

### The Semantic Grid: Past, Present and Future A Semantic Grid Masterclass

David De Roure University of Southampton www.semanticgrid.org



#### 1. The ambition

- 2. Enabling Technologies
  - Grid
  - Semantic Web
- 3. Semantic Grid
- 4. State of the Art
- 5. The Future



#### The ambition 1.

- **Enabling Technologies** 2.
  - Grid
  - Semantic Web
- Semantic Grid 3.
- State of the Art The Future 4.
- 5.

# Semantic Vision: J.C.R Licklider

"Lick had this concept of the intergalactic network which he believed was everybody could use computers anywhere and get at data anywhere in the world. He didn't envision the number of computers we have today by any means, but he had the same concept – all of the stuff linked together throughout the world, that you can use a remote computer, get data from a remote computer, or use lots of computers in your job."

> Larry Roberts, in Segaller, S (1998). "Nerds: A brief history of the internet", New York, TV Books Amsterdam

# Semantic Vision: Collaboratory

#### A collaboratory is

...a center without walls, in which the nation's researchers can perform their research without regard to geographical location, interacting with colleagues, accessing instrumentation, sharing data and computational resources, and accessing information in digital libraries

> William Wulf, 1989 U.S. National Science Foundation

# Semantic Vision: e-Science

e-Science is about global collaboration in key areas of science and the next generation of [computing] infrastructure that will enable it. e-Science will change the dynamic of the way science is undertaken.

John Taylor, Director General of UK Research Councils



Grid computing has emerged as an important new field, distinguished from conventional distributed computing by its focus on large-scale resource sharing, innovative applications, and, in some cases, high-performance orientation...we [define] the "Grid problem"...as flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources - what we refer to as virtual organizations

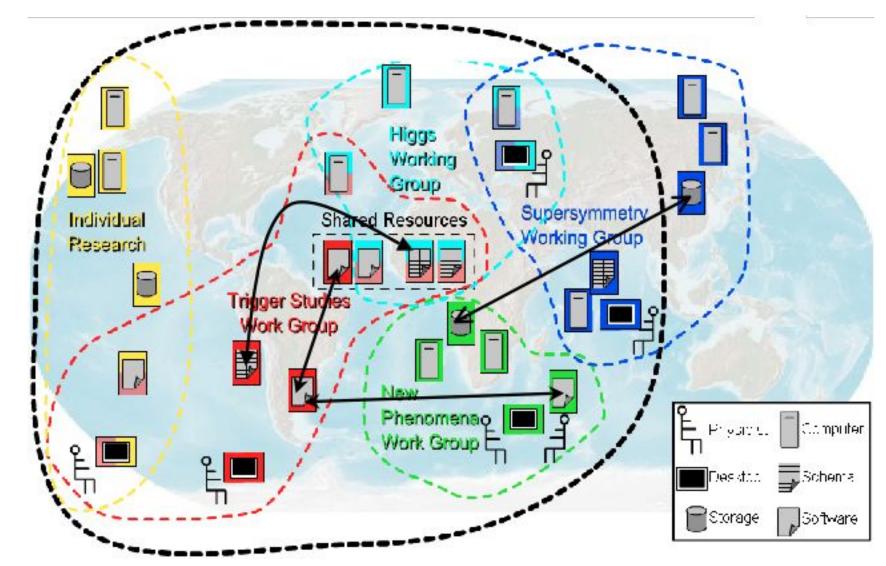
> From "The Anatomy of the Grid: Enabling Scalable Virtual Organizations" by Foster, Kesselman and Tuecke

# Semantic Vision: The Grid

"The ongoing convergence between Grids, Web Services and the Semantic Web is a fundamental step towards the realisation of a common serviceoriented architecture empowering people to create, provide, access and use a variety of intelligent services, anywhere, anytime, in a secure, costeffective and trustworthy way."

> Next Generation Grids 2 Requirements and Options for European Grids Research 2005-2010 and Beyond EU Expert Group Report July 2004

## Semantic Vision: The Grid

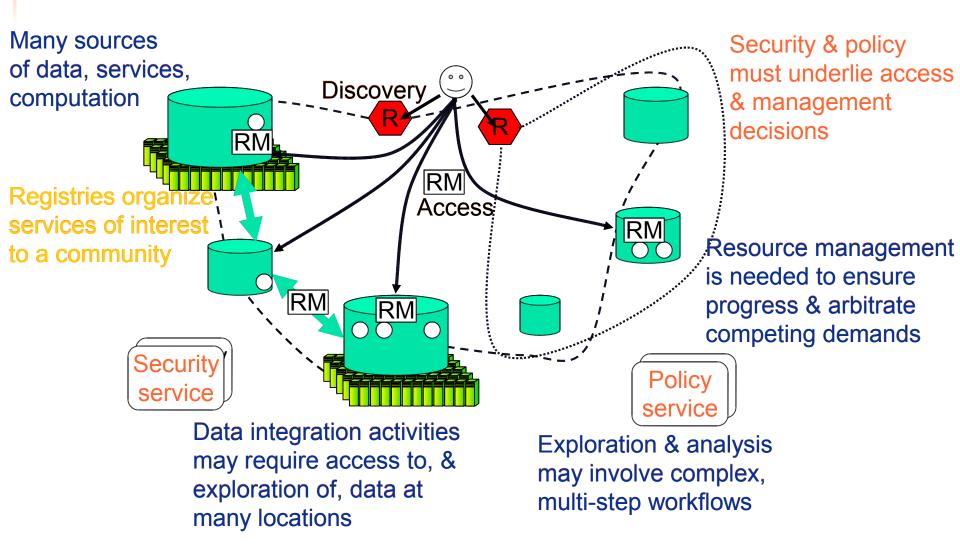


# Semantic Challenges: virtual orgs

- Resource configurations are transient, dynamic and volatile as services (databases, sensors, compute servers) switched in and out
- They are ad-hoc as service consortia have no central location or control, and no existing trust relationships
- They may be large, with hundreds of services orchestrated at any time
- They may be long-lived, for example a protein folding simulation could take weeks

- Scale of data and compute resources is large
- Quality of Service and performance criteria are severe
- Platform must be scalable, able to evolve, fault-tolerant, robust, persistent and reliable
- It should work seamlessly, and transparently – the user might not know or care where their calculation is done using how many machines, or where data is actually held

# Semantic Challenges: integration



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# Semantic Challenges: interop and reuse

# A SEC / UCSD & NCSA / UIC & Caltect A Mark

ADVANCED KNOWLEDGE TECHNOLOGIES

in the Grid

Collaborative

April 2005

- Wish to reuse
  - Data
  - Services
  - Knowledge
  - Software
- Anticipated useUnanticipated use



**UniGrids** 

Advanced Networ

Onto

t

nteroperability

Project

Enabling Grids for E-science in Europe

n

# Semantic Vision: The Grid

The Grid is fundamentally about joining things up, in an automated fashion, in order to do things that weren't possible before

**Data Computation People Instruments Services** 

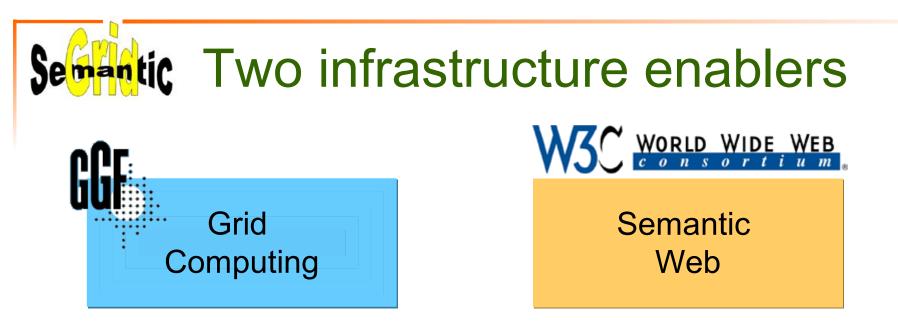
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#### The ambition 1.

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- On demand transparently constructed multiorganisational federations of distributed services
- Distributed computing middleware
- Computational Integration

- An automatically processable, machine understandable web
- Distributed knowledge and information management
- Information integration





By linking digital processors, storage systems and software on a global scale, grid technology is poised to transform computing from an Individual and corporate activity into a general utility

THE GRID: Computing without Bounds

By Ian Foster

# Semantic Grid Infrastructure

#### Application Specific Services such as "Run BLAST" or "Look at Houses for sale"

#### **Generally Useful Services and Features**

Such as "Access a Database" or "Submit a Job" or "Manage Cluster" or "Support a Portal" or "Collaborative Visualization"

#### **System Services and Features**

Handlers like WS-RM, Security, Programming Models like BPEL or Registries like UDDI

#### Container

can focus here

So we

Clarify these areas

Fox

# Semantic Grid Services

**Grid Applications** 

Open Grid Service Architecture

WSRF Profile for OGSA

Web Services

Building systems by composition of heterogeneous components demands that we standardise common patterns

- Approach to resource identification
- Lifetime management interfaces
- Inspection & monitoring interfaces
- Base fault representation
- Service and resource groups
- Notification

More than basic Web Services!

# Semantic OGSA Design Philosophy

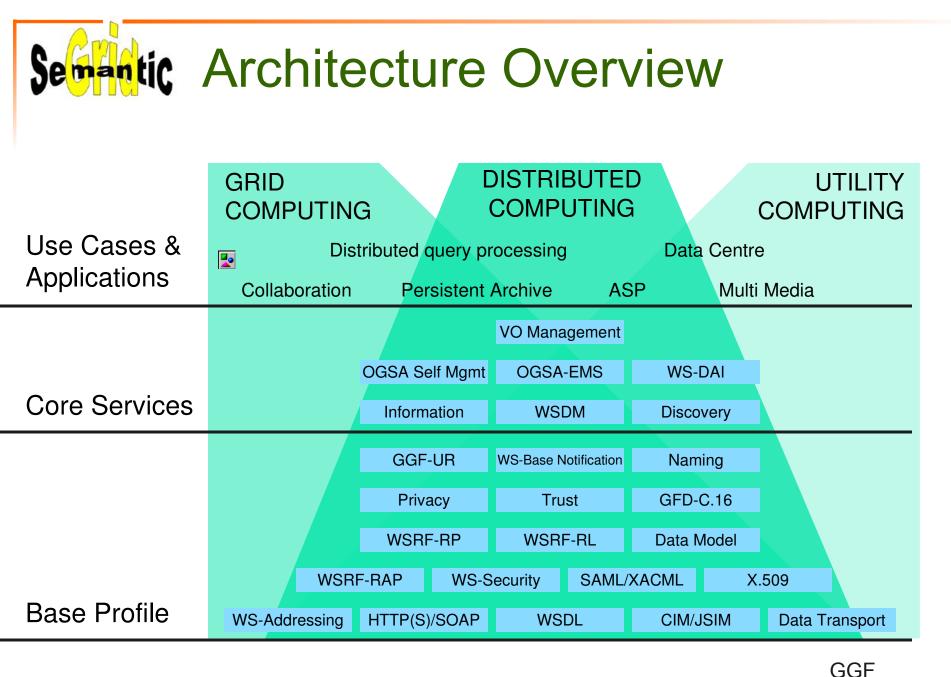
(Enhanced) Service Oriented Architecture

- Implicit Interface Extension (WSDL 2.0 'extends')
- Resources as First Class Entities (WSRF-Resources)
- Data type extensibility and introspection
- Dynamic service/resource/property creation and destruction

#### Use Case Driven

- Big and Small Science plus Industry and Commerce
- Component Based
  - Elements of the architecture are pluggable
- Customizable
  - Support for dynamic, domain-specific content, ...
  - Within the same standardized framework

#### Amsterdam



# Semantic Five Myths busted!

#### 1. Isn't it just for Physics?

- No e.g. Grids for Life Science and Medicine could dominate Grid applications
- Think of the range and scale of data and the community
- 2. Isn't it just High Performance computing?
  - No it's a generic mechanism for forming, managing and disbanding dynamic federations of services
  - Data integration, data access, data transport will dominate
  - Application integration is the key

# Semantic Five Myths busted!

1. Isn't it just a bag of protocols glued together?

 No – the Open Grid Service Architecture gives a well specified middleware stack built on industry standard web services

#### 2. Isn't it just Globus toolkit?

- No that is one implementation
- 3. Isn't it just a bunch of academics?
  - No commercial vendors are making serious investment

# Semantic GGF Leading the pervasive adoption of grid computing for research and industry

Defining grid specifications that lead to broadly adopted standards and interoperable software Building a broad international community for the exchange of ideas, experiences, requirements, and best practices

Operations Ensuring ongoing support of our mission and communication of our progress

Standards

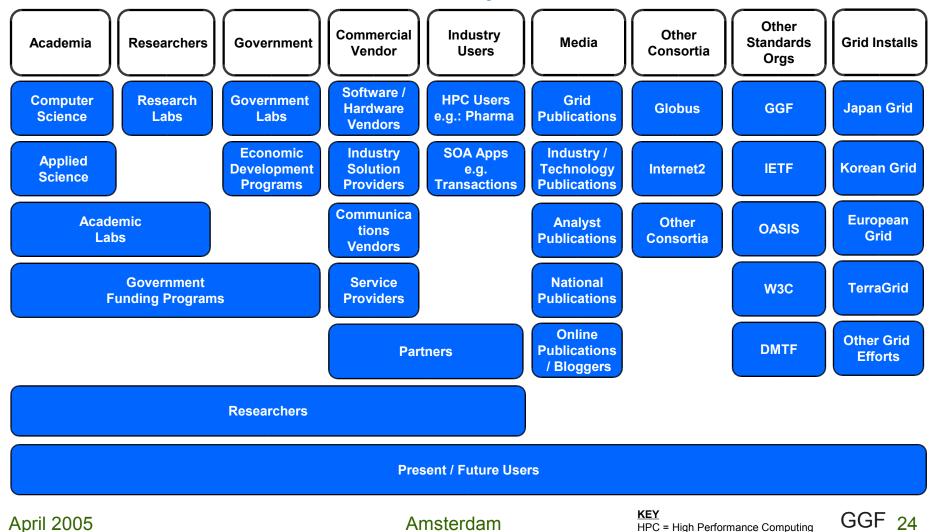
Community

Amsterdam

GGF

# Semantic The Grid ecosystem

#### **Grid Ecosystem**



SOA = Services Oriented Architecture

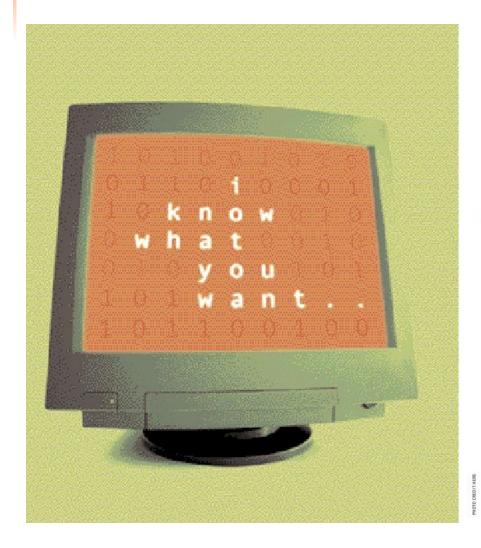


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# SEMANTIC

A new form of Web content that is meaningful to computers will unleash a revolution of new abilities

> by TIM BERNERS-LEE, JAMES HENDLER and ORA LASSILA

#### April 2005

#### Amsterdam

# Semantic Origins of the Semantic Web

The Semantic Web is an extension of the current Web in which information is given a well-defined meaning, better enabling computers and people to work in cooperation.

It is the idea of having data on the Web defined and linked in a way that it can be used for more effective discovery, automation, integration and reuse across various applications.

The Web can reach its full potential if it becomes a place where data can be processed by automated tools as well as people.

W3C Activity Statement

WEAVING

The Past, Present and Future

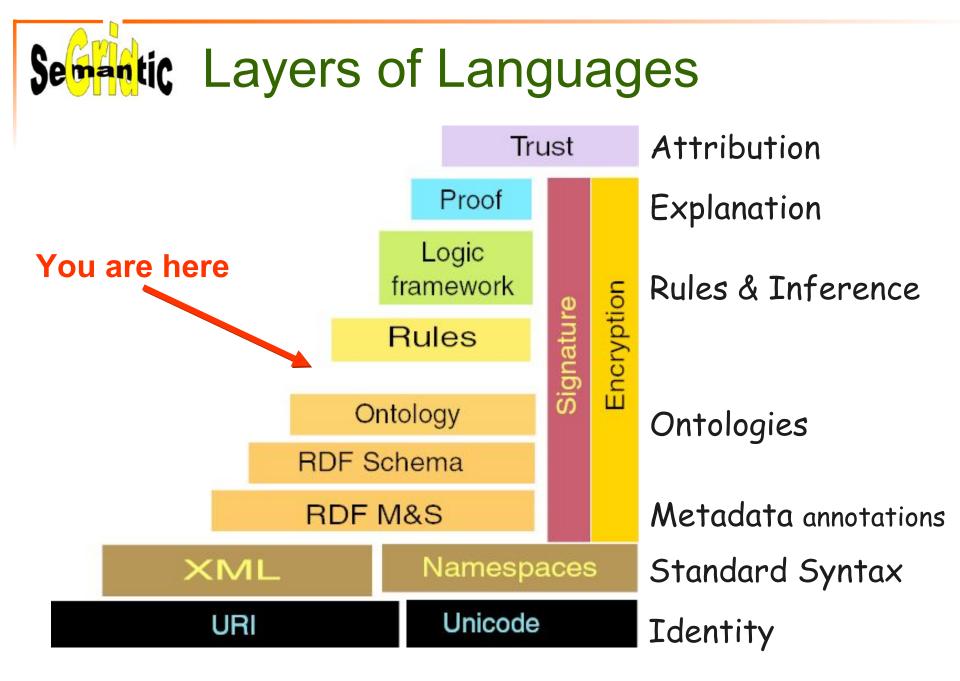
THE

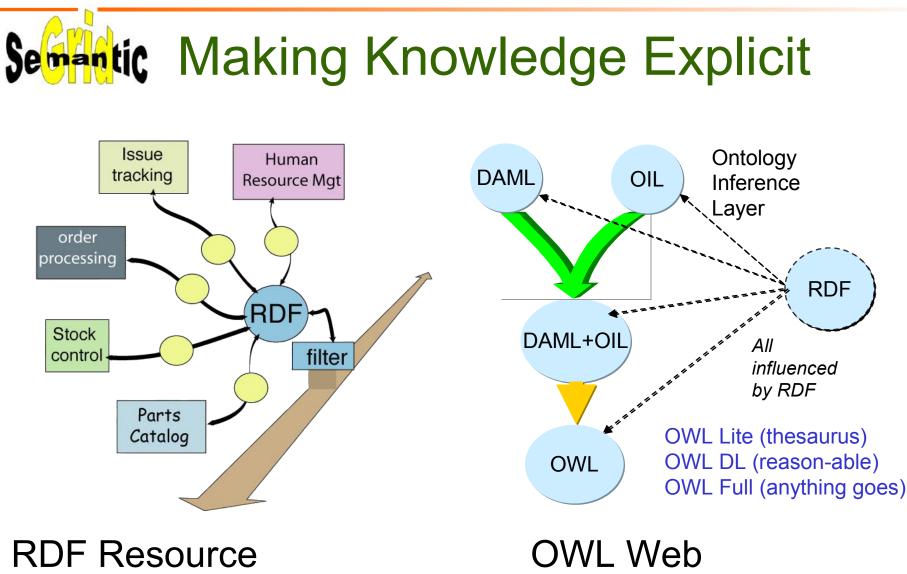
of the World Wide Web

by its Inventor

TIM BERNERS-LEE

FR





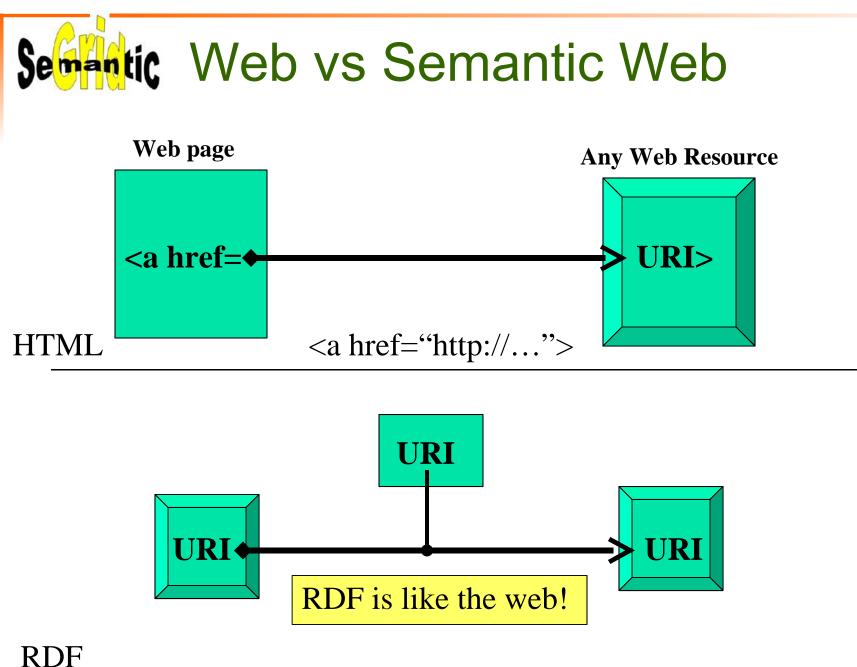
Description Framework

OWL Web Ontology Language

# Semantic Rocket Science (not)

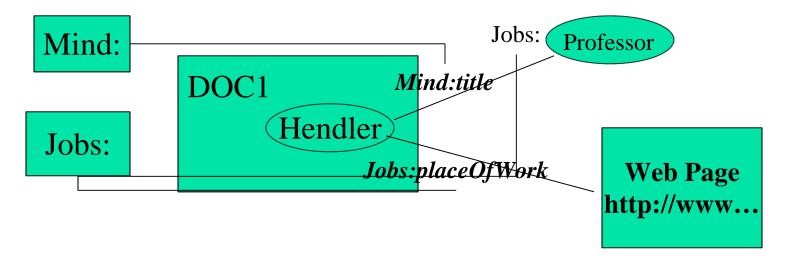
Is this rocket science? Well, not really. The Semantic Web, like the World Wide Web, is just taking well established ideas, and making them work interoperably over the **Internet**. This is done with standards, which is what the World Wide Web Consortium is all about. We are not inventing relational models for data, or query systems or rule-based systems. We are just webizing them. We are just allowing them to work together in a decentralized system - without a human having to custom handcraft every connection.

Tim Berners-Lee, Business Case for the Semantic Web, http://www.w3.org/DesignIssues/Business



# Semantic Sem Web models start from RDF...

DOC1 <mind:Person rdf:id="Hendler"> <mind:title jobs:Professor> <jobs:placeOfWork http://www.cs.umd.edu> </mind:Person>





In RDF, information is simply a collection of statements, each with a subject, verb and object - and nothing else.

In N3, you can write an RDF triple just like that, with a period:

<#pat> <#knows> <#jo> .

Everything, be it subject, verb, or object, is identified with a Universal Resource Identifier. This is something like

<http://www.w3.org/> or <http://www.w3.org/2000/10/swap/test/s1.n3#includes>

Primer: Getting into RDF & Semantic Web using N3, W3C

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		Age	Eyecol
	Pat	24	blue
	Al	3	green
	Jo	5	green

<#pat> <#age> 24; <#eyecolor> "blue" .
<#al> <#age> 3; <#eyecolor> "green" .
<#jo> <#age> 5; <#eyecolor> "green" .

# Semantic The O-Word

- An ontology is an explicit specification of a conceptualization [Gruber93]
- An ontology is a shared understanding of some domain of interest. [Uschold, Gruninger96]
- There are many definitions
  - a formal specification EXECUTABLE
  - of a conceptualization of a domain COMMUNITY
  - of some part of world that is of interest APPLICATION
- Defines
  - A common vocabulary of terms
  - Some specification of the meaning of the terms
- April 2005 A shared understanding for people and machines Tutorial 35

# Semantic 5 Myths Busted!

- **1.** Isn't it just AI and distributed agents (again)?
  - No It is primarily metadata integration and querying
- 2. Don't you need all that reasoning stuff?
  - No A little bit of semantics goes a long way! (Hendler)
- **3.** It only applies to the Web?
  - No the technologies are being used for Enterprise integration, exposing data in a common model, common ontology languages, representing terminologies.
- 4. One big ontology of everything never works!
  - No multiple ontologies; multiple everything!
- **5.** One big Semantic Web!
  - No lots of Semantic Web-lets, and expect it to break!

## Semantic Compare and contrast

The Grid	The Semantic Web
On demand transparently constructed multi-organisational federations of distributed services	An automatically processable, machine understandable web
Distributed computing middleware	Distributed knowledge and information management
Programmatic integration, originally based on protocols & toolkits	Information integration, based on metadata, ontologies and reasoning
Information & compute power <i>as</i> a utility	Information & knowledge <i>is</i> the new utility
Application pull: pioneers are application scientists with large scale collaboration problems, originally computationally-oriented.	Technology push: pioneers are primarily from the knowledge, agent and A.I. communities.
Scalability and performance	Er, yet to be proven



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### Semantic So what is the Semantic Grid?

- The Grid vision is about large scale distributed collaboration virtual organisations
- Fundamentally, this means that information and knowledge in and about the system must be 'machine processable'
- The Semantic Grid is an extension of the current Grid in which information and services are given well-defined meaning, better enabling computers and people to work in cooperation
- The full richness of the Grid ambition depends upon realising the Semantic Grid

#### Semantic The Semantic Grid Report 2001

- At this time, there are a number of grid applications being developed and there is a whole raft of computer technologies that provide fragments of the necessary functionality.
- However there is currently a major gap between these endeavours and the vision of e-Science in which there is a high degree of easy-to-use and seamless automation and in which there are flexible collaborations and computations on a global scale.

www.semanticgrid.org

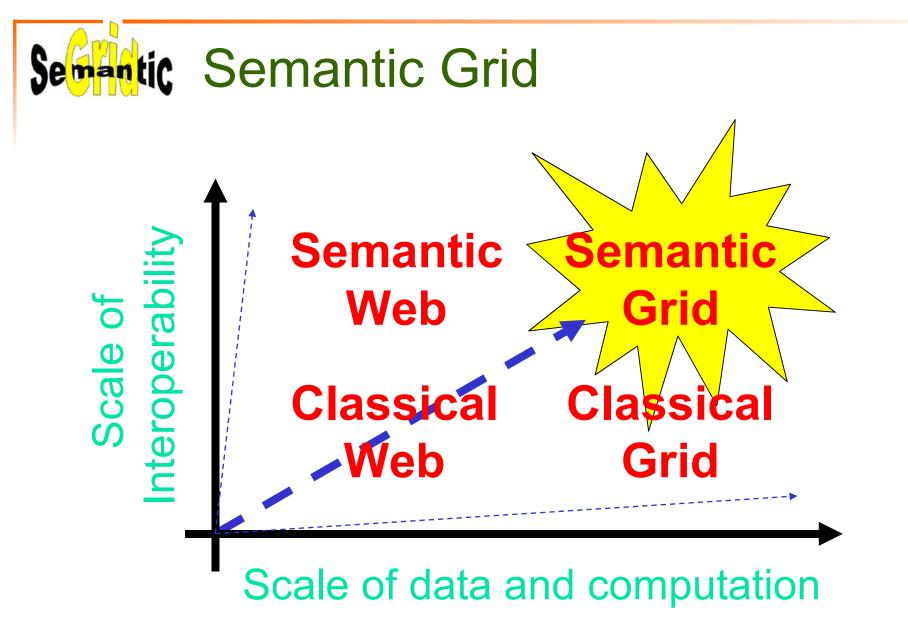
NB Report updated – March 2005 issue of Proceedings of the IEEE

## Semantic Building bridges





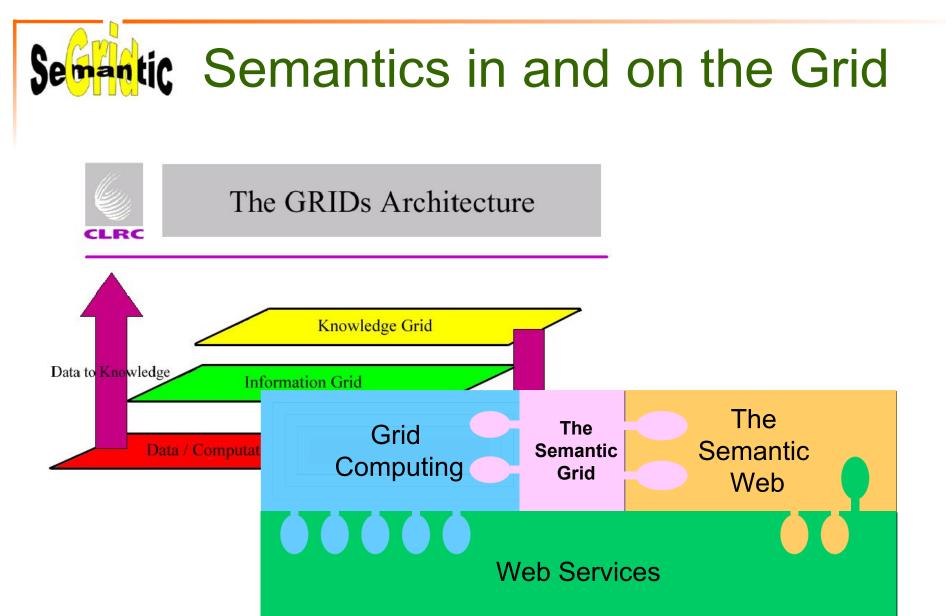
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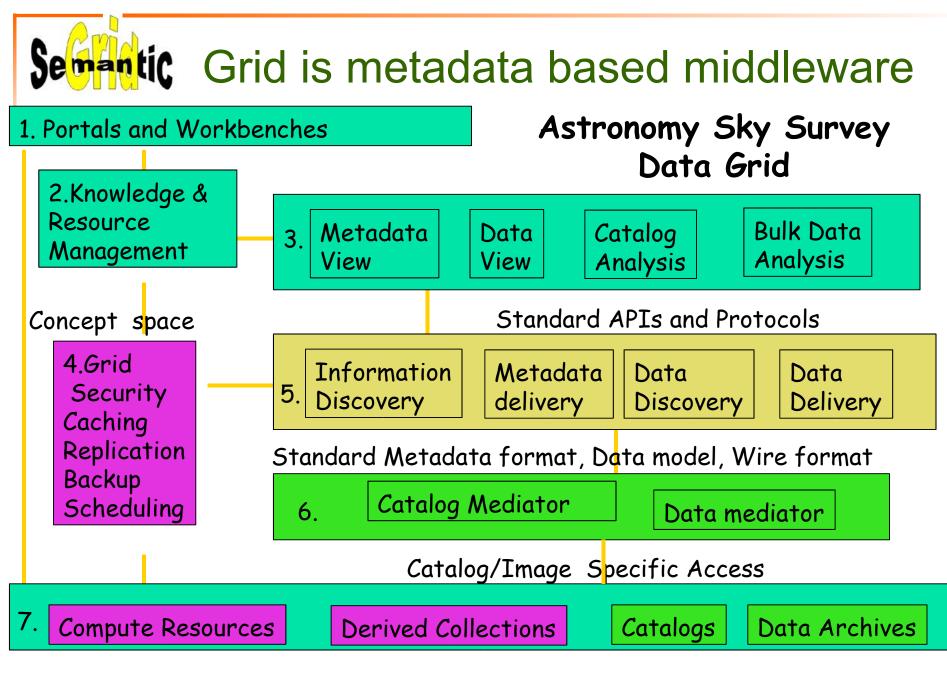


# Semantic Semantics in and on the Grid

The Semantic Grid is an extension of the current Grid in which information and services are given well-defined meaning, better enabling computers and people to work in cooperation







## Semantic For example...

Annotations of results, workflows and database entries could be represented by RDF graphs using controlled vocabularies described in RDF Schema and DAML+OIL

*Personal notes* can be XML documents annotated with metadata or RDF graphs linked to results or experimental plans

Exporting *results* as RDF makes them available to be reasoned over

RDF graphs can be the "glue" that associates all the components (literature, notes, code, databases, intermediate results, sketches, images, workflows, the person doing the experiment, the lab they are in, the final paper)

The *provenance* trails that keep a record of how a collection of services were orchestrated so they can be replicated or replayed, or act as evidence



At the data/computation layer: classification of computational and data resources, performance metrics, job control, management of physical and logical resources

At the information layer: schema integration, workflow descriptions, provenance trail

At the knowledge layer: problem solving selection, intelligent portals

Governance of the Grid, for example access rights to databases, personal profiles and security groupings

Charging infrastructure, computational economy, support for negotiation; e.g. through auction model

# Semantic Yet more ...

Represent the syntactic data types of e-Science objects using XML Schema data types

Represent domain ontologies for the semantic mediation between database schema, an application's inputs and outputs, and workflow work items

Represent domain ontologies and rules for parameters of machines or algorithms to reason over allowed configurations

Use reasoning over execution plans, workflows and other combinations of services to ensure the semantic validity of the composition

Use RDF as a common data model for merging results drawn from different resources or instruments

Capture the structure of messages that are exchanged between components

## GGF Semantic Grid RG

#### Goals

Many grid applications are set to benefit from semantic web tools and techniques. The semantic web includes standards and tools for immediate use (e.g RDF), ongoing activities (such as the W3C Web Ontology Working Group) and an active community of researchers. This RG provides a forum to track semantic web community activities, determine relevance to grid activities, provide a route for transfer of information and ideas between the communities and coordinate activities as appropriate.

### Semantic Motivating examples

- "Correlate the new molecular structure with the existing structural databases; what are the likely physical properties of the crystal?"
- "Retrieve & align 2000nt 5' from every serine/threonine kinase in Fabacae expressed exclusively in the root cortex whose expression increases 5x or more upon infection by Rhizobium but is not affected by osmotic or heavy-metal stresses & is <40% homologous in the active site to kinases known to be involved in cell-cycle regulation in any other species"

# Semantic Wikipedia entry

The Semantic Grid refers to an approach to Grid computing in which information, computing resources and services are described in standard ways that can be processed by computer. This makes it easier for resources to be discovered and joined up automatically, which helps bring resources together to create virtual organizations. The descriptions constitute metadata and are typically represented using the technologies of the Semantic Web, such as the Resource Description Framework (RDF).

By analogy with the Semantic Web, the Semantic Grid can be defined as "an extension of the current Grid in which information and services are given well-defined meaning, better enabling computers and people to work in cooperation."

This notion of the Semantic Grid was first articulated in the context of e-Science, observing that such an approach is necessary to achieve a high degree of easy-to-use and seamless automation enabling flexible collaborations and computations on a global scale.

The use of Semantic Web and other knowledge technologies in Grid applications is sometimes described as the Knowledge Grid. Semantic Grid extends this by also applying these technologies within the Grid middleware. Some Semantic Grid activities are coordinated through the Semantic Grid Research Group of the Global Grid Forum.

Amsterdam://en.wikipedia.org/wiki/Semantic\_Grid



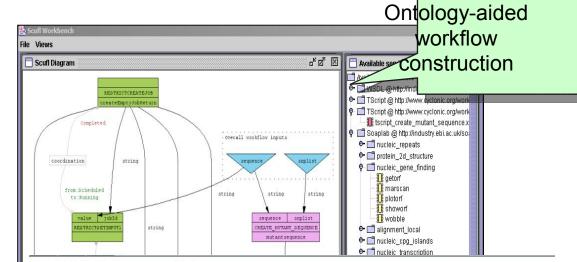
#### 1. The ambition

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### Semantics in e-Science

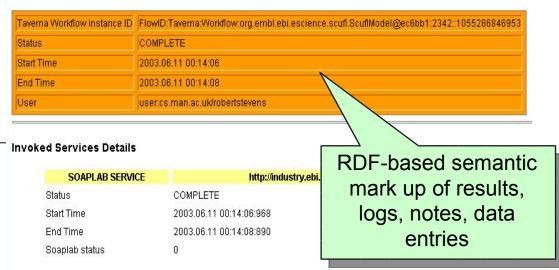
- RDF-based service and data registries
- RDF-based metadata for experimental components
- RDF-based provenance graphs
- OWL based controlled vocabularies for database content
- OWL based integration



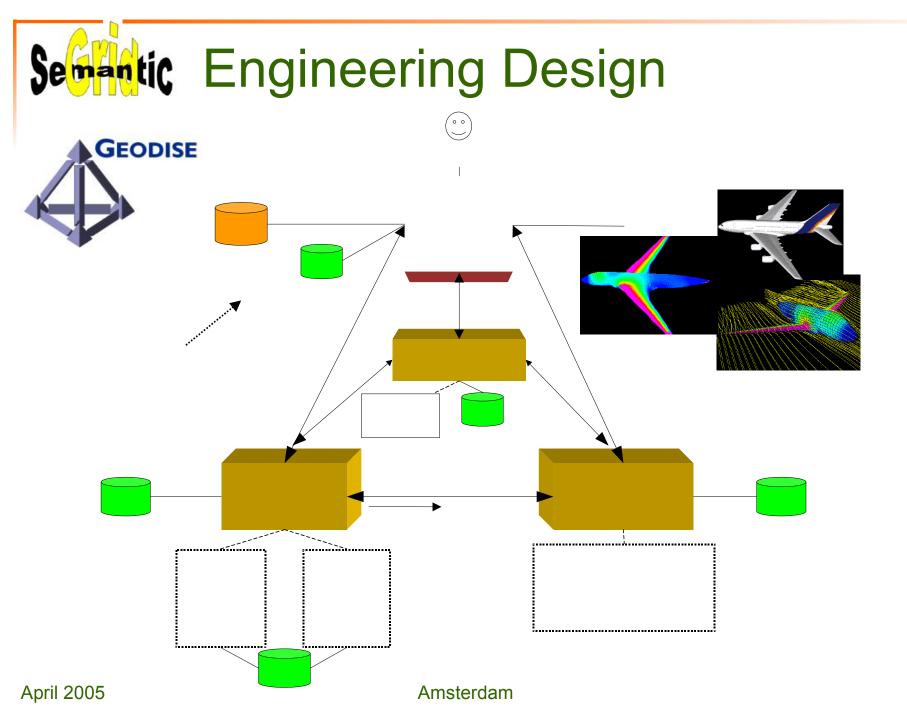


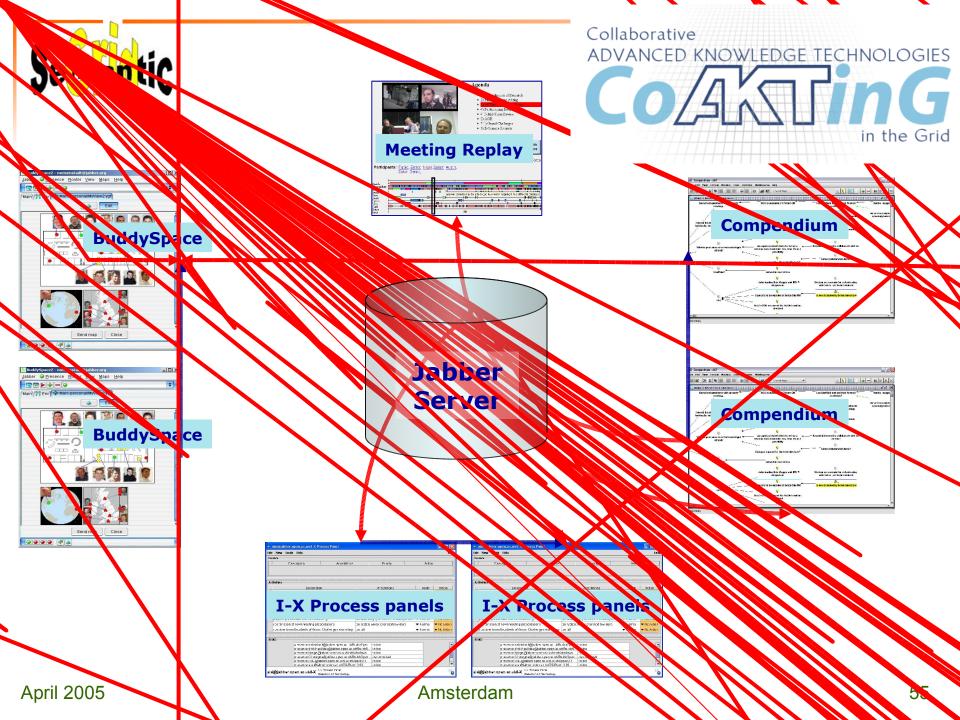
#### Workflow Provenance Data

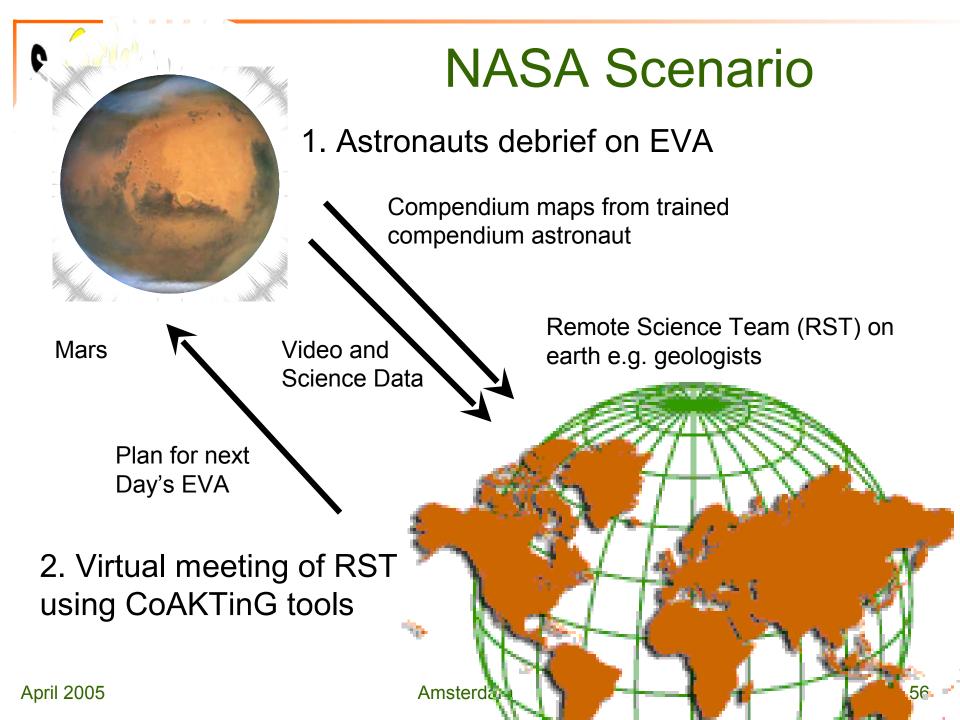
#### Workflow overall summary



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### Semantic GGF9 Semantic Grid Workshop

- The Role of Concepts in myGrid *Carole Goble*
- Planning and Metadata on the Computational Grid Jim Blythe
- Semantic support for Grid-Enabled Design Search in Engineering Simon Cox
- Knowledge Discovery and Ontology-based services on the Grid Mario Cannataro
- Attaching semantic annotations to service descriptions Luc Moreau
- Semantic Matching of Grid Resource Description Frameworks John Brooke
- Interoperability challenges in Grid for Industrial Applications *Mike Surridge*
- Semantic Grid and Pervasive Computing David De Roure

#### Semantic E-Science Special Issue

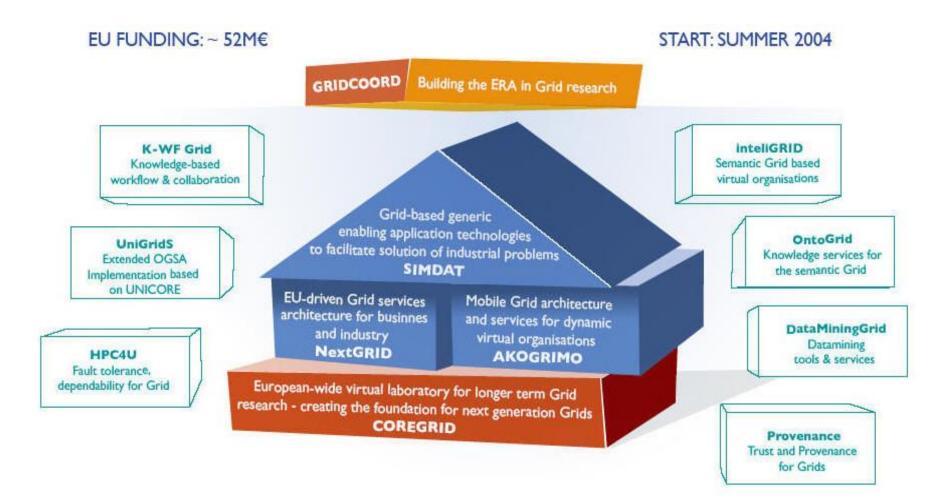
- IEEE Intelligent Issue Special Issue on E-Science, Jan-Feb 2004
  - De Roure, Gil, Hendler
- Challenges:
  - Realising the network effect
  - Moving beyond centralized stores
  - Automated assembly
  - Collaboration tools

## Semantic GGF11 Semantic Grid Workshop

- Engineering semantics: Costs and Benefits Simon Cox
- Designing Ontologies and Distributed Resource Discovery Services for an Earthquake Simulation Grid Marlon Pierce
- Exploring Williams-Beuren Syndrome Using myGrid Carole Goble
- Distributed Data Management and Integration Framework: The Mobius Project Shannon Hastings
- eBank UK Linking Research Data, Scholarly Communication and Learning David De Roure
- Using the Semantic Grid to Build Bridges between Museums and Indigenous Communities Ronald Schroeter

- Collaborative Tools in the Semantic Grid *David De Roure*
- The Integration of Peer-to-peer and the Grid to Support Scientific Collaboration
- OWL-Based Resource Discovery for Inter-Cluster Resource Borrowing *Hideki* YOSHIDA
- Semantic Annotation of Computational Components Peter Vanderbilt
- Interoperability and Transformability through Semantic Annotation of a Job Description Language Jeffrey Hau

**NEW GRID RESEARCH PROJECTS IN FP6** 





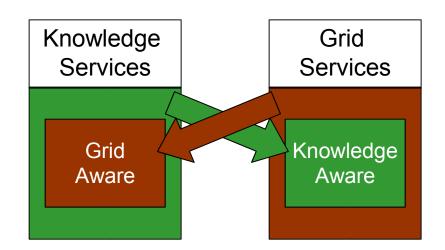
## Semantic OntoGrid Objectives

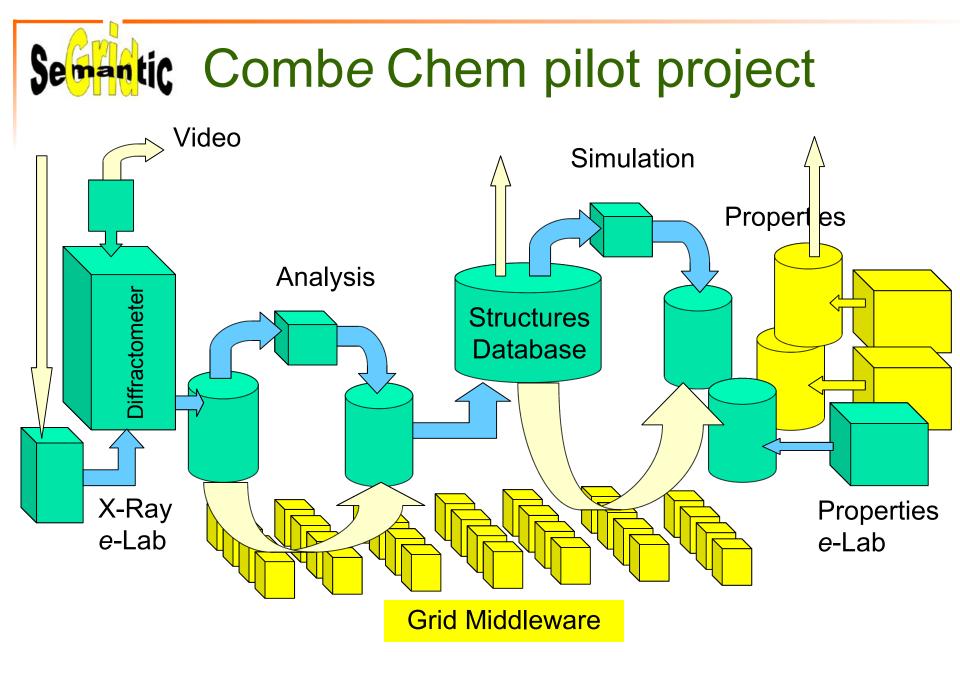
#### Strategic

- Pioneer the use of Knowledge Technologies (KT) to enhance and extend architecture and design of Grid computing systems
- Enable Deployment of Knowledge Technologies in Grid Architectures
- Deploy prototypes in the context of real world
   Business Applications

#### Technical

- Knowledge Services that are Grid Aware and Grid Compliant
- Grid Services that are Knowledge Aware





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#### Semantic CombeChem Smart Tea

#### the Smart Tea Project



is about improving the information environment for chemists doing chemistry - within and beyond the lab.

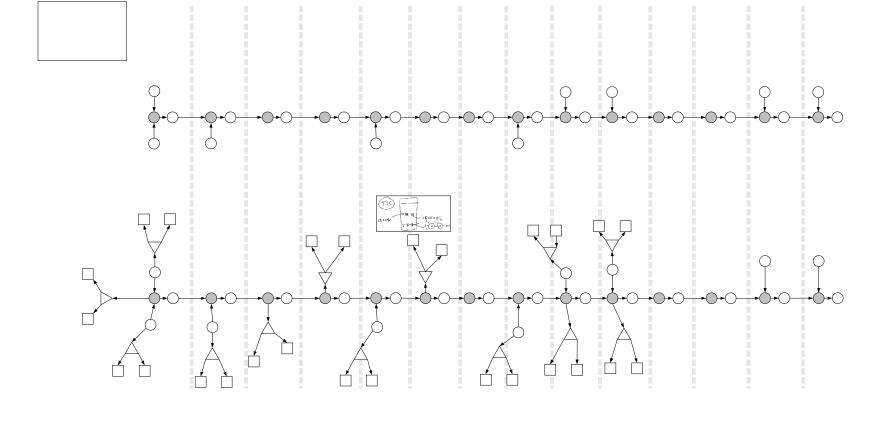
Smart Tea is about supporting chemists in the preparation, execution, analysis and dissemination of their experimental work.

#### www.smarttea.org











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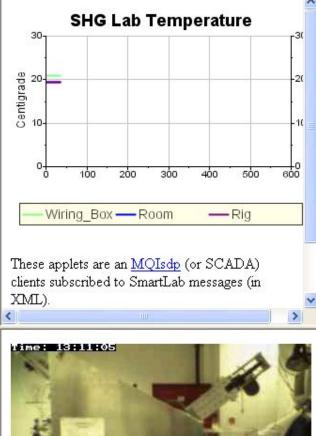


#### **Most Recent SHG Lab Status**

#### Interpreted

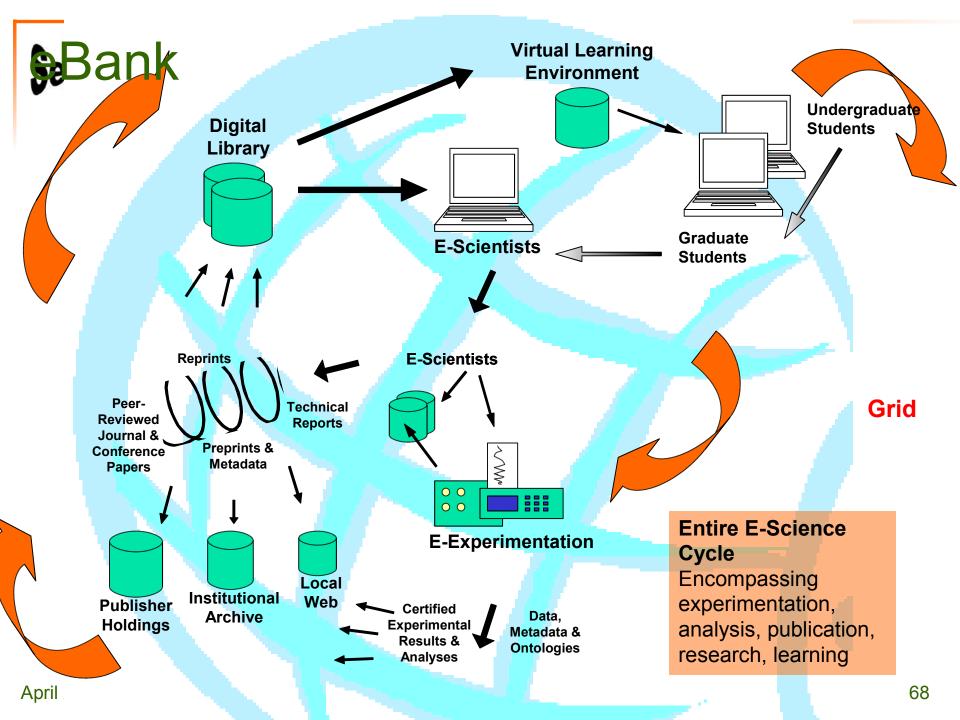
Item	Status	Last Updated
PIR Sensor 1	Not Triggered	Wed 01 Sep 2004 10:22:07
PIR Sensor 2	Not Triggered	Wed 01 Sep 2004 10:22:10
PIR Sensor 3	Not Triggered	Wed 01 Sep 2004 10:22:09
Door : Surface Science	Closed	Tue 31 Aug 2004 11:20:18
Door : Control Room	Closed	Wed 01 Sep 2004 10:22:09
InterLock	Engaged	Wed 01 Sep 2004 10:21:41
Light	On	Wed 01 Sep 2004 10:21:37
Wiring Box Temperature	20.996094C	Wed 01 Sep 2004 08:59:31
Room Temperature	19.531250C	Wed 01 Sep 2004 13:04:08
Rig Temperature	19.531250C	Wed 01 Sep 2004 13:04:38

#### **Smart Lab Snapshot**





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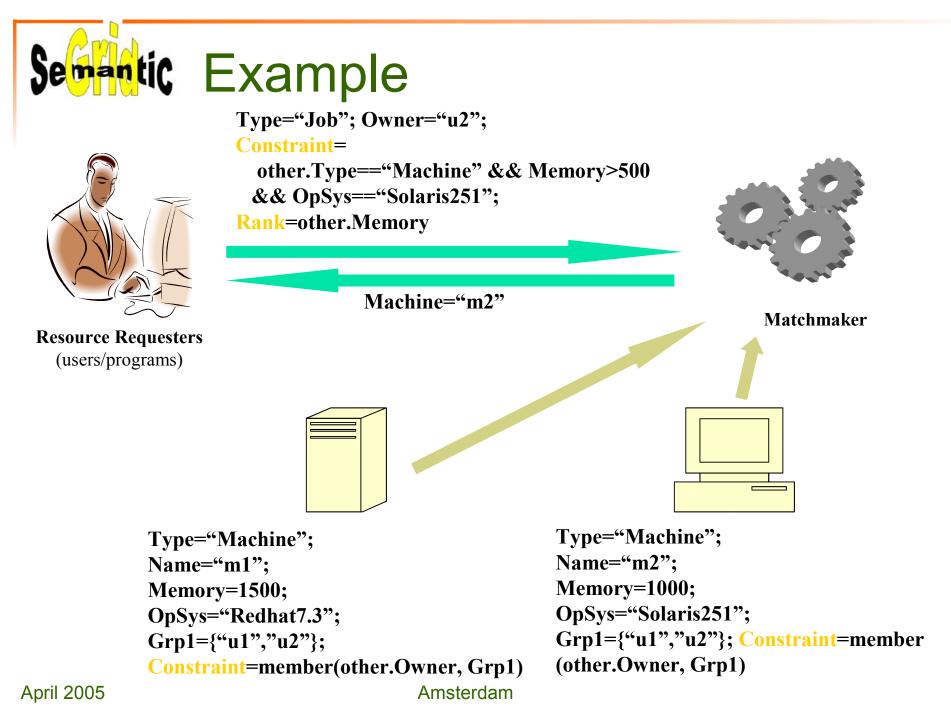
Ontology-based Resource Matching: The Grid Meets the Semantic Web

Hongsuda TangmunarunkitStefan DeckerCarl KesselmanCarl KesselmanCenter for Grid TechnologiesIntelligence Division

Information Sciences Institute University of Southern California

## Semantic Condor Matchmaker

- Exact syntactic matching
  - Examples: Condor Matchmaker, PBS
  - Use symmetric syntax (i.e., attribute-value pairs) to describe resources and requests
     Type="Machine"; Type="Job";
  - Constraints are specified by conjunctions and disjunctions of arithmetic/string comparisons and set membership Boolean operations
    - Memory > 1000

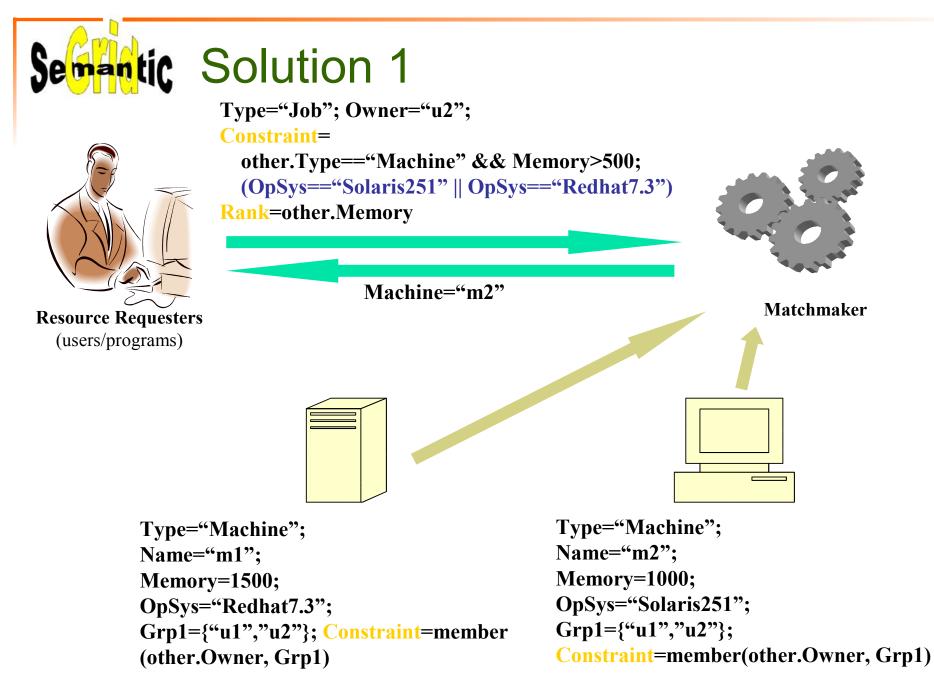


#### Semantic Finding the Unix machine

- A machine's operating system is described as "SunOS" or "Linux."
- To query for a machine that is "Unix" compatible, a user either has to:
  - Explicitly incorporate the Unix compatibility concept into the request requirements by requesting a disjunction of all Unix-variant operating systems

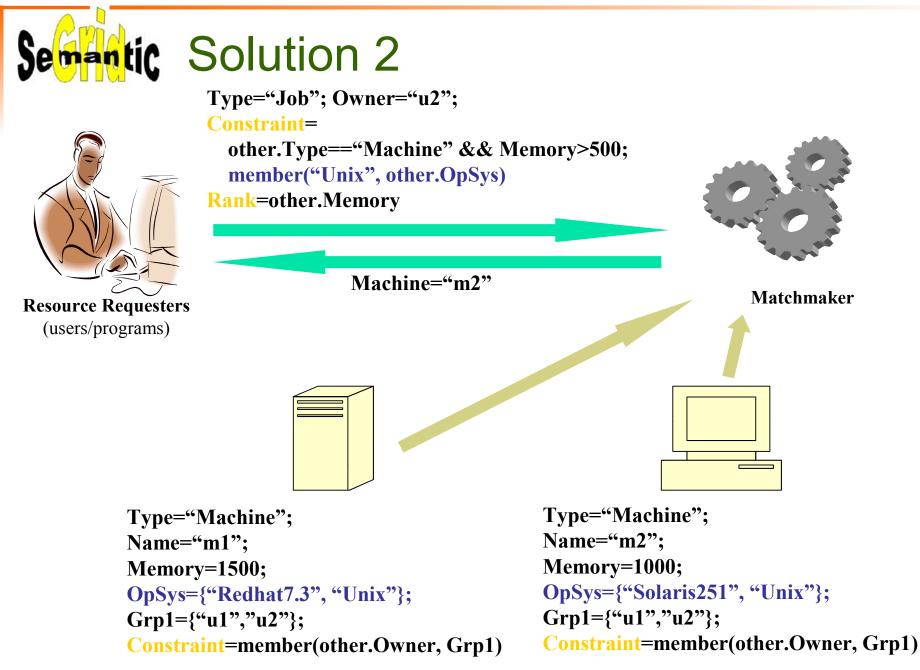
e.g., (OpSys="SunOS" OpSys="Linux")

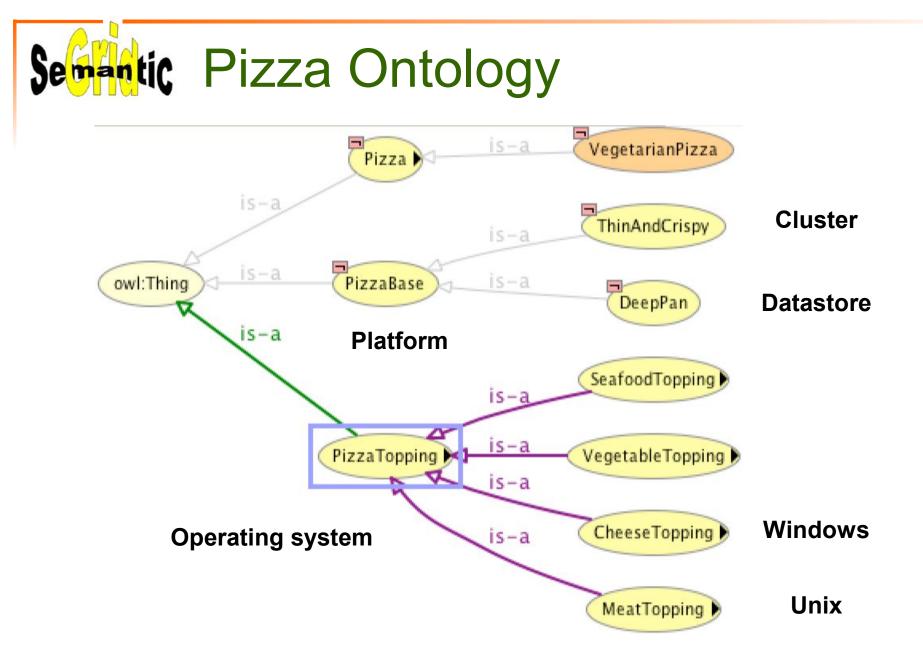
- The disjunctive requirements become unwieldy as more abstract concepts are developed.
- 5. Wait for all interesting resources to advertise their operating system as Unix as well as either Linux or SunOS e.g., (OpSys= "SunOS," "Unix"), and then express a match as setmembership of the desired Unix value in the OpSys value set e.g., hasMember(OpSys, "Unix").
- The advertisements become more complex and all resources must be updated before a match can occur.



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#### tic Insight from GRIP

- The process of building the ontologies gave insight into the fundamental differences in conceptualisation and hence the barriers to interoperability
- Globus (via the GLUE schema) attempts to model the abstract structure of the resources
  - · "This is what we are, this is what we can do"
- Unicore AJO abstracts the request for resources
  - "I want this work done in time for this event."



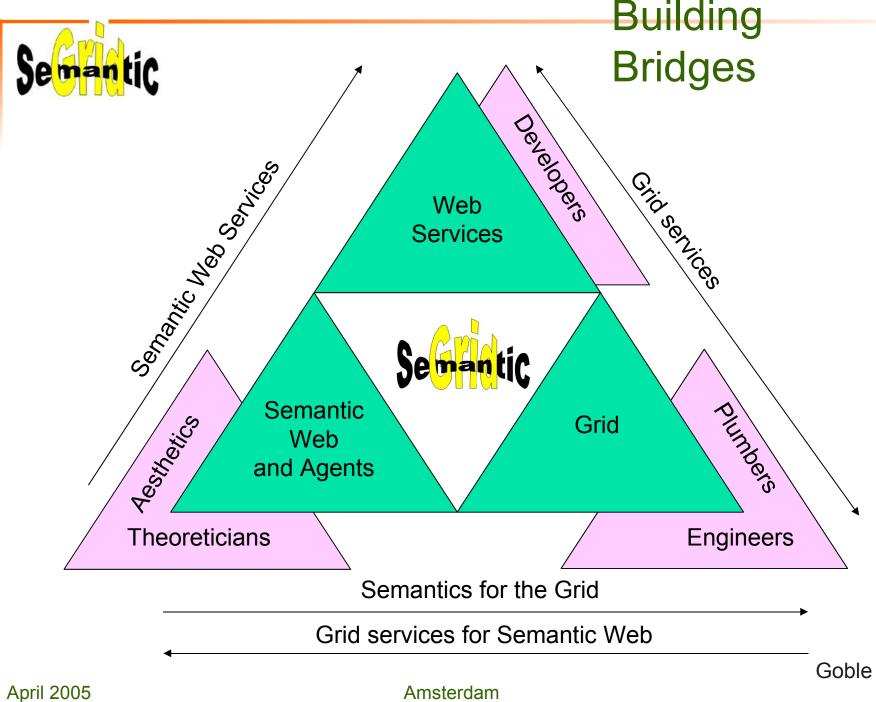
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Semantic Grid security and trust policies, management and frameworks **Resource** selection & scheduling **Ontologies for service classification Resource brokering** Knowledge Semantic aware Grid services **Representation for** Semantic Semantic Grid Services interoperability and integration Semantics in Agent Workflow and schedule repair Communication Knowledge-Languages based Semantics for service delegation provenance and knowledge aggregation and audit trails Service Quality of service and service (Semantic) event Negotiation notification level agreement management Models for quality and accessibility of data Lifetime sources, incl. versioning, recoverability, etc. management New models for Architectures for (Semantic) supporting Semantic Grid fault tolerance and Service state Services dependability Virtualisation and Grid aware provisioning of Audit trails over **Semantic services** Naming knowledge service transient state Scaleable service composition for

Apheterogeneous environments

Service enactment/invocation frameworks



#### Semantic Semantic Grid Services

- Service description, discovery
- Service composition, workflow
- Semantic matching vs e.g. Condor matchmaking
- Quality of Service, availability
- WSI+, WSRF, …
- Rules language compatibility
- Autonomy?

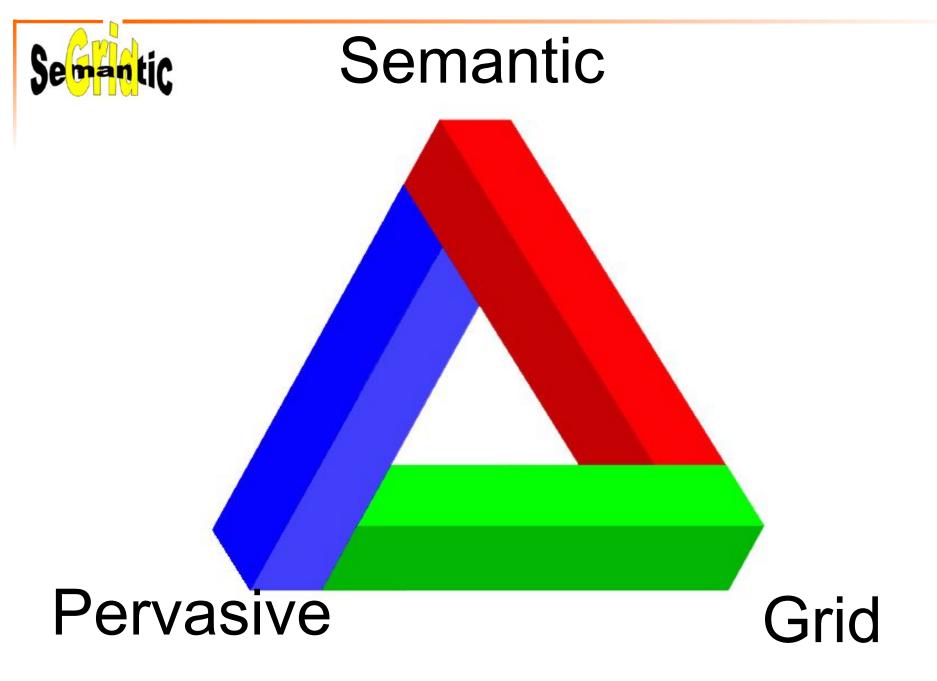
#### www.semanticgrid.org



David De Roure Carole Goble Geoffrey Fox

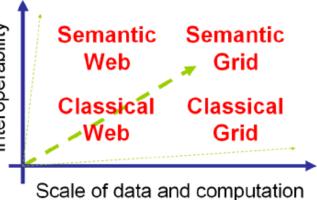
#### Semantic Agenda

- GGF IP policy, sign-up sheet, notetaker
- 2. Introduction to Semantic Grid (30mins)
- 3. Grid Resource Description ontology (5mins)
- 4. Semantic Web Services Kashif Iqbal (20mins)
- 5. Aspects of agent-based computing and Grid computing
  - 1. Agents and the Grid Hiroki Suguri (15mins)
  - 2. WS-Agreement Wolfgang Ziegler (10mins)
- 6. Discussion to inform charter review (5mins)



Trust Proof Logic framework Rules Ontology RDF Schema RDF M&S XML Namespaces URI Unicode

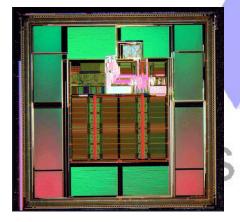
Semantic Fundamentally about Interoperability and inference





Grid and Pervasive share issues in large scale distributed systems. e.g. service description, discovery, composition; autonomic computing. These can be aided with semantics.





Pervasive applications need the Grid, e.g. Sensor Networks

> Grid applications need Pervasive Computing e.g. Smart Laboratory



### Semantic Research agenda March 2005

- 1. Automated Virtual Organisation Formation and Management
- 2. Service Negotiation and Contracts
- 3. Security, Trust and Provenance
- 4. Metadata and Annotation
- 5. Content Processing and Curation
- 6. Knowledge Technologies
- 7. Design and Deploy
- 8. Interaction
- 9. Collaboration
- 10. Pervasive Computing

## Semantic Discussion: single global system?

Knowledge representation, as this technology is often called, is currently in a state comparable to that of hypertext before the advent of the web: it is clearly a good idea, and some very nice demonstrations exist, but it has not yet changed the world. It contains the seeds of important applications, but to unleash its full power it must be linked into a single global system.

Tim Berners-Lee, inventor of the WWW, 2001

#### Semantic Community Events

- Attend...
  - CCGrid 2005 Semantic infrastructure for Grid Applications workshop (May)
  - Ubiquitous Computing for e-Research workshop at NeSC (May)
  - Semantic Grid: The Convergence of Technologies, Dagstuhl (July)
  - GGF14 and/or GGF15
  - Semantic Grid conference in China, late 2005
  - WWW2006 in Edinburgh, May 2006



# Thank you

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