



VAMDC

Virtual Atomic and Molecular Data Centre



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With the collaboration of:

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Uncertainties in atomic data and how they propagate in chemical abundances

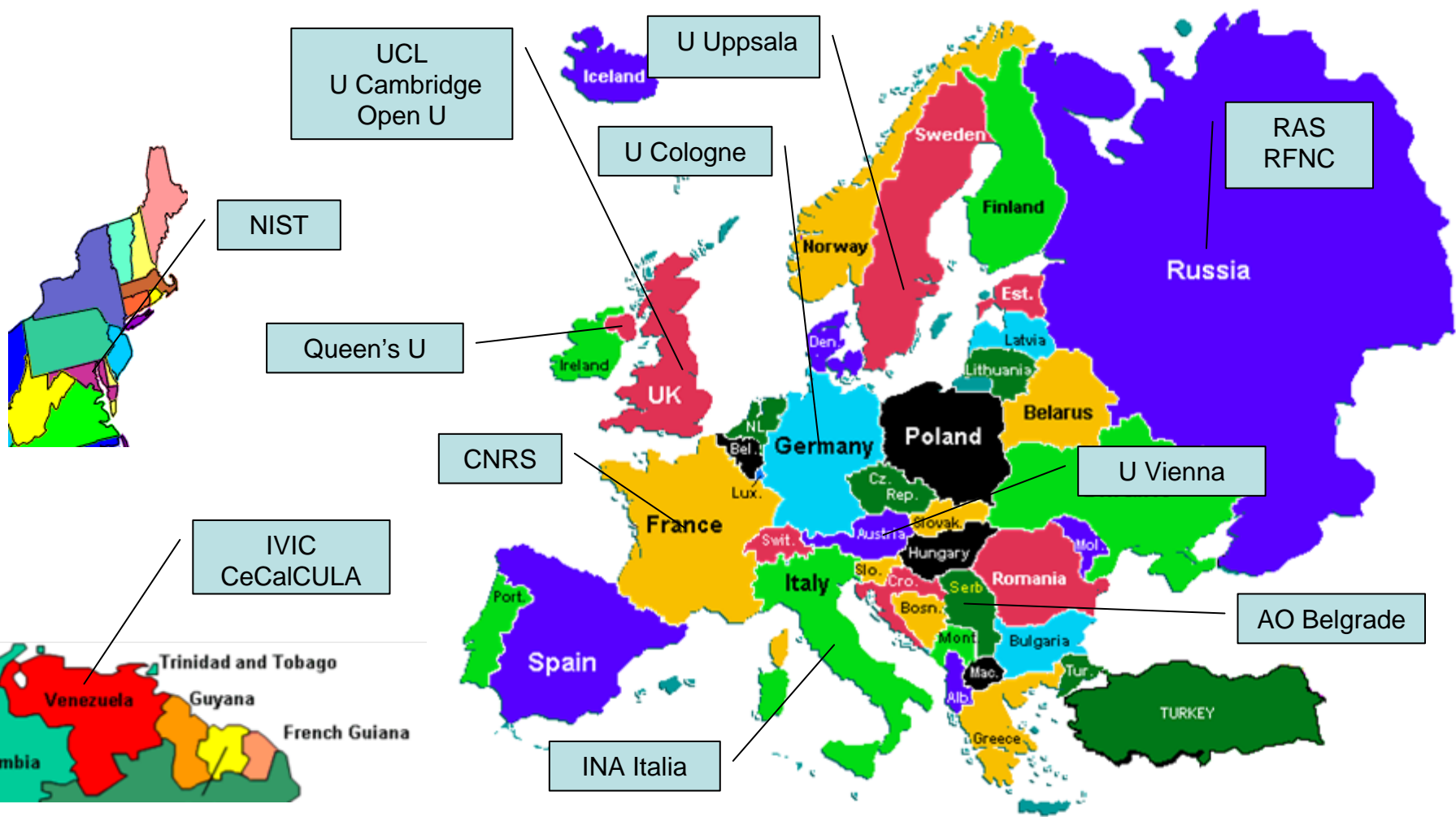
Instituto de Astrofísica de Canarias

27 October 2010

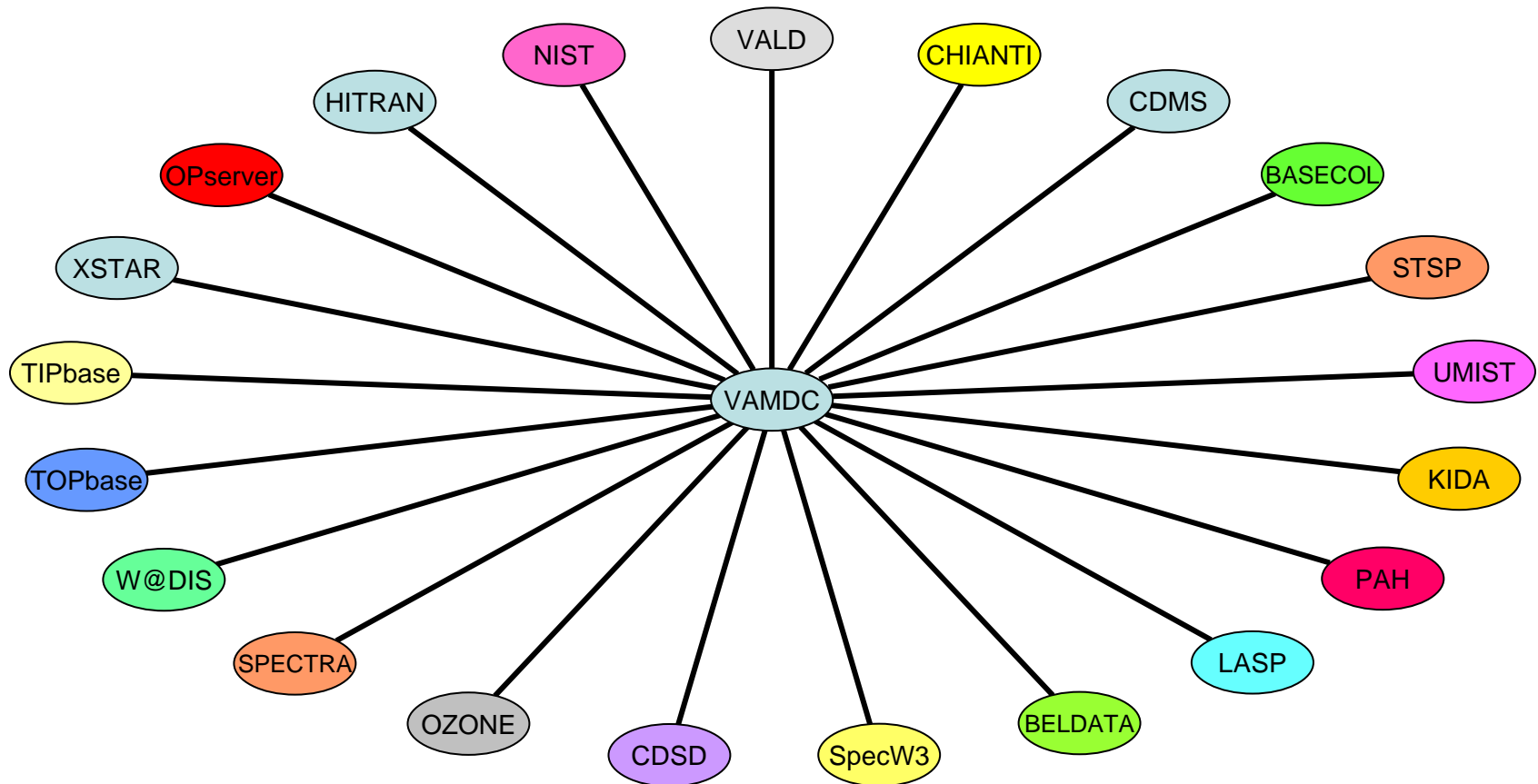
- VAMDC aims at building an interoperable e-infrastructure for the exchange of atomic and molecular data. VAMDC involves 15 administrative partners representing 24 teams from 6 European Union member states, Serbia, the Russian Federation and Venezuela.
- VAMDC is supported by EU in the framework of the FP7 "Research Infrastructures - INFRA-2008-1.2.2 - Scientific Data Infrastructures" initiative. It started on the 1st of July for a duration of 42 months.



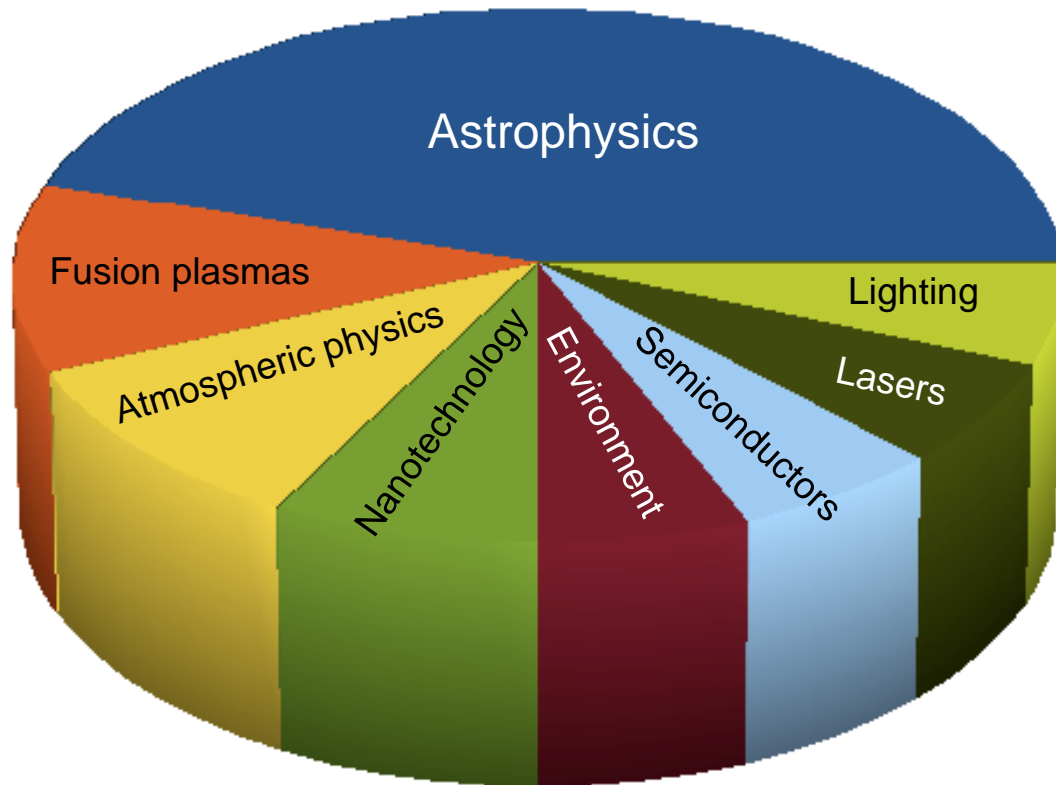
VAMDC integrates several research groups mainly from the European Research Area



Users will navigate seamlessly and retrieve data from 21 A&M databases



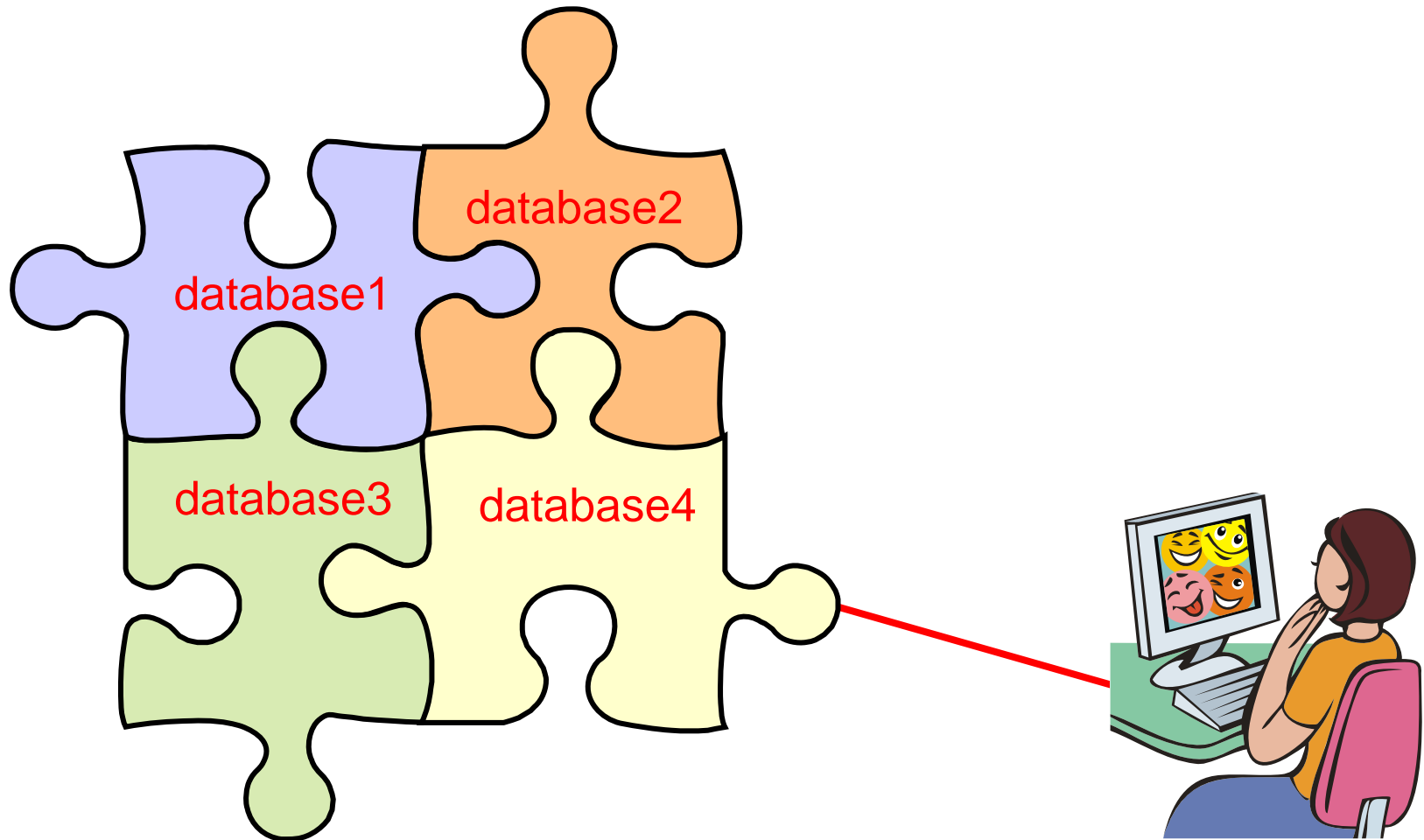
A&M data are used in a wide variety of research and industrial fields



Outstanding problems in existing A&M databases are interoperability and data interfaces



VAMDC intends to deploy an interoperable e-environment for distributed A&M databases



E-science is collaborative data-intensive science

Science Paradigms

- Thousand years ago:
science was **empirical**
describing natural phenomena
- Last few hundred years:
theoretical branch
using models, generalizations
- Last few decades:
a **computational** branch
simulating complex phenomena
- Today: **data exploration** (eScience)
unify theory, experiment, and simulation
 - Data captured by instruments
or generated by simulator
 - Processed by software
 - Information/knowledge stored in computer
 - Scientist analyzes database/files
using data management and statistics



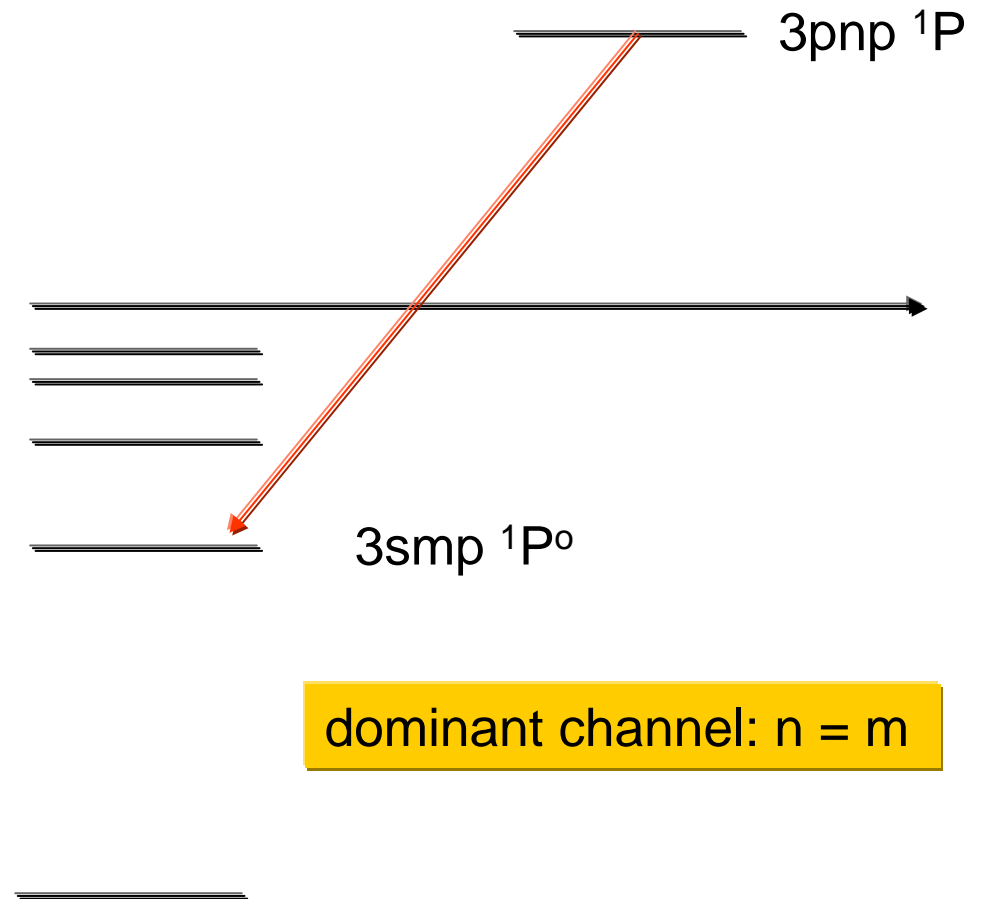
$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - K\frac{c^2}{a^2}$$



Radiative decay of $3pnp$ 1P states in Mg-like ions

Mg I

State	RLT (ns)
$3p4p$ 1P	$3.47E+00$
$3p5p$	$3.67E+00$
$3p5p$	$3.72E+00$
$3p6p$	$3.73E+00$
$3p7p$	$3.74E+00$
$3p8p$	$3.75E+00$
$3p9p$	$3.78E+00$
$3p10p$	$3.87E+00$



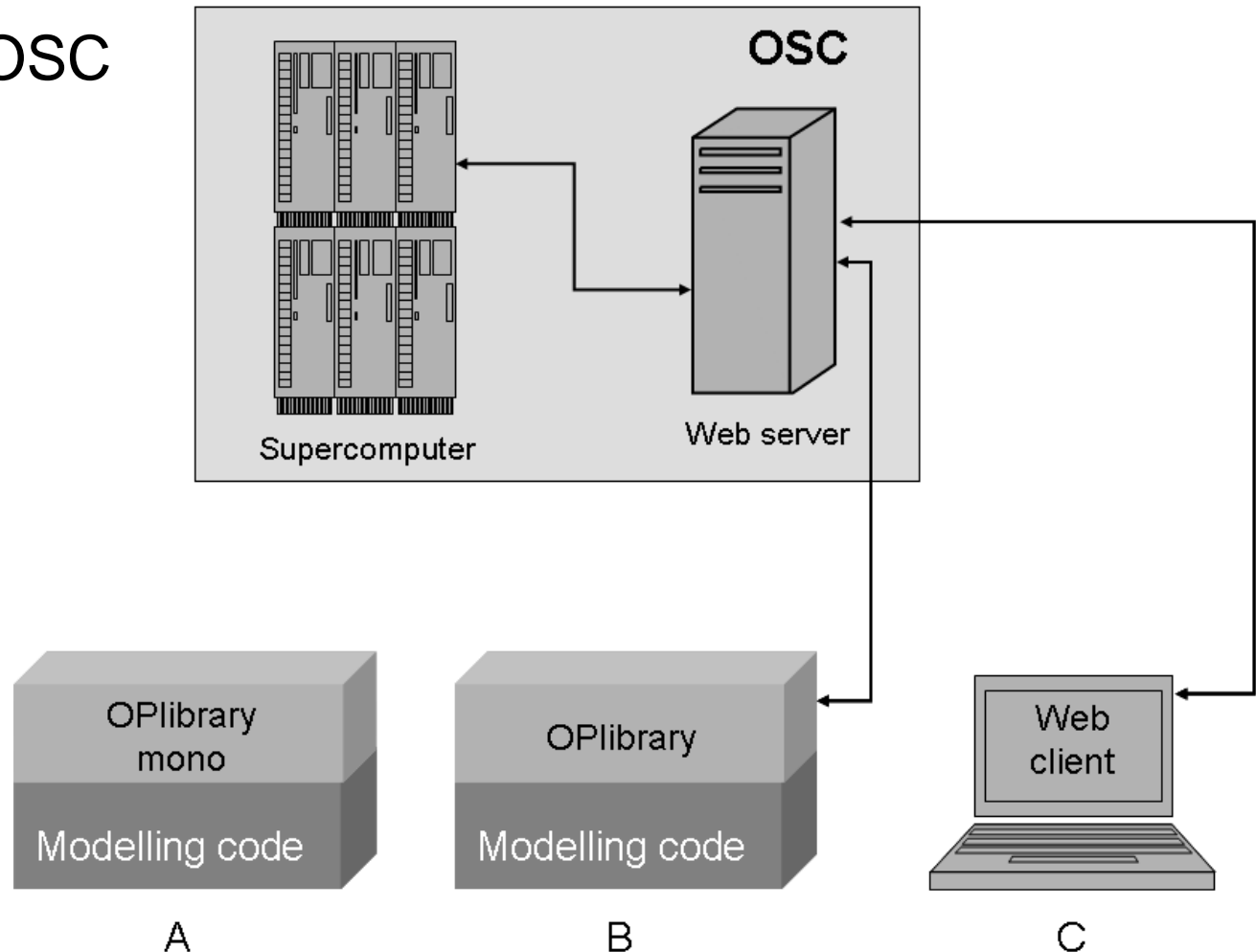
Butler et al (1990)

E-science is changing scientific research dynamics

- Distributed computer environments
 - Virtual organizations
 - Grids
 - Clouds
- Data-base centric computing
 - Warehousing (IVOA, VAMDC)
 - Data mining
- Applications accessible as WSDL/SOAP web services
- Service integrators
 - Scripts
 - Workflows
- Social networks as end users
- Data-curation environments
 - XML-based data exchange (XSAMS)
 - Metadata
 - Data preservation

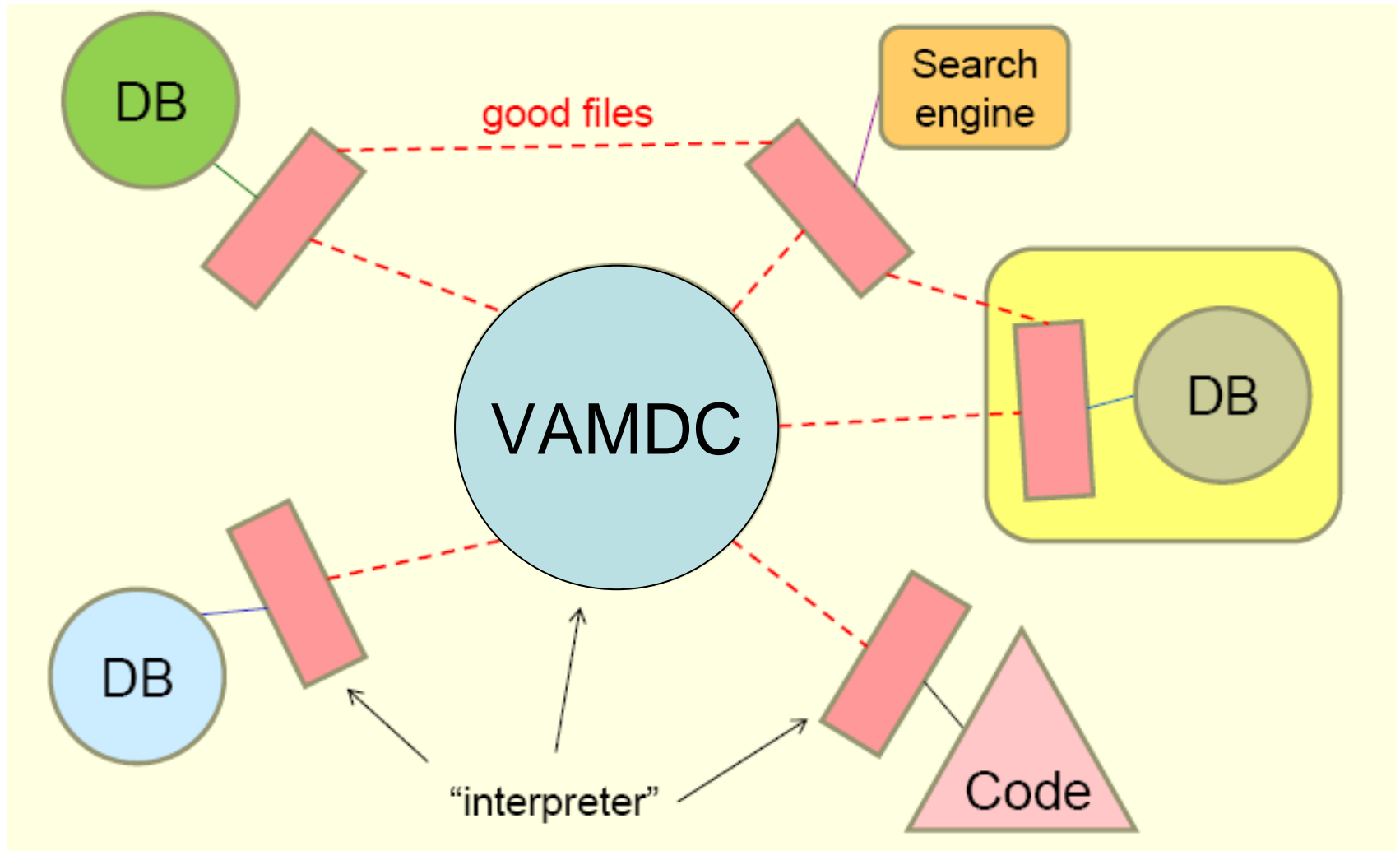
The OPserver is a good example of database-centric computing

OPserver at OSC

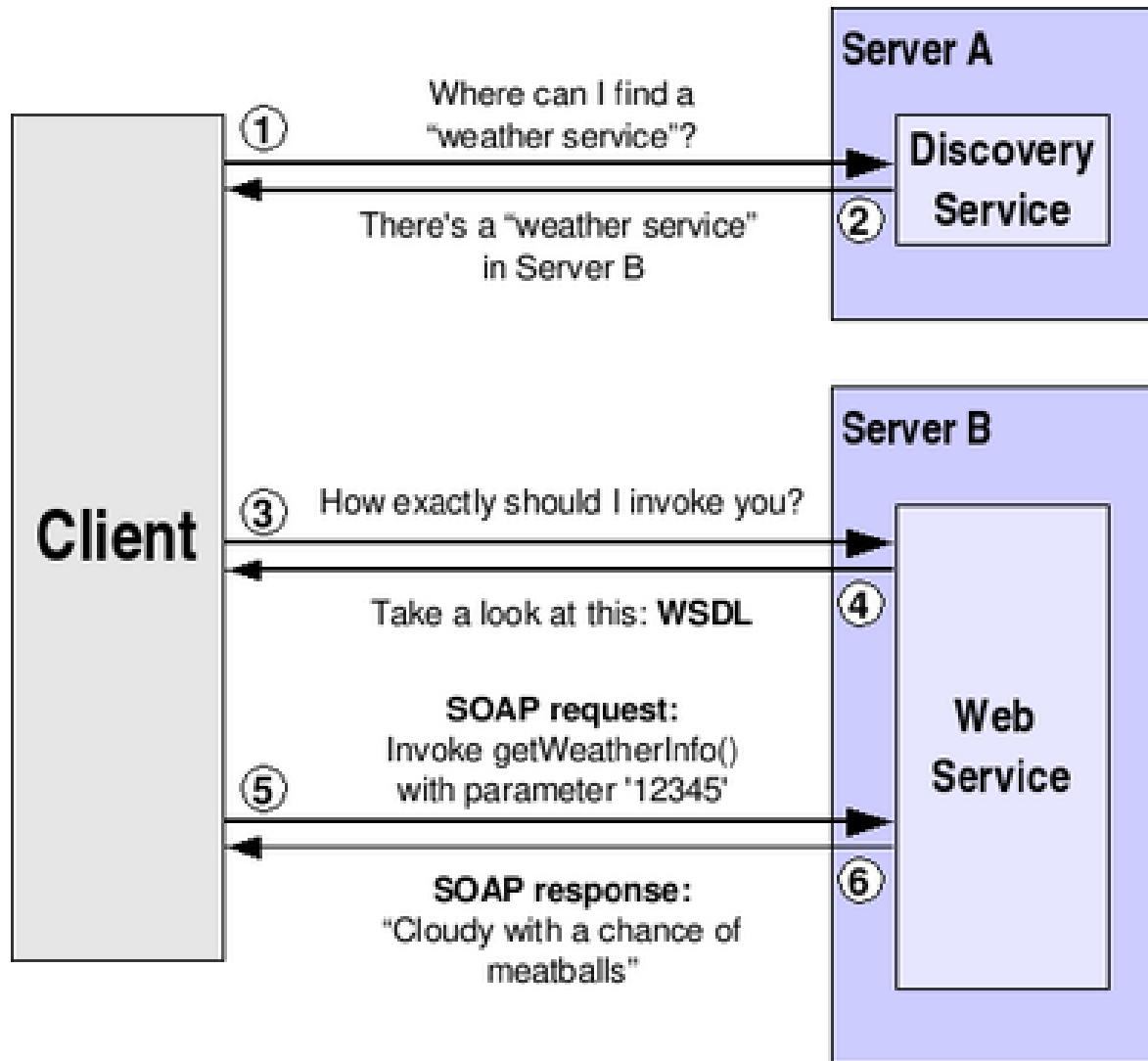


From Mendoza et al. (2007)

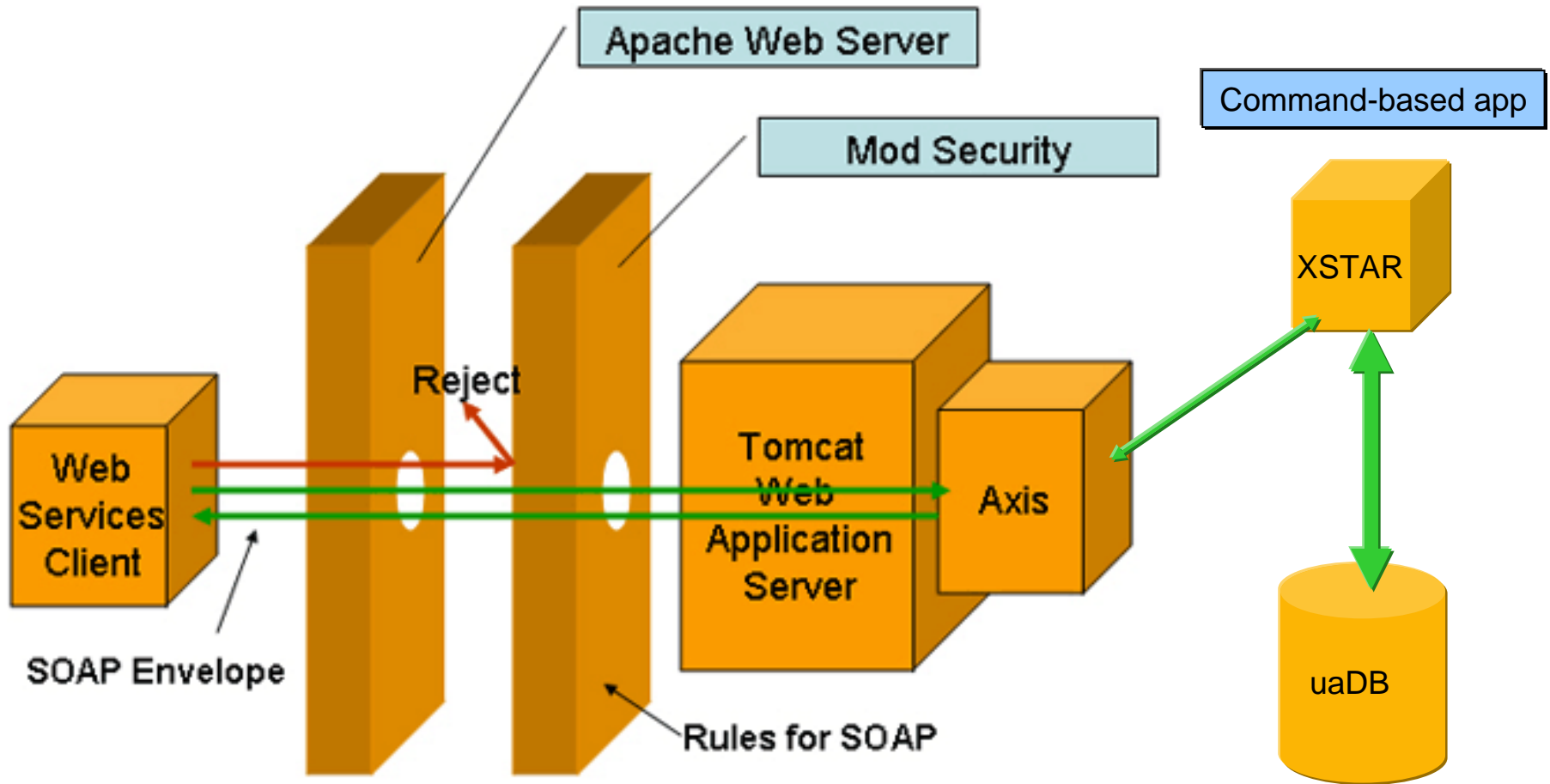
Data exchange strategy



VAMDC will provide a registry of A&M web services



The XSTAR spectral modeling code is being offered as a SOAP web service



Once XSTAR is available as a web service, it can be integrated in a web page

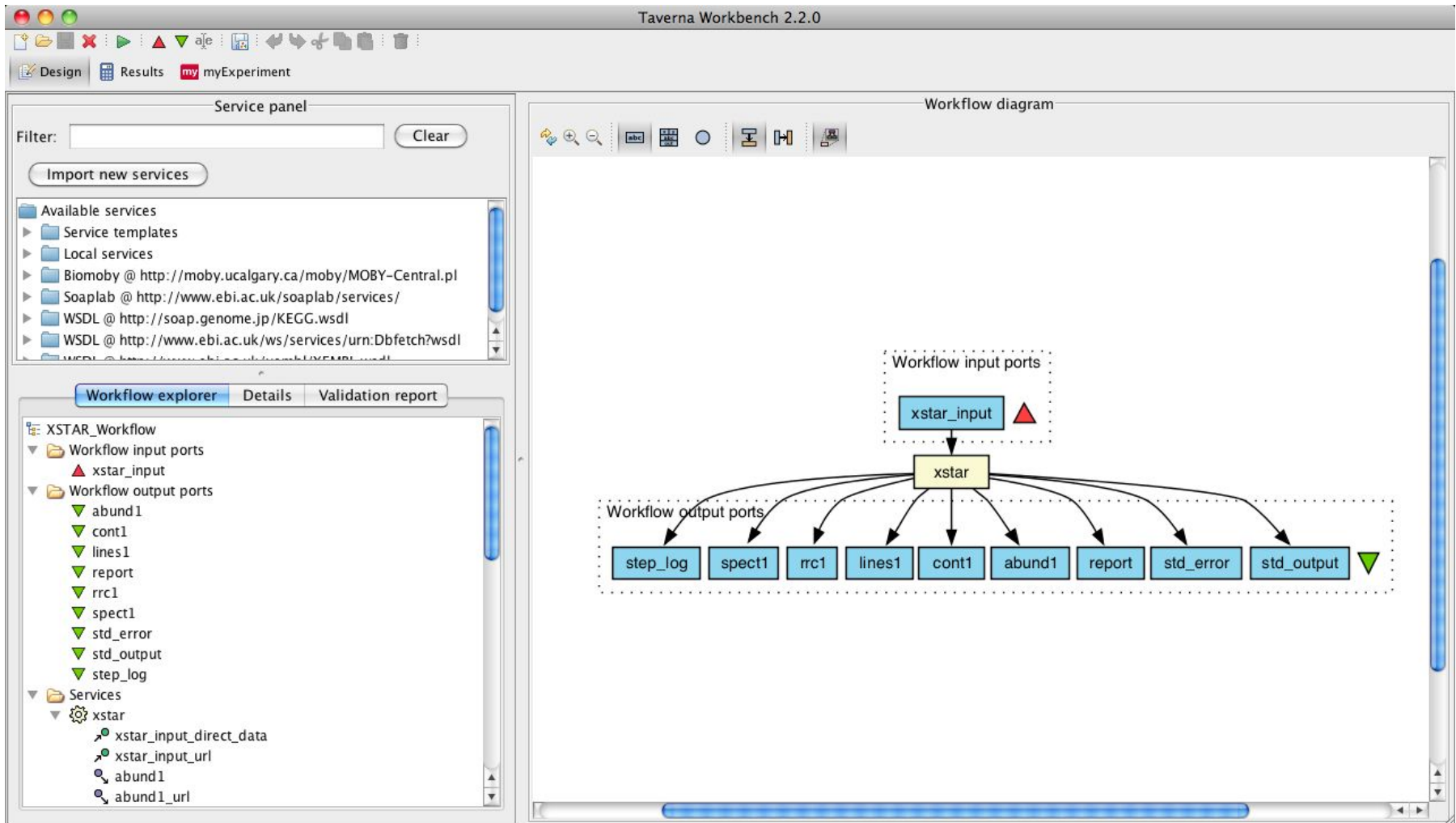
The screenshot shows a Windows Internet Explorer browser window displaying a web service interface for XSTAR. The browser's address bar shows the URL `http://caoba.ivic.ve:8180/soaplab2-axis/`. The page content includes:

- A Google search bar at the top with a translation notice: "Esta página está escrita en inglés. ¿Quieres traducirla con la barra Google? Más información ¿Esta página no está escrita en inglés? Ayúdanos a mejorar Traducir Desactivar traducción al inglés".
- Two search results:
 - [stgjk](#) Computer program for calculating...
 - [xstar](#) Computer program for calculating the physical conditions and emission spectra of photoionized gases.
- A text block: "You can get a couple of sample input files (for testing purposes) here:"
- A list of links:
 - [Simple job](#) (aprox. 25 sec.)
 - [Complex job](#) (aprox. 20 min.)
- A yellow background area containing a "Run service" button and a form for "Inputs".

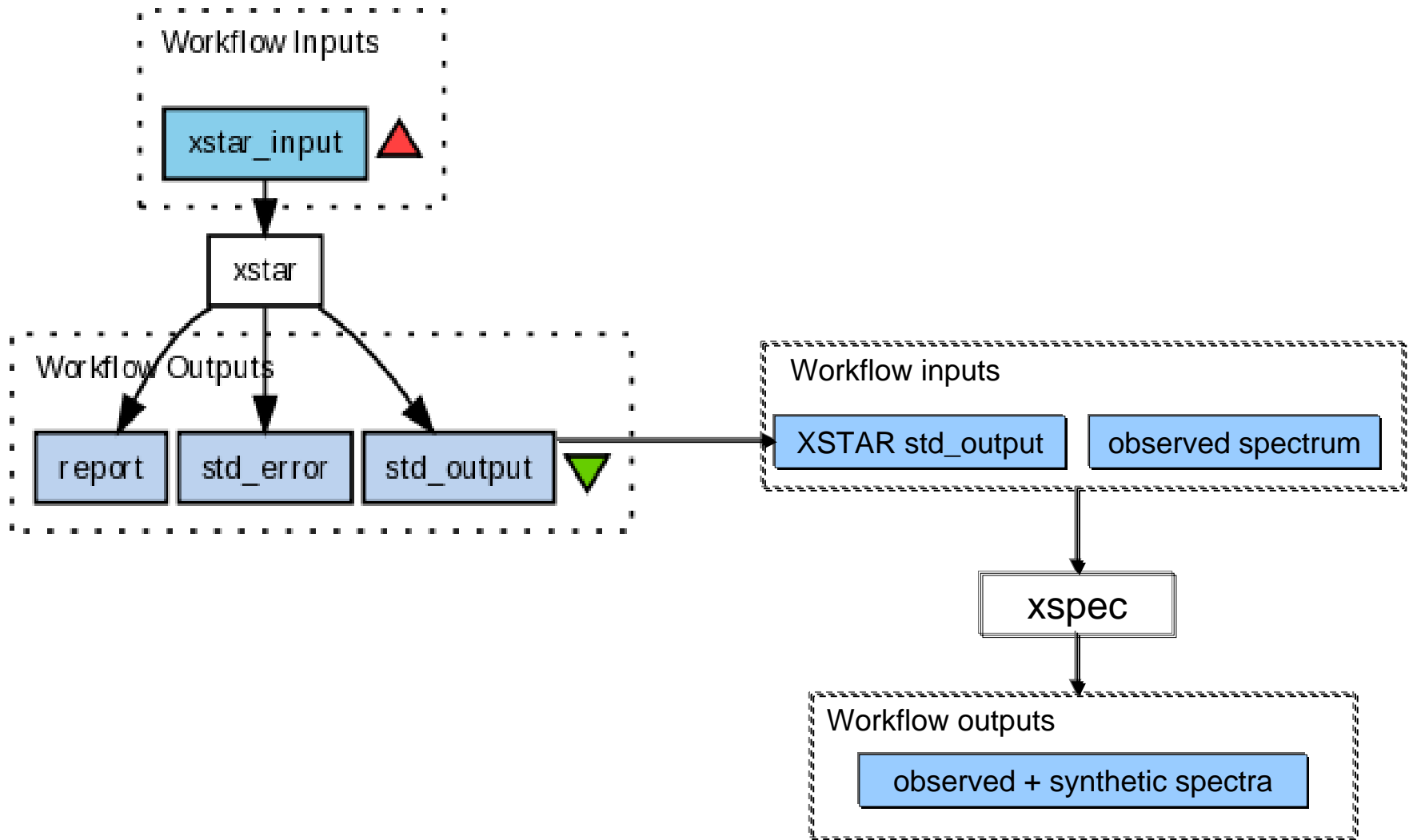
The "Inputs" section features a text field for "xstar_input", a radio button for "as URL", and a radio button for "direct data or local file" (which is selected). Below the text field is an "Examinar..." button. A "Reset fields" button is located at the bottom left of the yellow area. The "Report" section is currently empty.

The browser's status bar at the bottom indicates "Internet | Modo protegido: activado" and a zoom level of "100%".

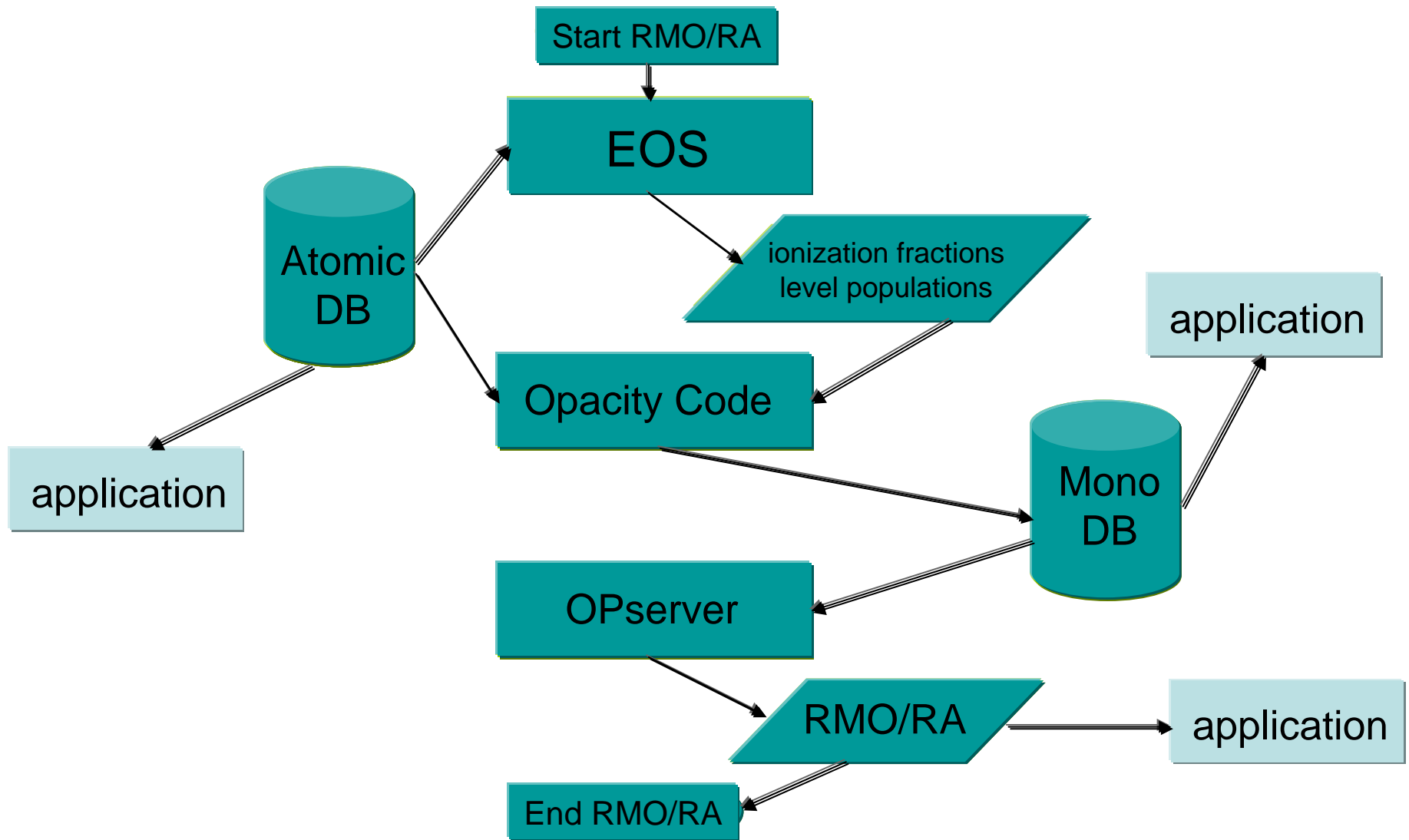
Once XSTAR is available as a web service, it can be integrated in a workflow system



Once XSTAR is available as a web service, it can be integrated in a workflow system



The computation of astrophysical opacities would be a topical example for a workflow system



Workflows maybe published in scientific social network systems

XSTAR All Search

Home »

BOOKMARK f t e ...

Didn't find what you need? [Click here](#) to search external workflow repositories.

Search results for "XSTAR"

Note: some items may not be visible to you, due to viewing permissions.

Users (1) Groups (1) Workflows (2)

Taverna 2

XSTAR (v2)

View

Download (v2)

Created: 02/04/10 @ 19:52:35 | Last updated: 04/08/10 @ 23:25:51

License: Creative Commons Attribution-No Derivative Works 3.0 Unported License

Original Uploader



This is a simple workflow designed to run XSTAR with an user selected input. XSTAR is a computer program for calculating the physical conditions and emission spectra of photoionized gases. More information can be found here: - XSTAR home page:

New/Upload

Workflow GO

Log in / Register

Username or Email:

Password:

Remember me:

OR

Use OpenID:

(eg: name.myopenid.com)

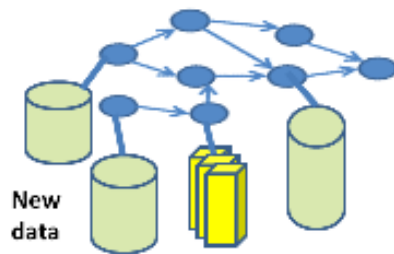
Log in

Workflow may become the blueprints of reproducible & adaptable scientific methods

Paul Fisher is a bioinformatician studying disease in African cattle

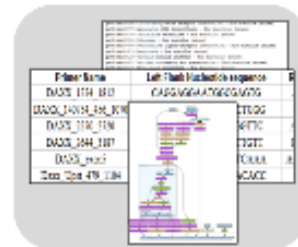


1 Paul **designs** a workflow and **executes** it over shared Web Services



3

The data and workflow are **discovered** by others for **reuse** in other areas of science



2 Paul **publishes** the workflow and results on the Web and the paper online

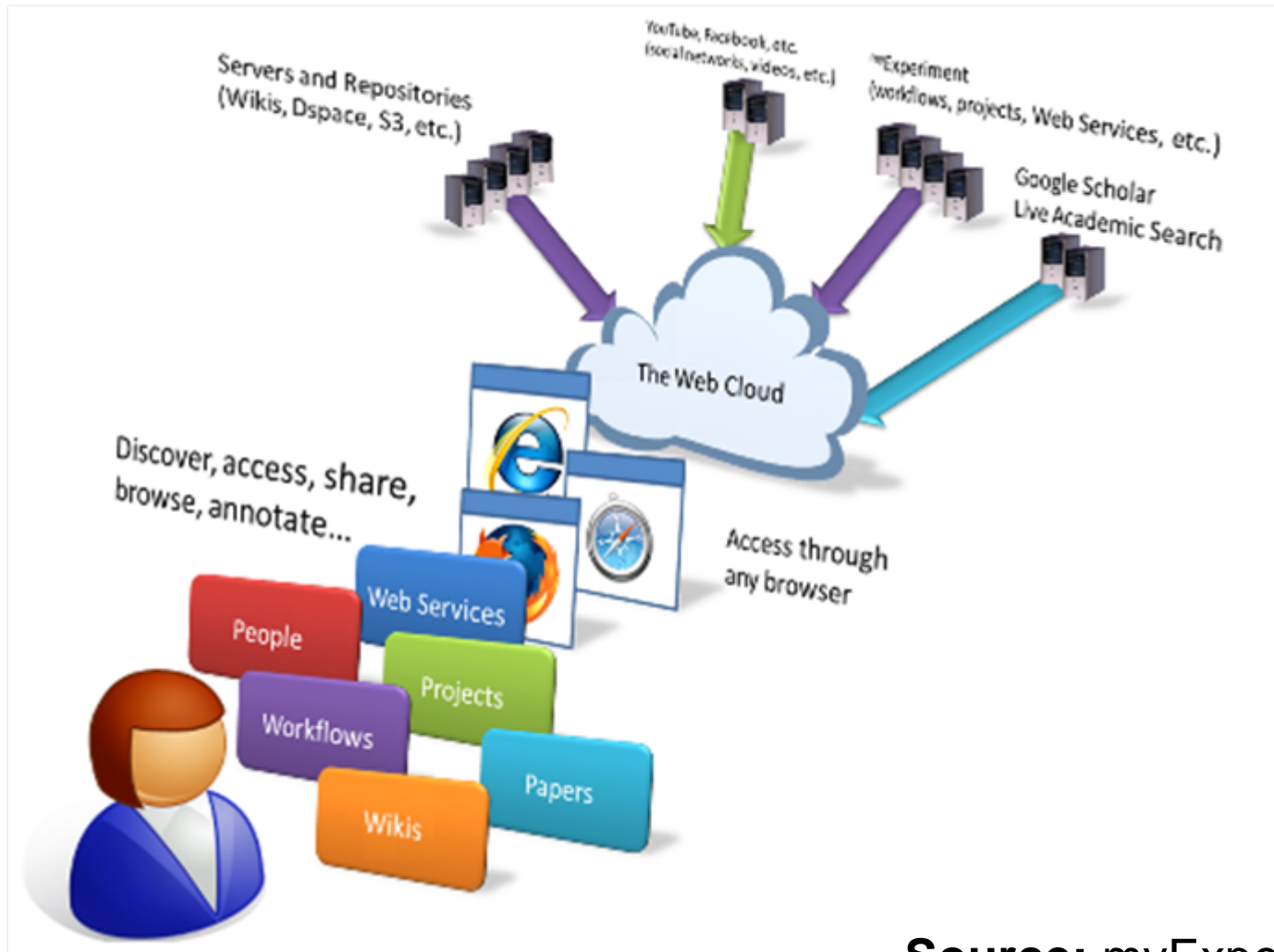


4 The workflow is tagged, reviewed and **curated** by its user community and by specialists



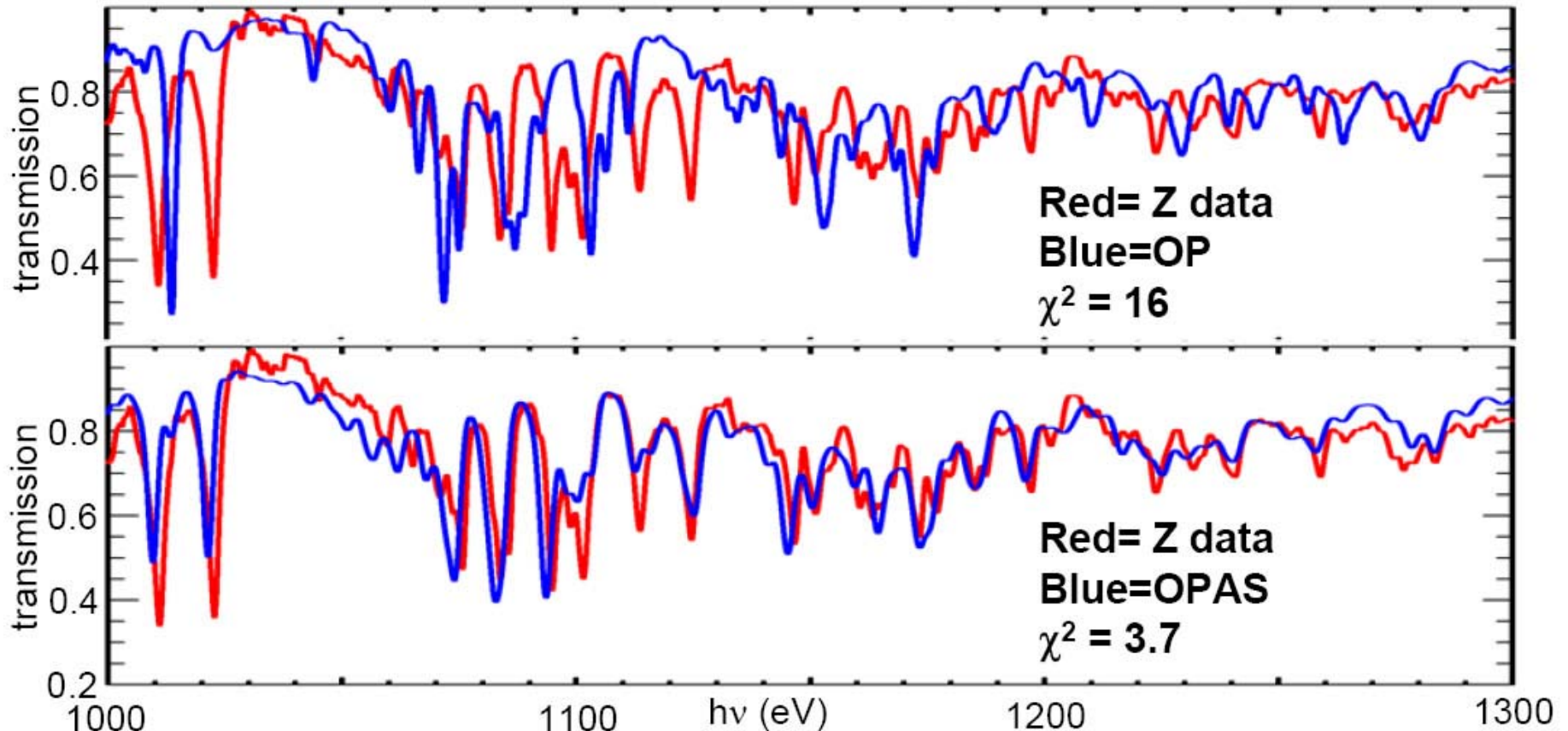
Source: myExperiment

We should attempt to form A&M data producer/user communities



Source: myExperiment

OP Fe RMO at Z conditions is being questioned

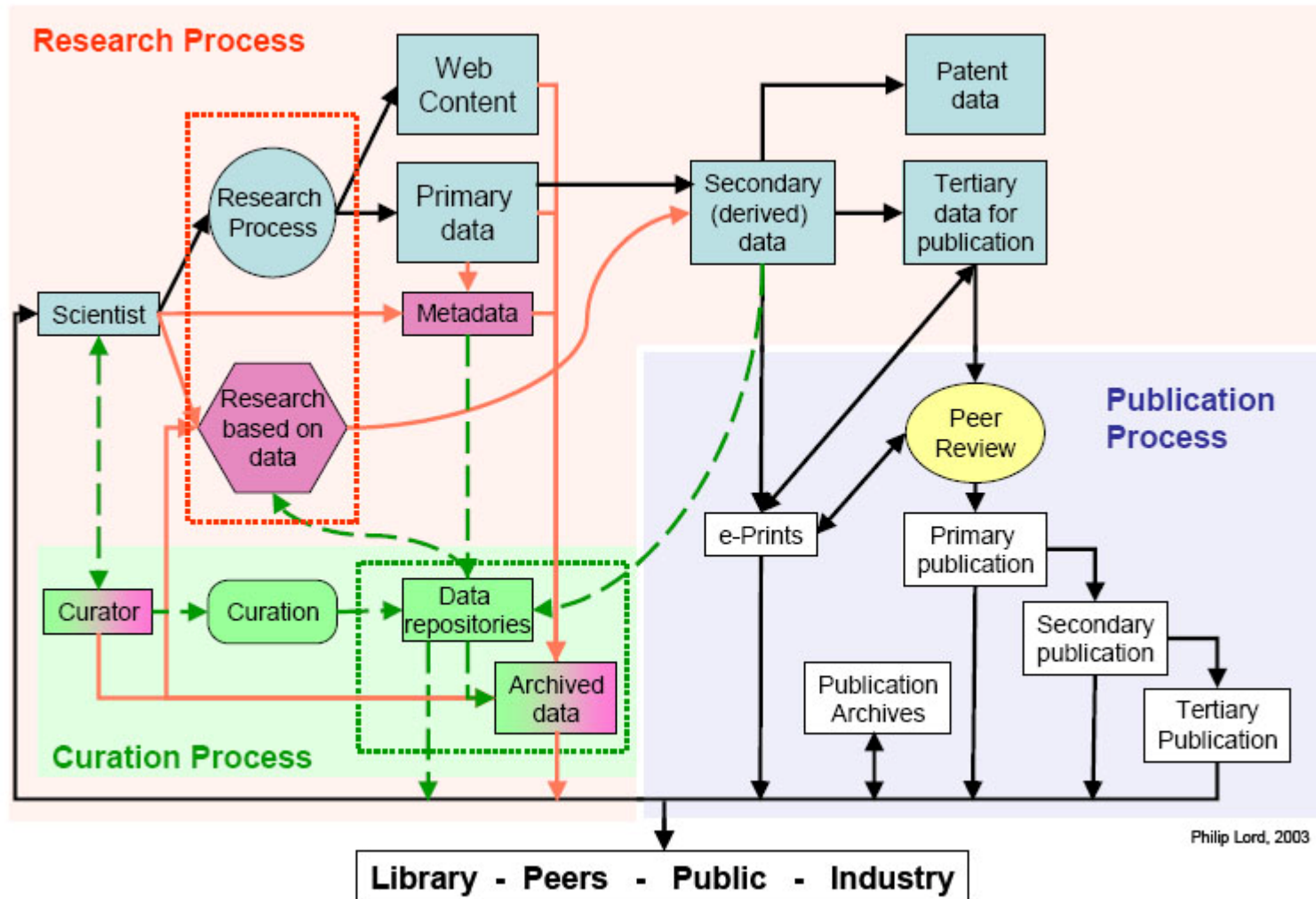


**OP Rosseland mean is $\sim 1.5x$ lower than OPAS at Z conditions.
If this difference persisted at solar conditions, it would solve the CZ problem**

Z conditions: $T \sim 156$ eV, $n_e \sim 10^{22}$ cm $^{-3}$

From Bailey (2008)

Model of the curation process



Conclusions

- ✓ Scientific research is becoming increasingly collaborative and data-intensive (e-science)
- ✓ Atomic data production must be scaled up to the extreme requirements of virtual organizations
- ✓ Data repositories must be kept fit and integral for contemporary purpose, discovery and reuse (e-science curation)
- ✓ Data preservation is of vital importance