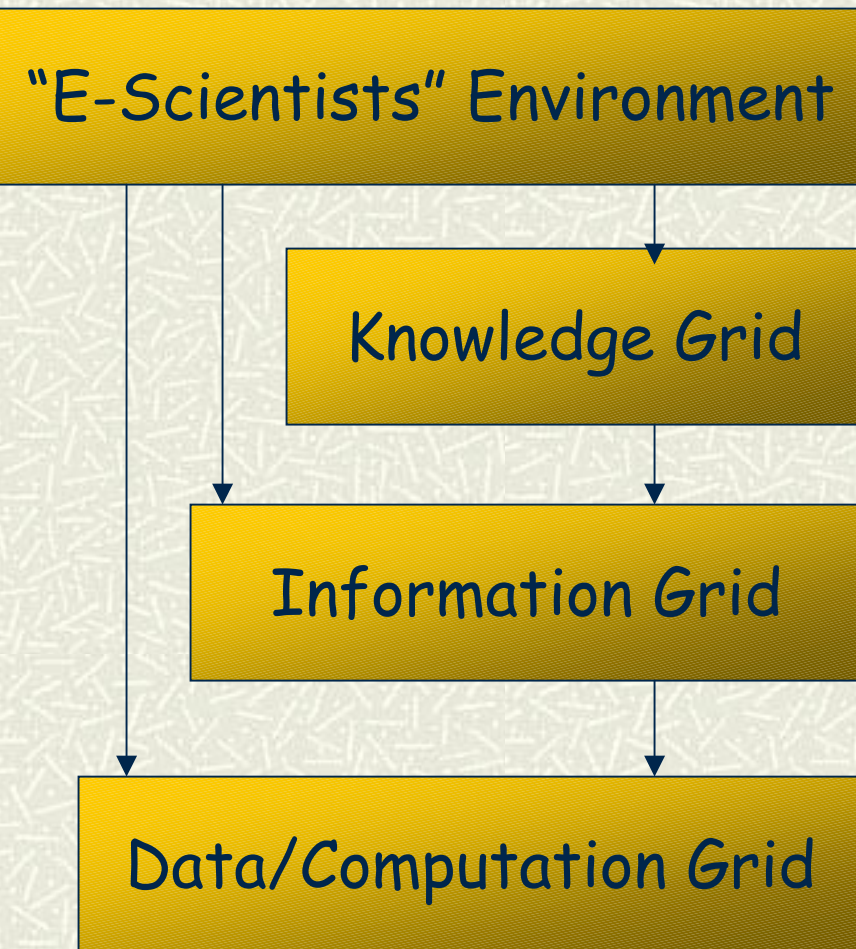


# What is the Grid?



## # In silico experiments

- Information harvesting & PSE
- Dynamically forming virtual organisations to solve problems.
- Describing, searching for and weaving resources: people, applications, db, content, instruments
- Orchestrating resources
- Support for scientific method: provenance, argumentation, opinion contextualisation etc

# Grid is metadata based middleware

## Astronomy Sky Survey Data Grid

1. Portals and Workbenches

2. Knowledge &  
Resource  
Management

3. Metadata  
View

Data  
View

Catalog  
Analysis

Bulk Data  
Analysis

Concept space

Standard APIs and Protocols

4. Grid  
Security  
Caching  
Replication  
Backup  
Scheduling

5. Information  
Discovery

Metadata  
delivery

Data  
Discovery

Data  
Delivery

Standard Metadata format, Data model, Wire format

6. Catalog Mediator

Data mediator

Catalog/Image Specific Access

7. Compute Resources

Derived Collections

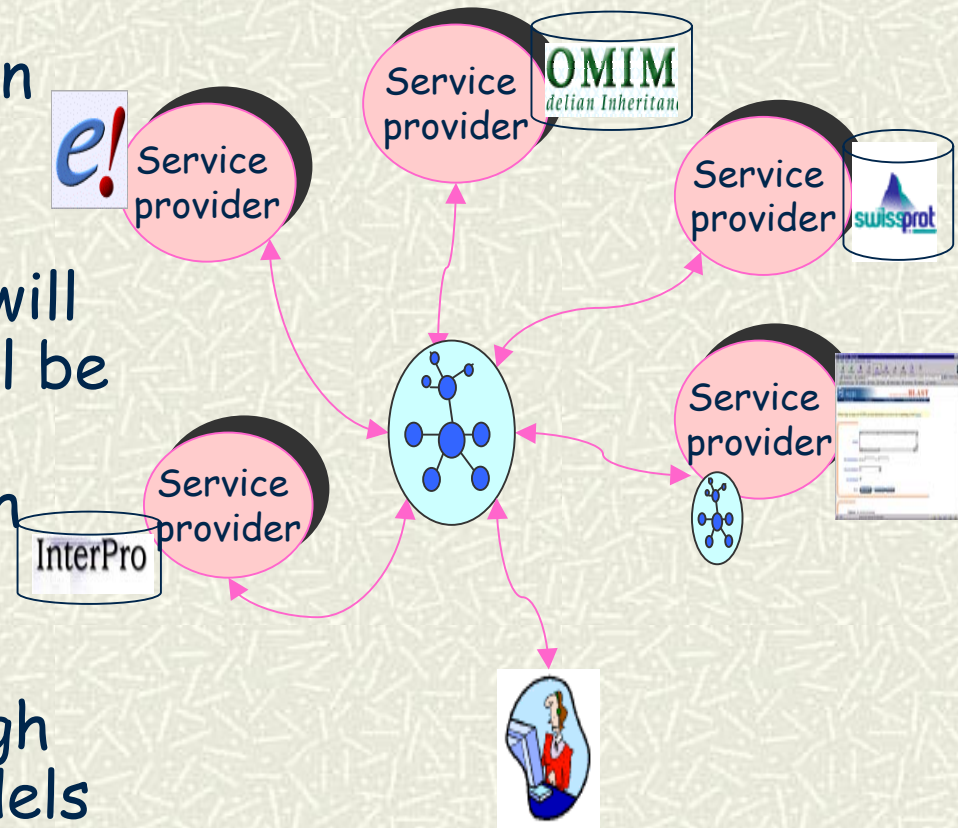
Catalogs

Data Archives

# Grid is...

## dynamic marshalling of resources

- Needs describing the resources, mapping between resources.
- Resources include BIG databases - the instances will not be on the web, they will be inside applications and databases (there isn't much difference).
- Semantic web technologies for shared meaning (through ontologies) and shared models (e.g. exporting results through RDF and using inference over them).



# Isn't information all computationally accessible already?

- Document publishing paradigm.
- Descriptive knowledge.
- Ontologies for controlling content already used.
- Evolving, non-predictive schemas
- XML is king.

InterPro Entry IPR000025 - Netscape

Database	InterPro
Accession	IPR000025; Melatonin_receptor (matches 22 proteins)
Name	Melatonin receptor
Type	Family
Dates	08-OCT-1999 (created) 27-MAR-2000 (last modified)
Signatures	<a href="#">PR00857</a> ; MELATONINR (22 proteins)
Parent	<a href="#">IPR000276</a> ; Rhodopsin-like GPCR superfamily (3990 proteins)
Children	<a href="#">IPR002278</a> ; Melatonin 1A receptor (12 proteins) <a href="#">IPR002279</a> ; Melatonin 1C receptor (5 proteins) <a href="#">IPR002280</a> ; Melatonin-related 1X receptor (3 proteins)
Function	melatonin receptor ( <a href="#">GO:0008502</a> )
Component	membrane ( <a href="#">GO:0016020</a> )

**Abstract**

G-protein-coupled receptors (GPCRs) constitute a vast protein family that encompasses a wide range of functions (including various autocrine, paracrine and endocrine processes). They show considerable diversity at the sequence level, on the basis of which they can be separated into distinct groups. We use the term clan to describe the GPCRs, as they embrace a group of families for which there are indications of evolutionary relationship, but between which there is no statistically significant similarity in sequence [1]. The currently known clan members include the rhodopsin-like GPCRs, the secretin-like GPCRs, the cAMP receptors, the fungal mating pheromone receptors, and the metabotropic glutamate receptor family.

The rhodopsin-like GPCRs themselves represent a widespread protein family that includes hormone, neurotransmitter and light receptors, all of which transduce extracellular signals through interaction with guanine nucleotide-binding (G) proteins. Although their activating ligands vary widely in structure and character, the amino acid sequences of the receptors are very similar and are believed to adopt a common structural framework comprising 7 transmembrane (TM) helices [2, 3, 4].

Melatonin is secreted by the pineal gland during darkness [5]. It regulates a variety of neuroendocrine functions and is thought to play an essential role in circadian rhythms. Drugs that modify the action of melatonin, and hence influence circadian cycles, are of clinical interest (for example, in the treatment of jet-lag). Melatonin receptors are found in the retina, in the pars tuberalis of the pituitary, and in discrete areas of the brain. The receptor inhibits adenylyl cyclase via a pertussis toxin-sensitive G-protein, probably of the Gi/Go class [5].

**Examples**

- [P49288](#) ML1C\_CHICK
- [P49285](#) ML1A\_CHICK
- [P49219](#) ML1C\_XENLA
- [P49217](#) ML1A\_PHOSU

[View examples](#)

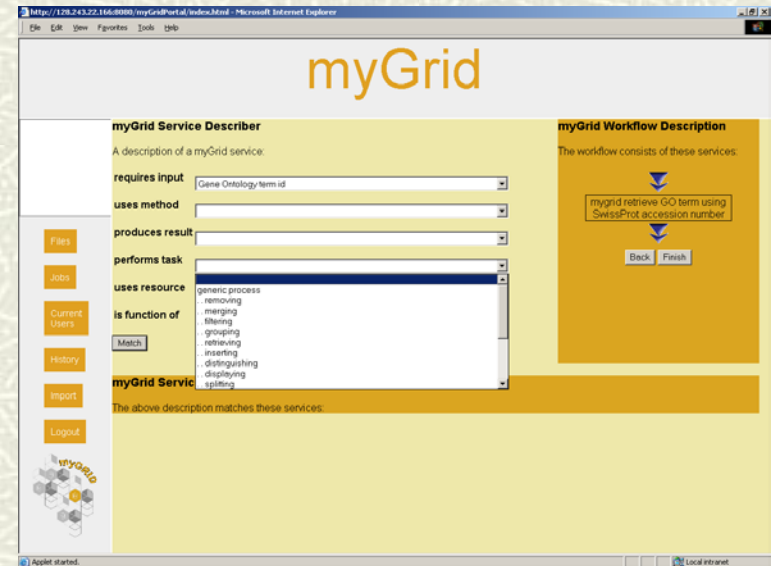
**References**

1. Attkwood T.K., Findlay J.B.C. *Fingerprinting G-protein-coupled receptors*. Protein Eng. 7: 195-203(1994). [IMEDLINE:94224751] [PUB00004961]

Document Done

# Grid is ... services, services, services

- # The first generation of Grid was protocol based.
- # Second generation is *service* based: Open Grid Service Architecture.
- # Semantic Web description and annotation technologies core to service sophisticated service description and processing.
- # Descriptions => Automated discovery & search, selection, (imprecise) matching, composition & interoperation, invocation, execution monitoring
- # Reasoning is darn handy



# The Semantic Grid is ...knowledge management

Q: What ATPase superfamily proteins are found in mouse?

1. P21958 (from Swiss-Prot).
2. InterPro is a pattern database and could tell you if you had permission and paid.
3. Attwood's lab expertise is in nucleotide binding proteins
4. Jones published a new paper on this in Nature Genetics two weeks ago
5. Smith in your lab already asked this question...

# Remarks

- # Semantic Web is a part of the Grid vision?
- # Semantic Web technologies should be relevant for Grid metadata at all levels.
- # There isn't one Grid, there are collections of Grids for communities - might be a more tractable model for the Semantic Web.
- # Most facts will stay in databases. Metadata about the (scientific) process and facts could be in RDF.
- # E-Science (everyone?) loves XML and ignores RDF
  - Annotations sit in other (non RDF) databases.
- # Reliability, scalability, performance, explanation, longevity, evolution ...

# The Road Ahead: Scientific Data Integration with the Semantic Web !?



# The Road Ahead: Scientific Data Integration with the Semantic Web !?

*Internet2*

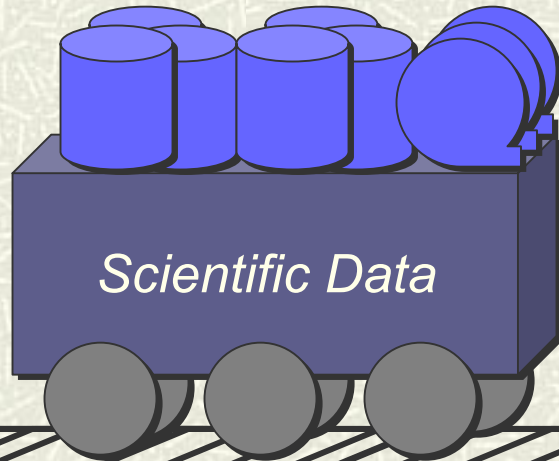


# The Road Ahead: Scientific Data Integration with the Semantic Web !?

*Internet2*

***Data-Grid***

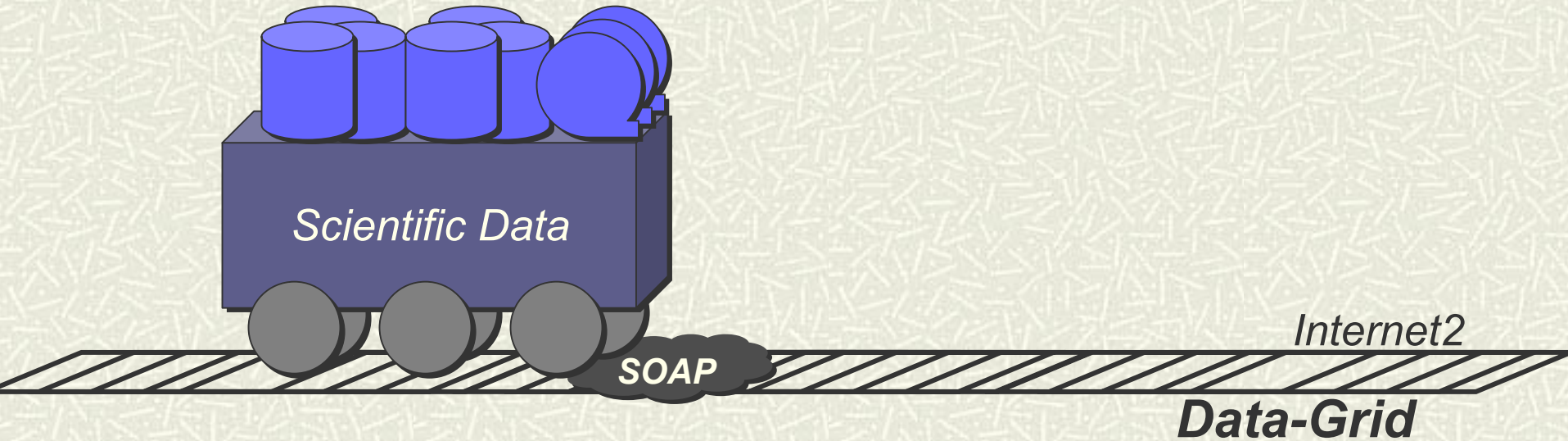
# The Road Ahead: Scientific Data Integration with the Semantic Web !?



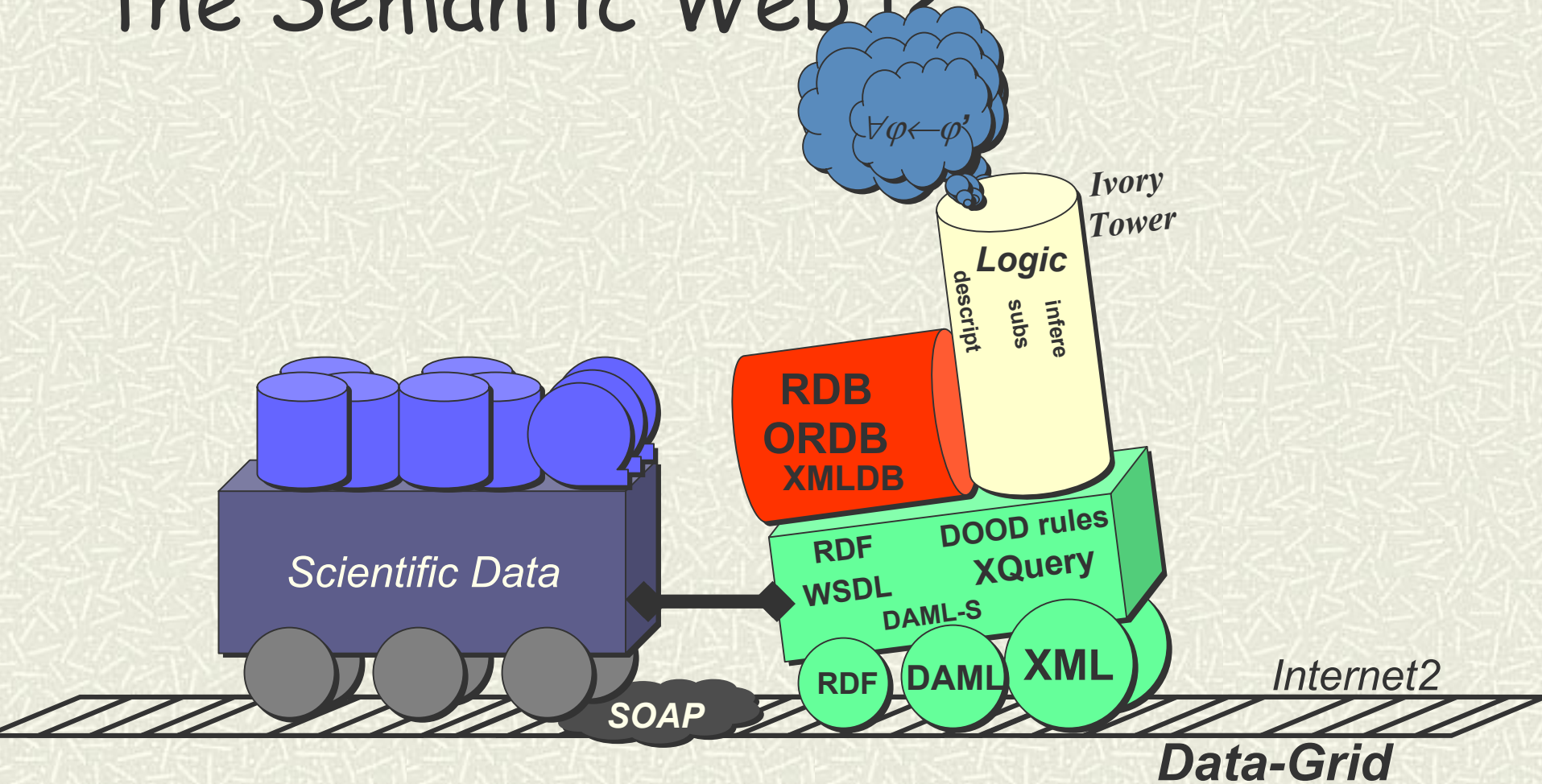
*Internet2*

**Data-Grid**

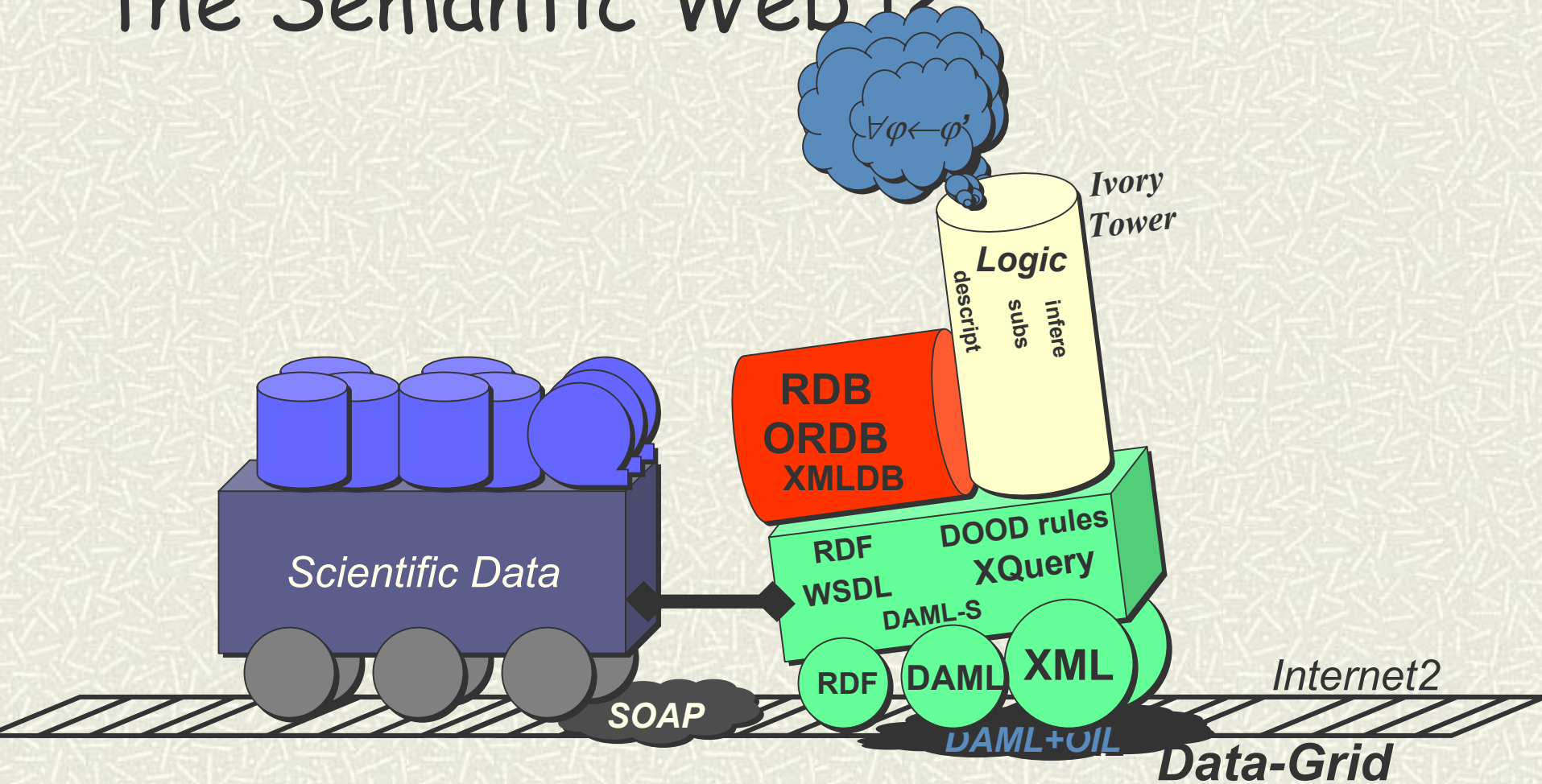
# The Road Ahead: Scientific Data Integration with the Semantic Web !?



# The Road Ahead: Scientific Data Integration with the Semantic Web I2



# The Road Ahead: Scientific Data Integration with the Semantic Web I2



# The Road Ahead: Scientific Data Integration with the Semantic Web I2

