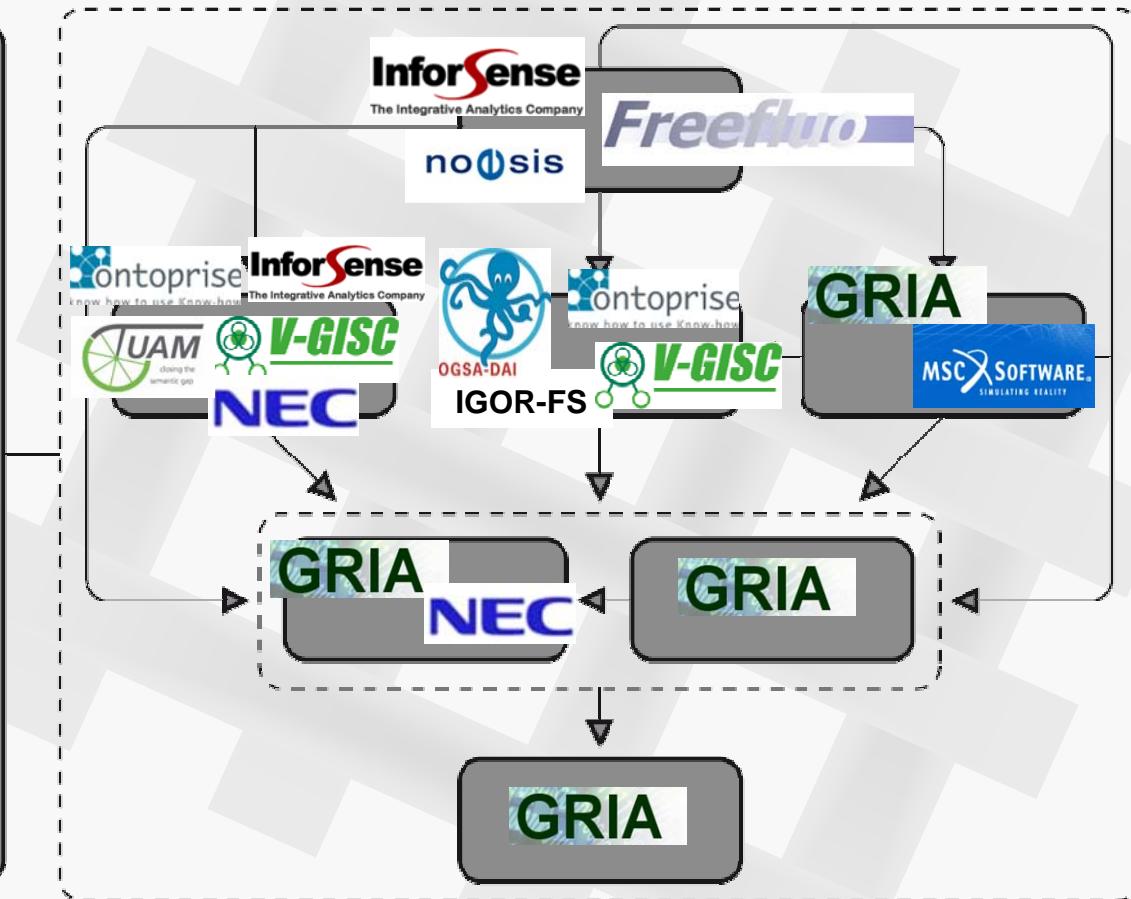
The SIMDAT Architecture



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SIMDAT Technologies

- Problem Solving Environments



- Analysis Services

- CAE Analysis Methods

- Design Optimisation

- Parametric Geometry

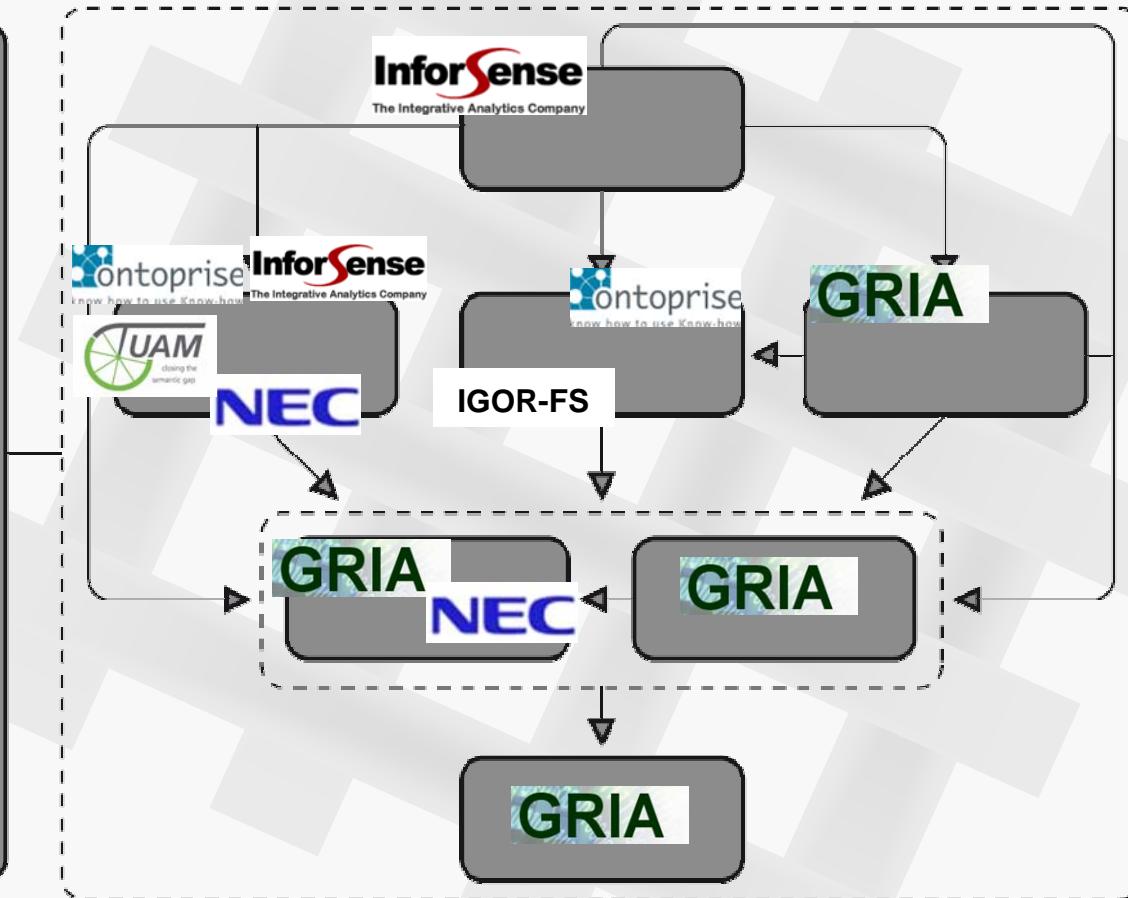
- Bioinformatics Analysis Methods

- Metadata- and Knowledge Extraction Services

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Pharmaceutical Domain Solution

- Problem Solving Environments



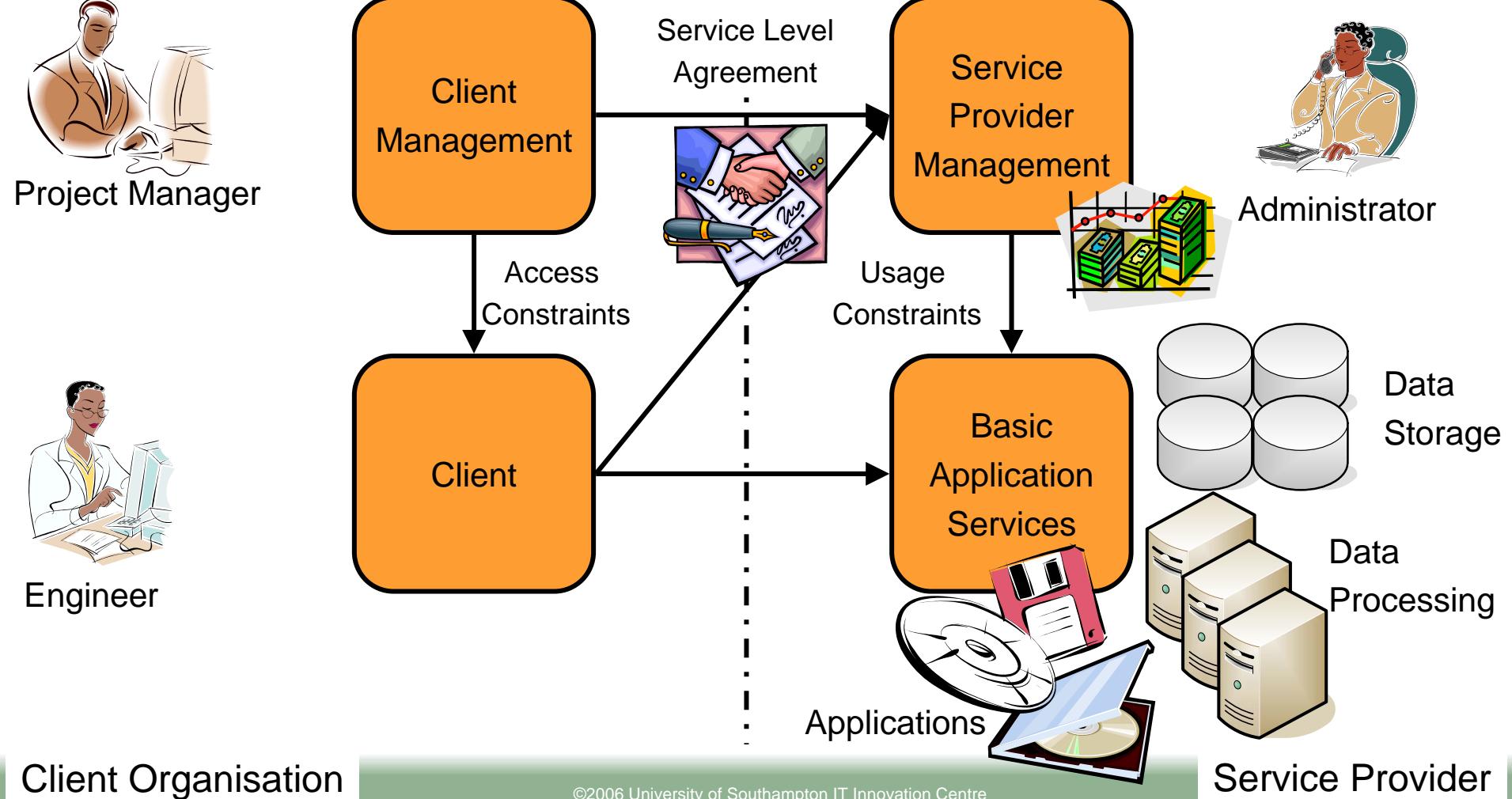
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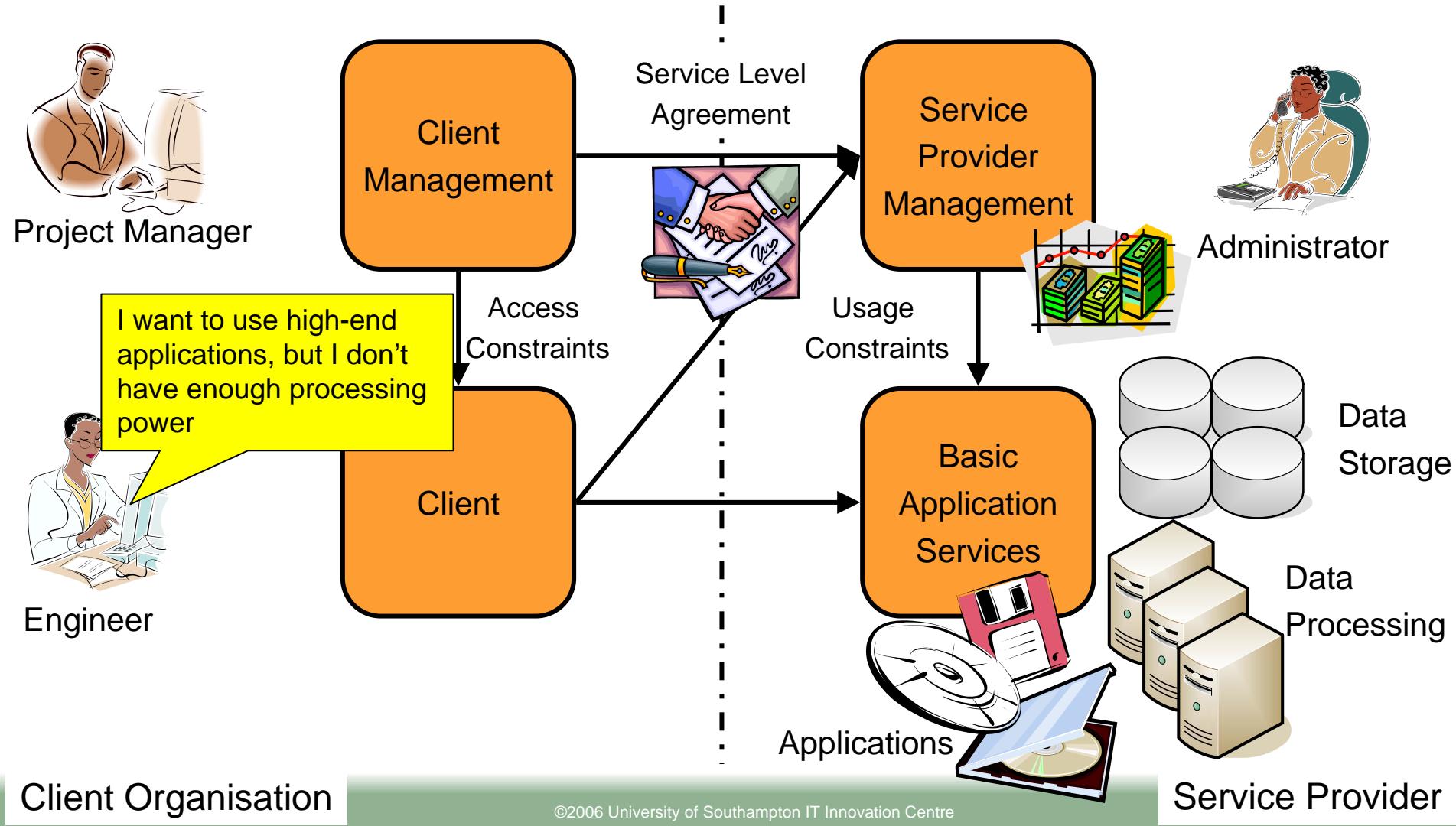
GRIA: A Grid for business

- 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>

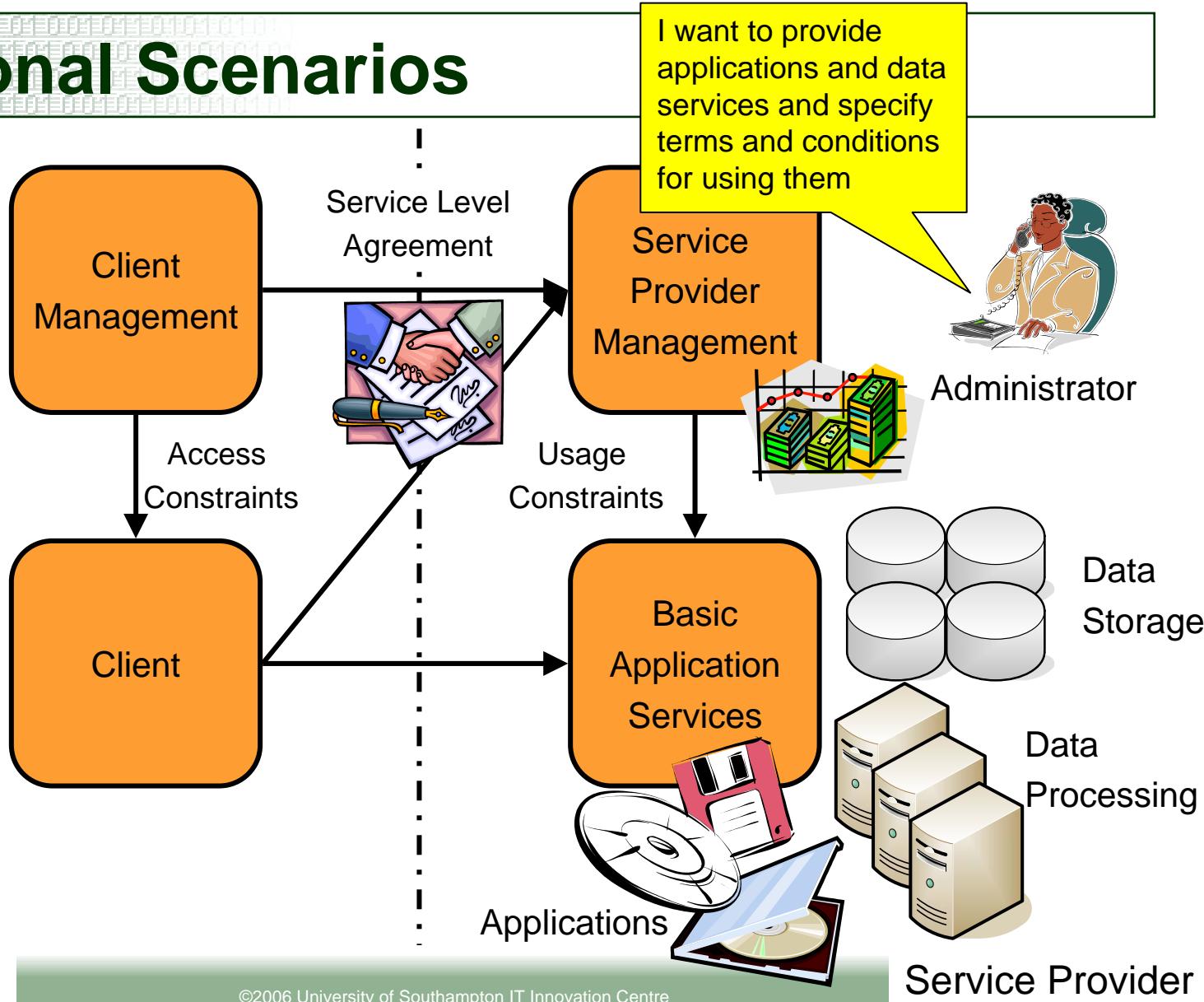
Operational Scenarios



Operational Scenarios



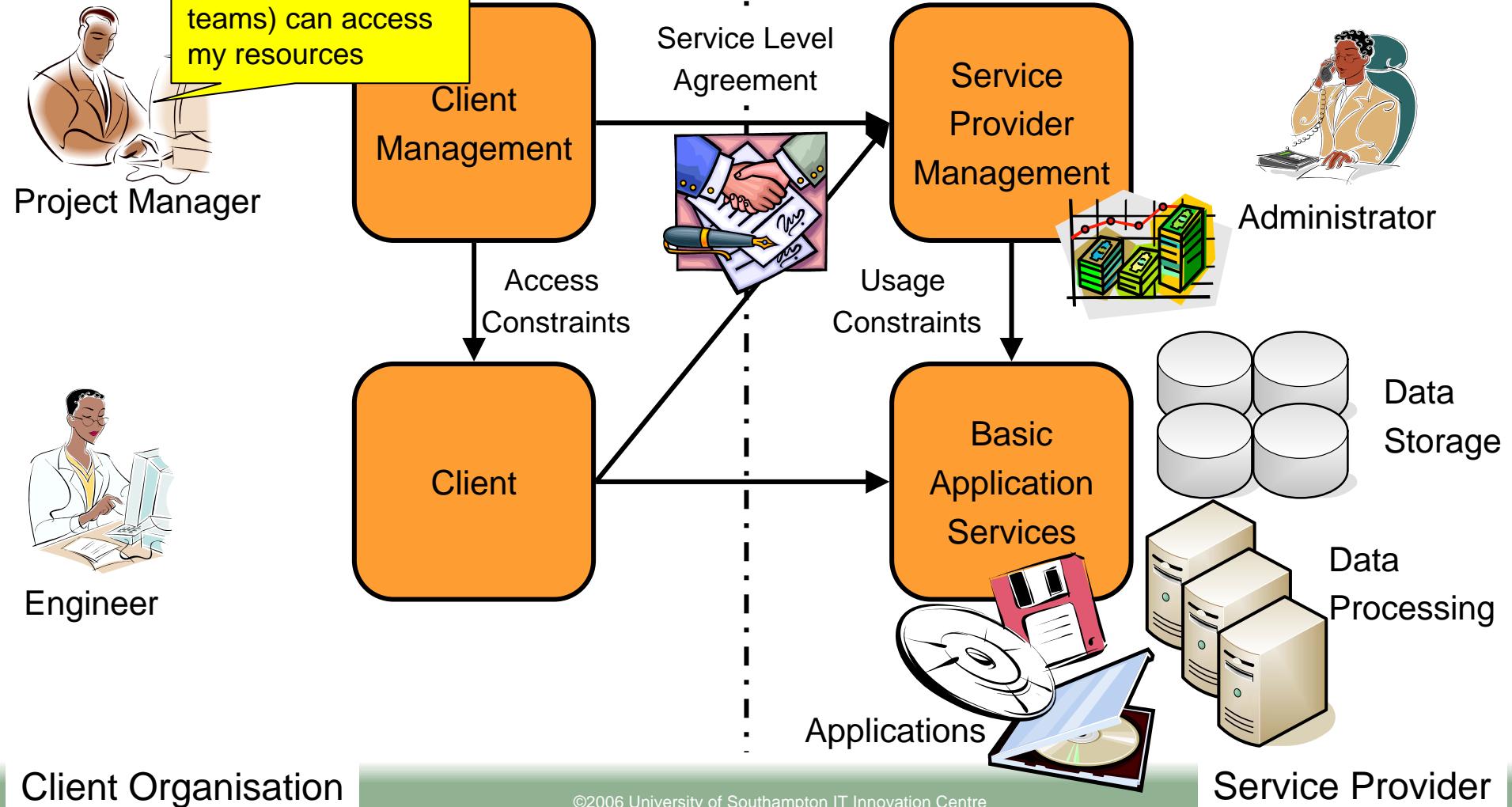
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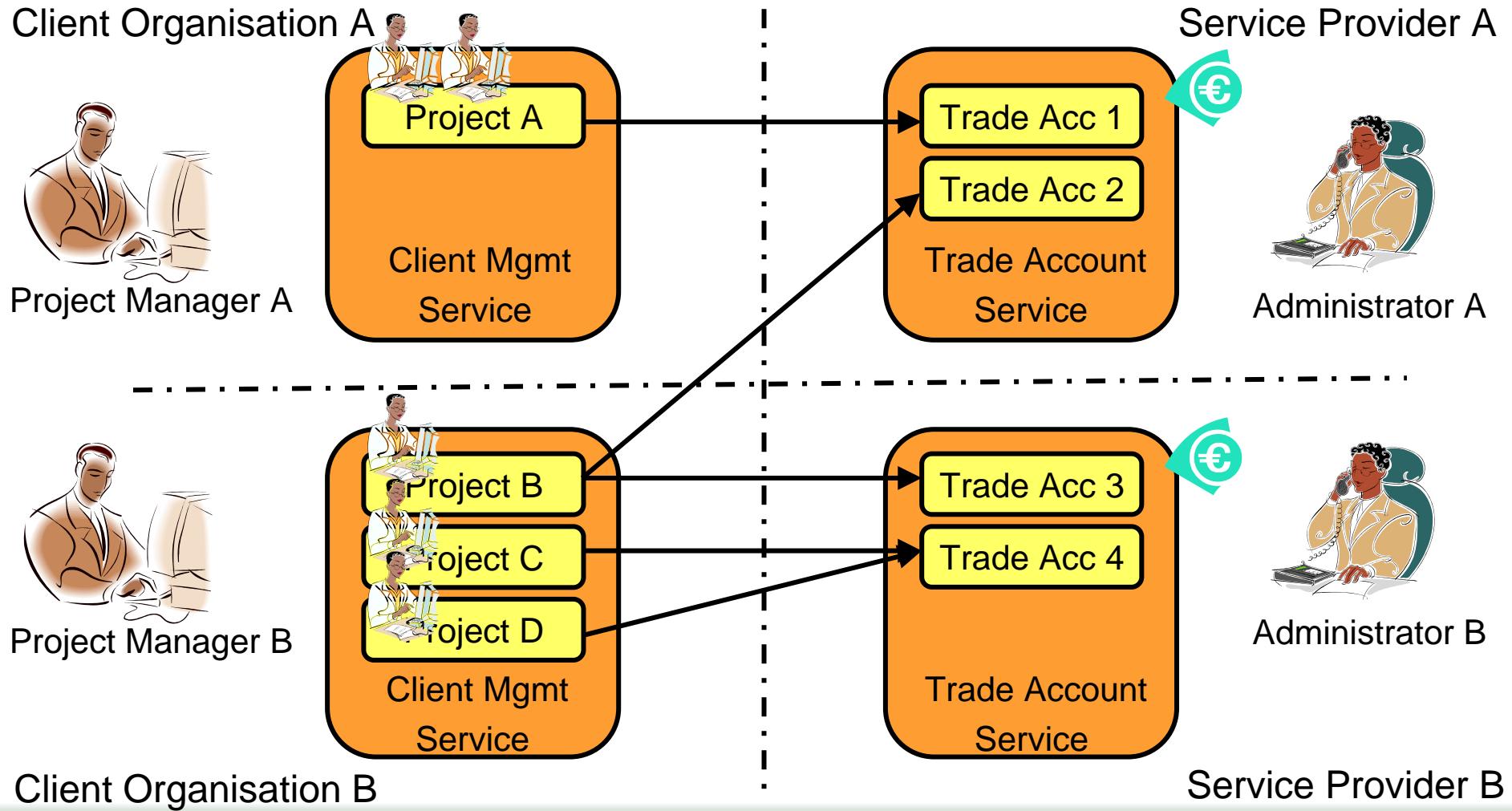
Op

I want to manage my organisation's relationships, and decide who in my team (and partners teams) can access my resources

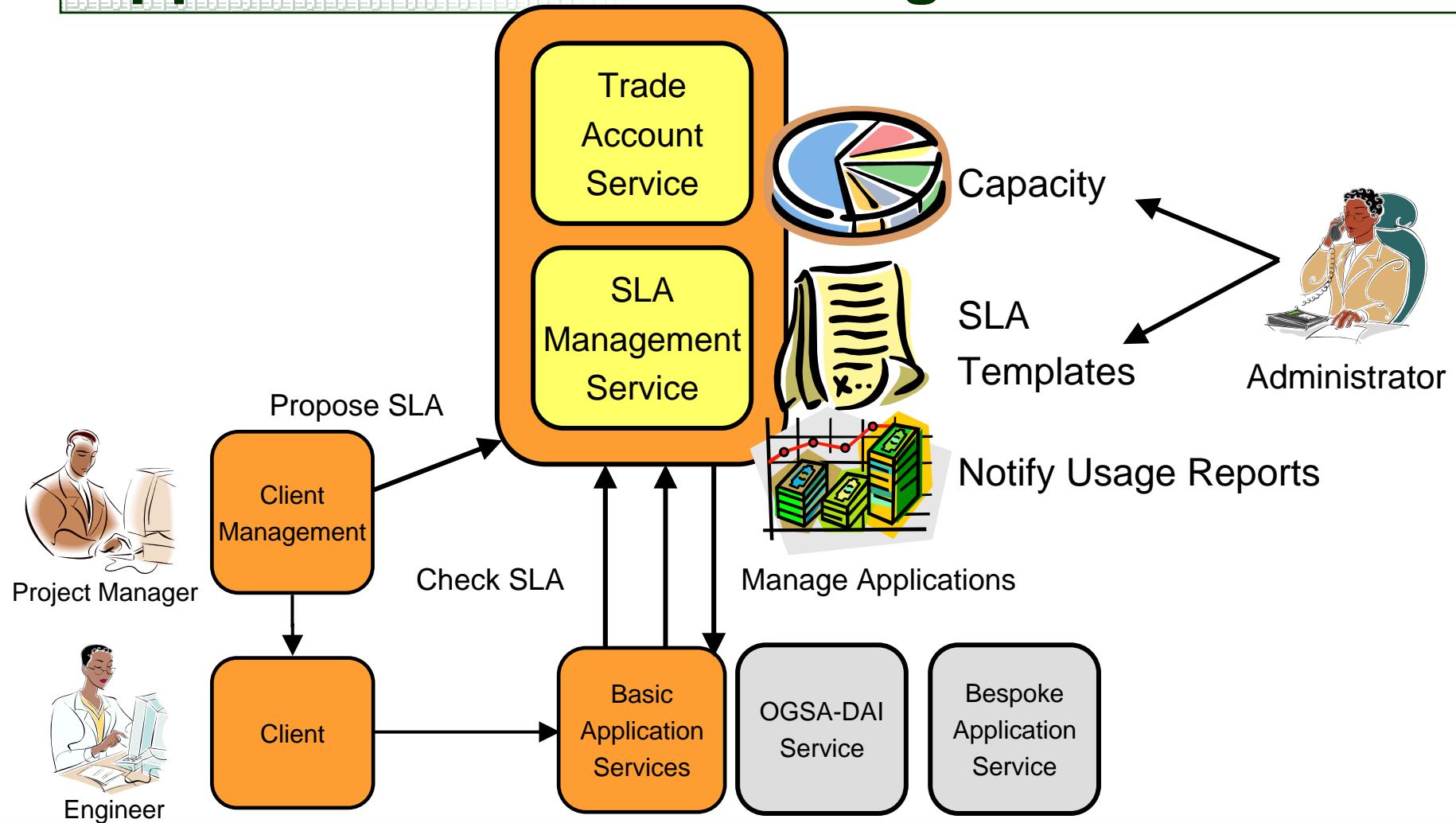
Scenarios



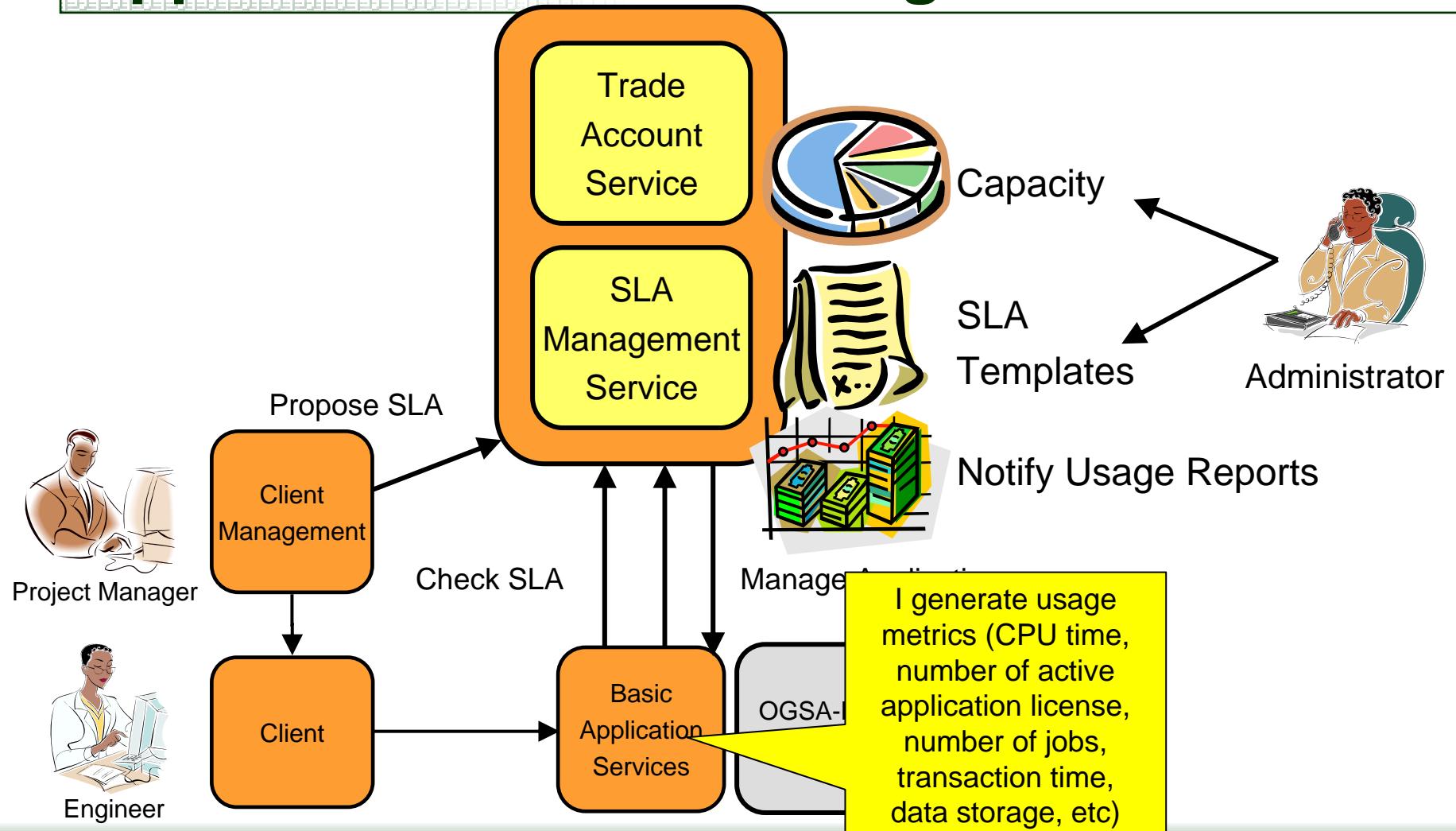
Managing Relationships



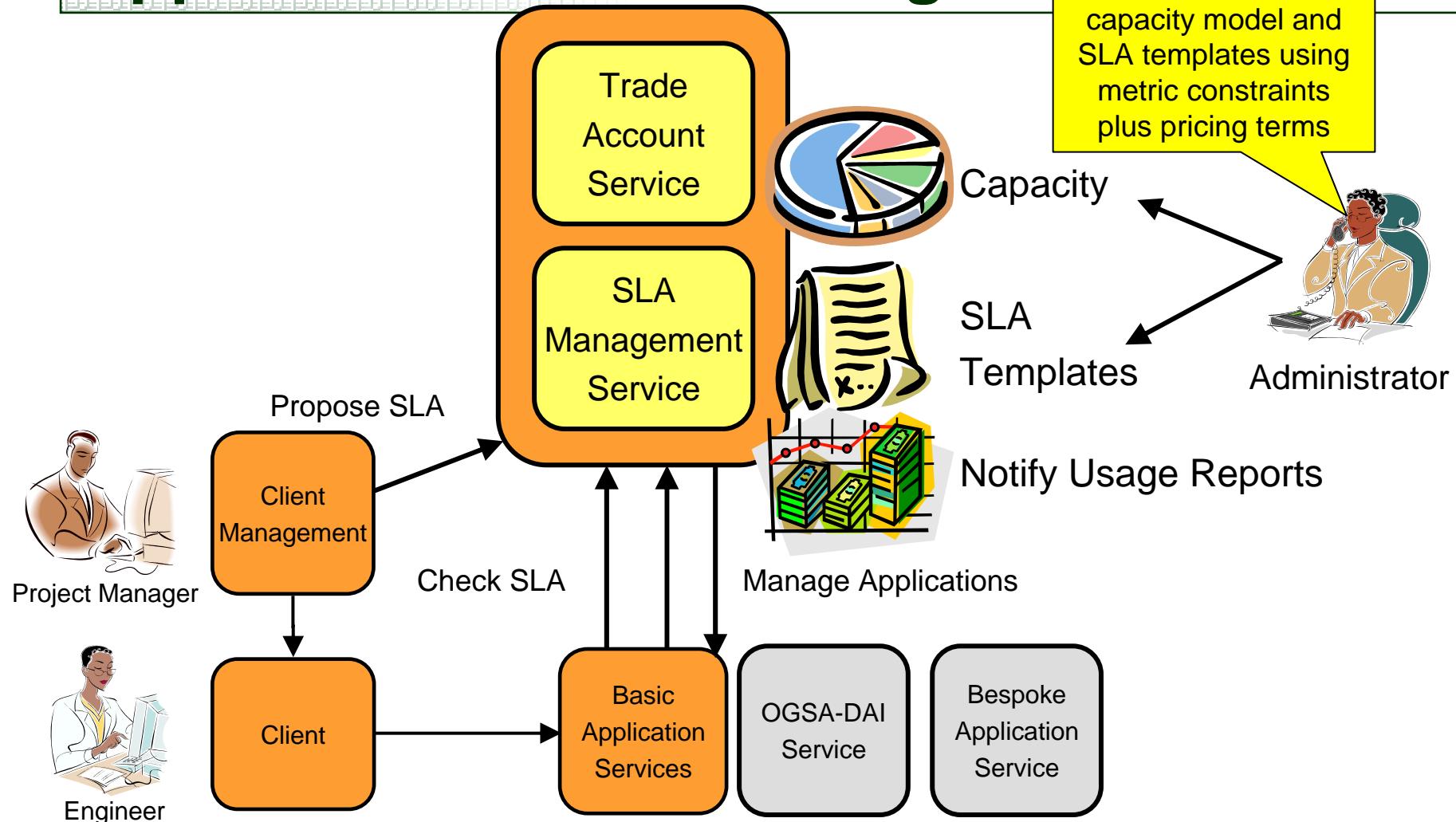
Application Service Management



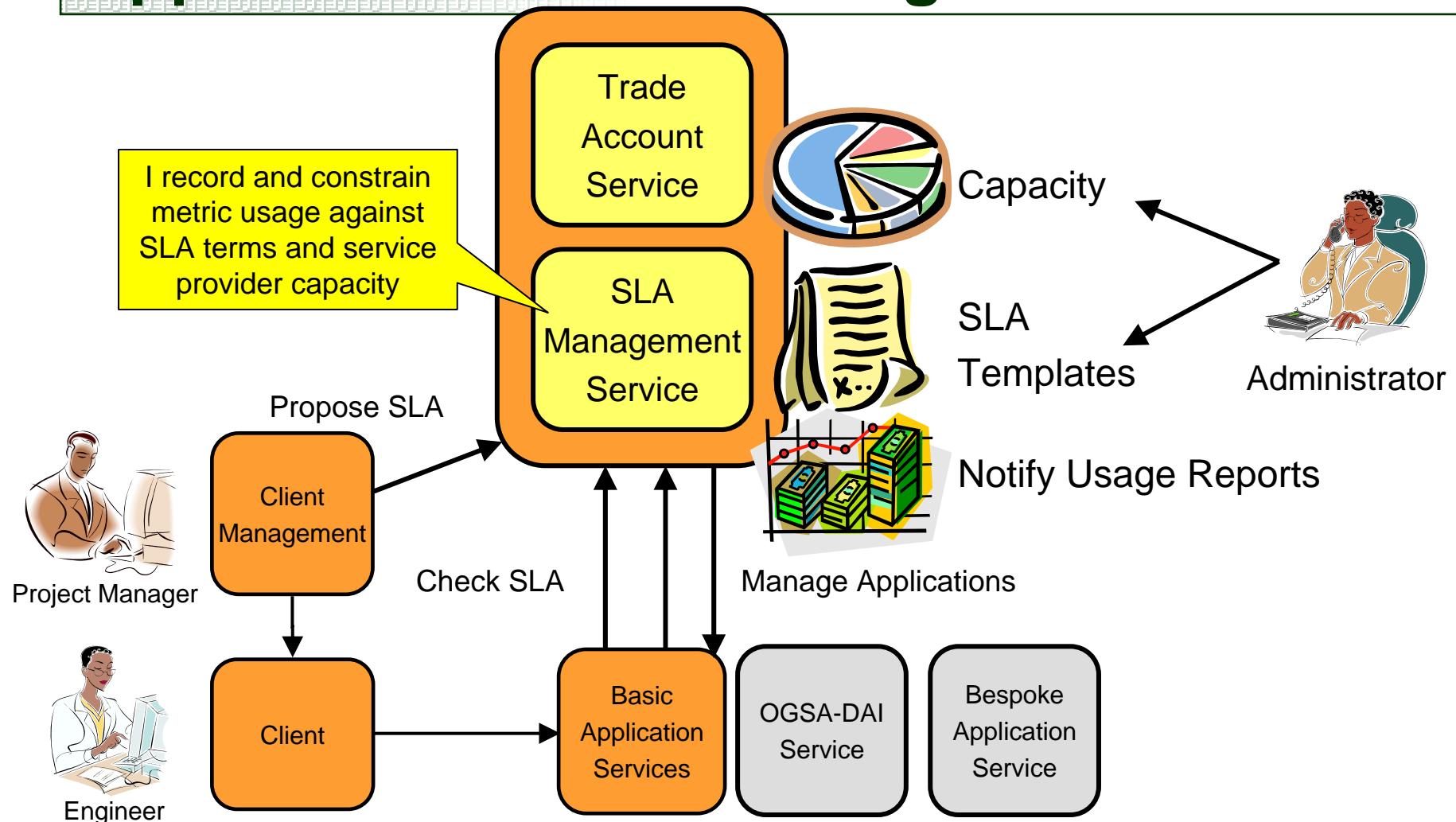
Application Service Management



Application Service Management



Application Service Management



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

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For more information



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

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SIMDAT

