XSTAR: application deployment on the global cyber-infrastructure

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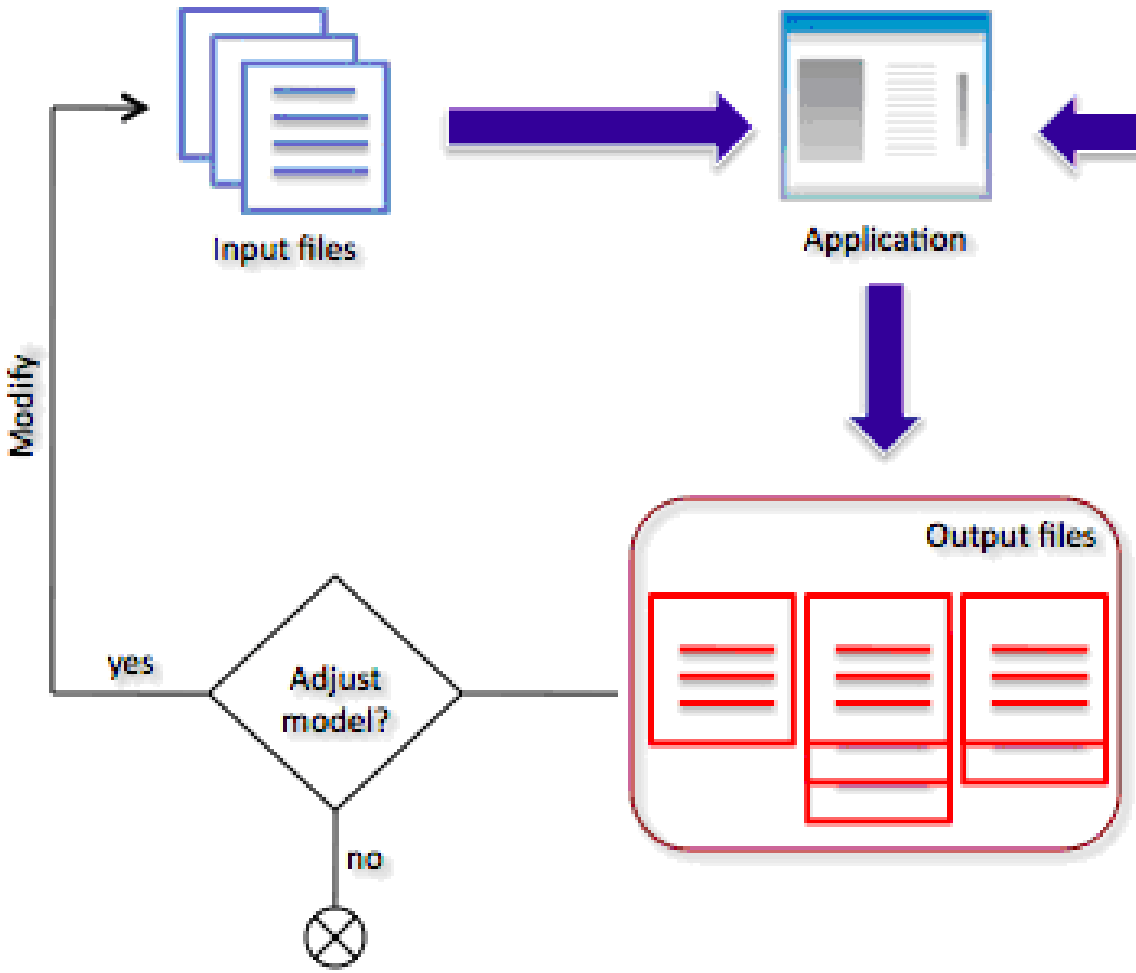
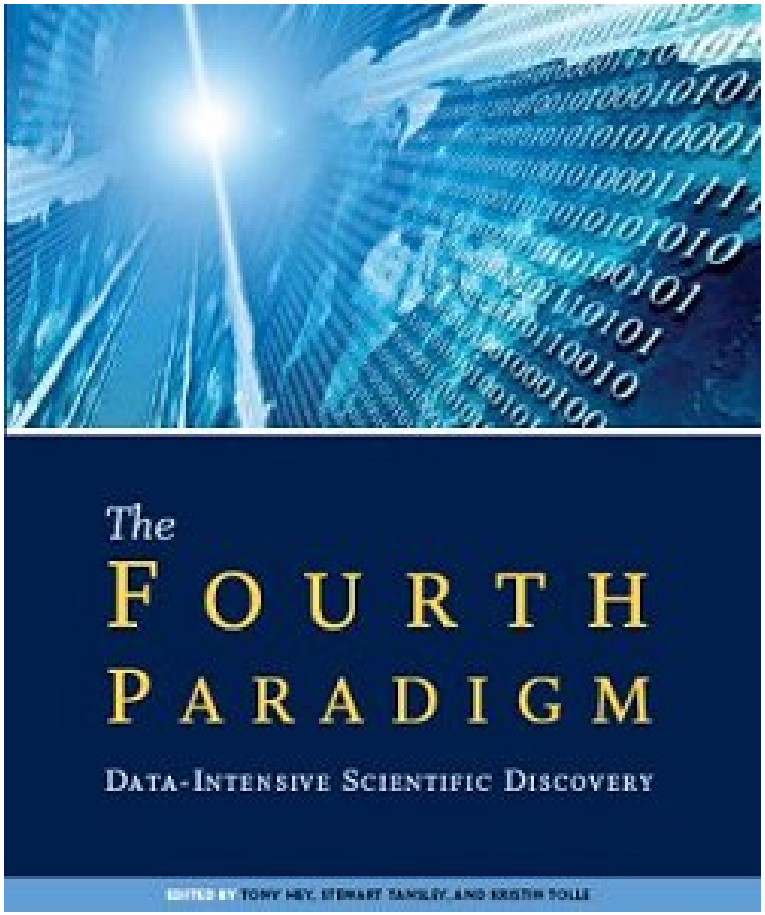
XSTAR: spectral modeling code as a case study



- XSTAR reads an extensive atomic DB to compute synthetic spectra
- We have been improving the atomic DB for past 8 years
- Grids of models are run sequentially
- XSTAR is downloaded from a web page, unpacked, installed and run from the command line

We attempt to map out VAMDC specifications in data-intensive research

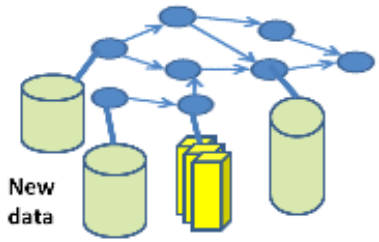


- Database-centric computing
- Application and database deployment as web services
- Service integration with workflows and mashups
- Social network (VO) as the end user

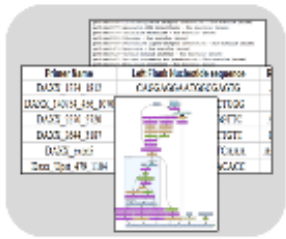
We can use e-science tools and methods from other data-intensive fields, e.g. bioinformatics, climatology

Paul Fisher is a bioinformatician studying disease in African cattle

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



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

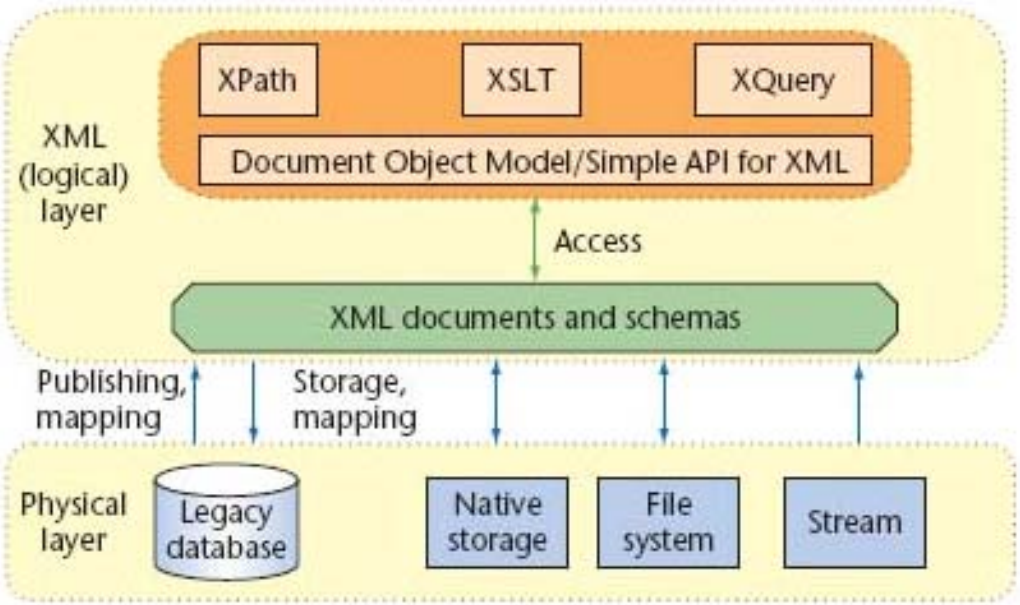


3 The data and workflow are **discovered** by others for **reuse** in other areas of science

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

Source: myExperiment

Integration of diverse DBs with XSAMS



XML DB integration:

- Publishing: SQL data → XML
- Storage: XML → SQL data
- Access: Xquery → SQL query

- XSTAR database (DB) (uaDB) can now be used standalone
- uaDB has been implemented with MySQL
- We have experimented with XSAMS and eXist, and discard native XML DB due to very slow query responses
- Diverse DB integration on the logical layer with XML
- Must develop XML/SQL map for each DB which supports DB-DB interaction

Source: Freire &Benedikt (2004)

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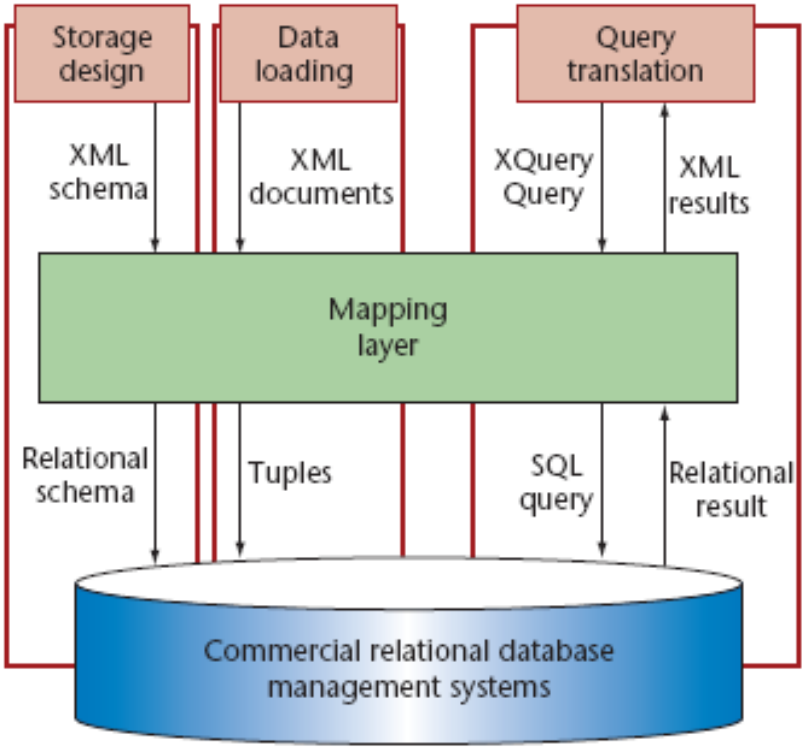

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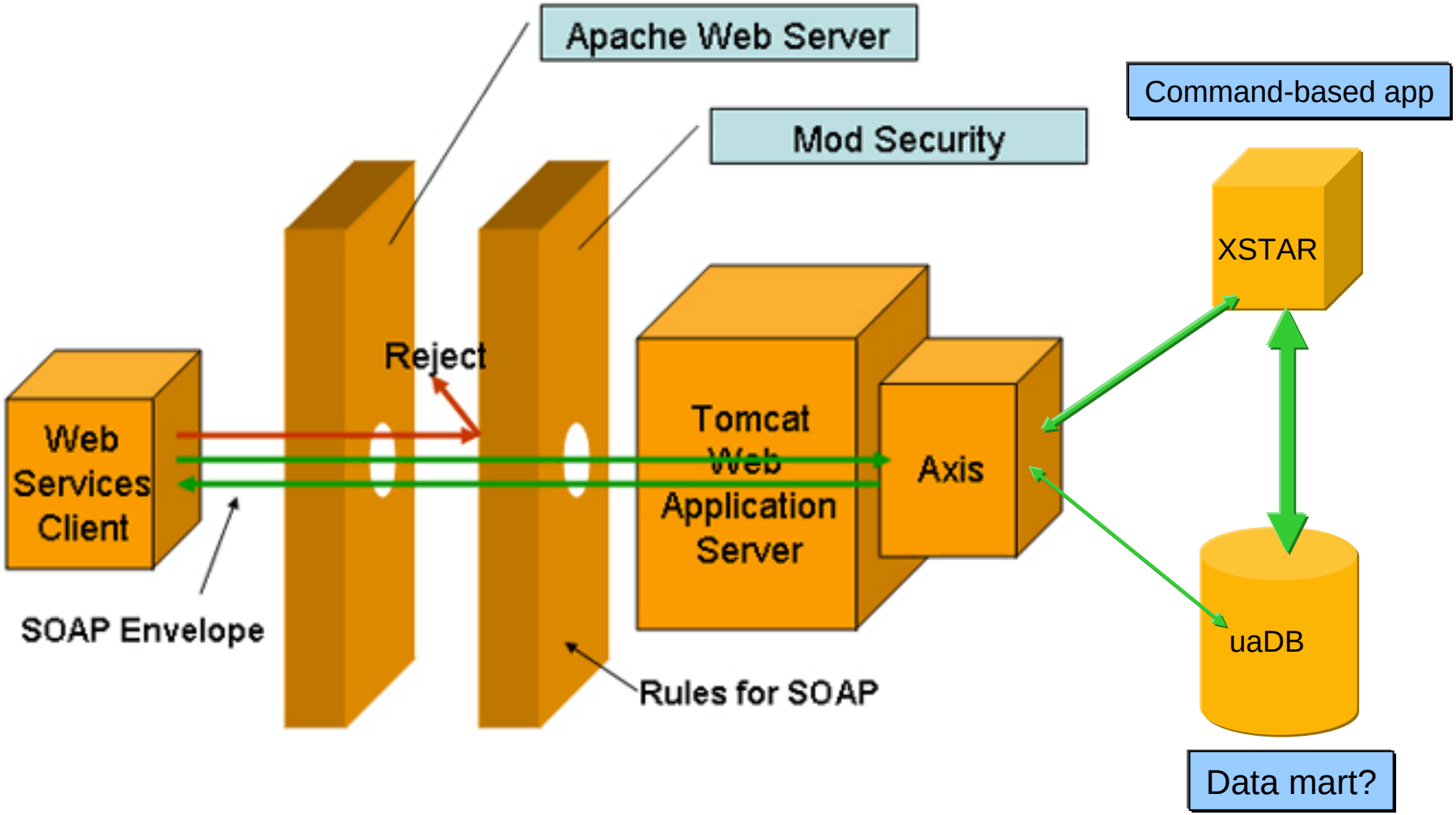
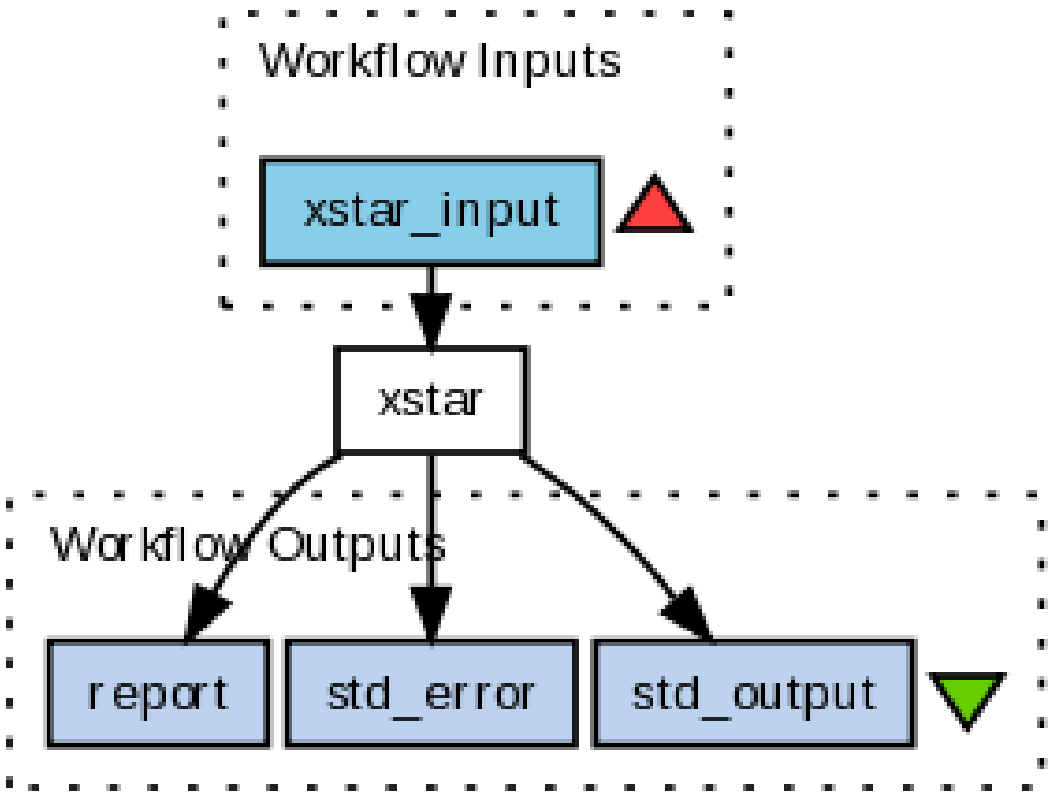
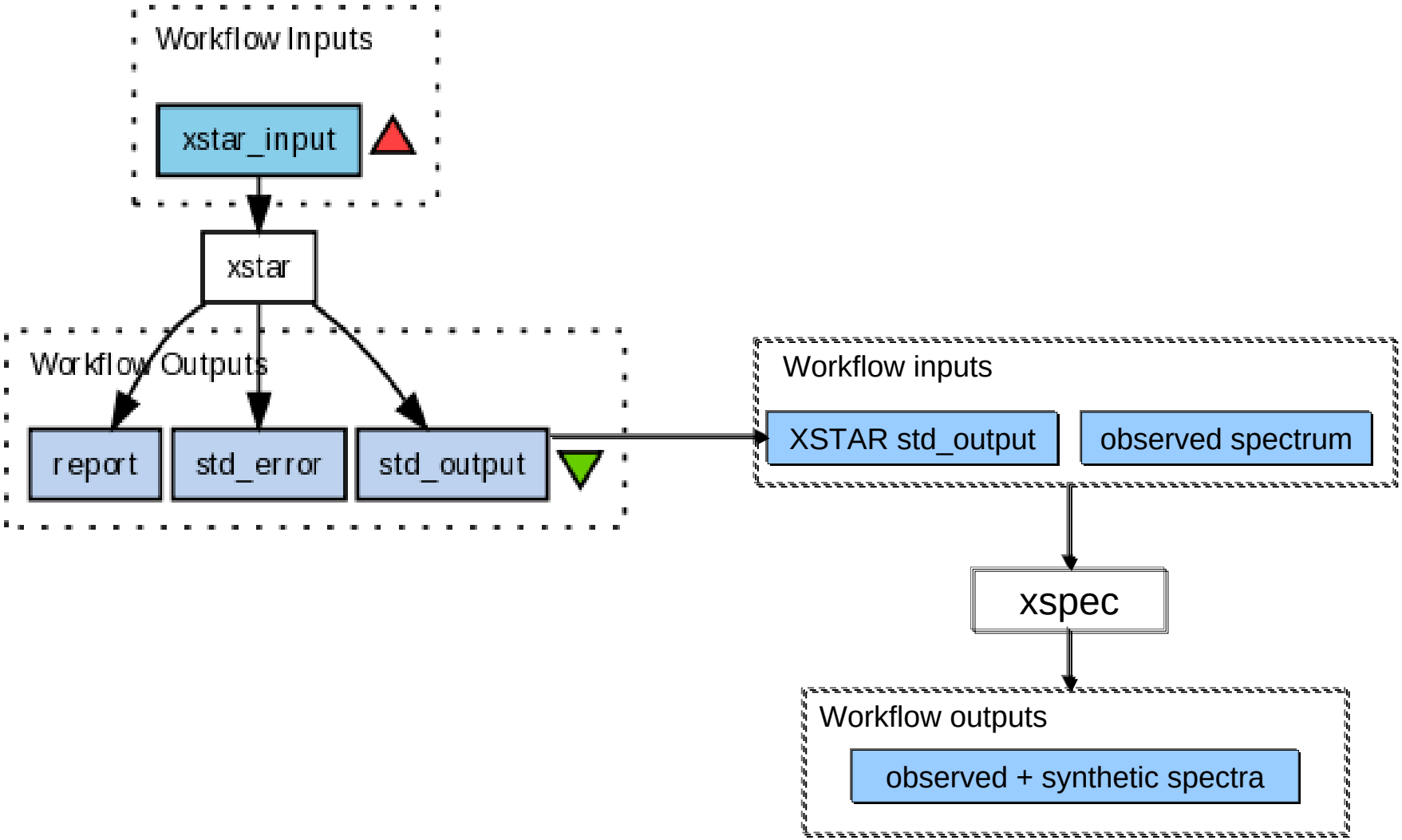
XSTAR web service implemented with SOAP2



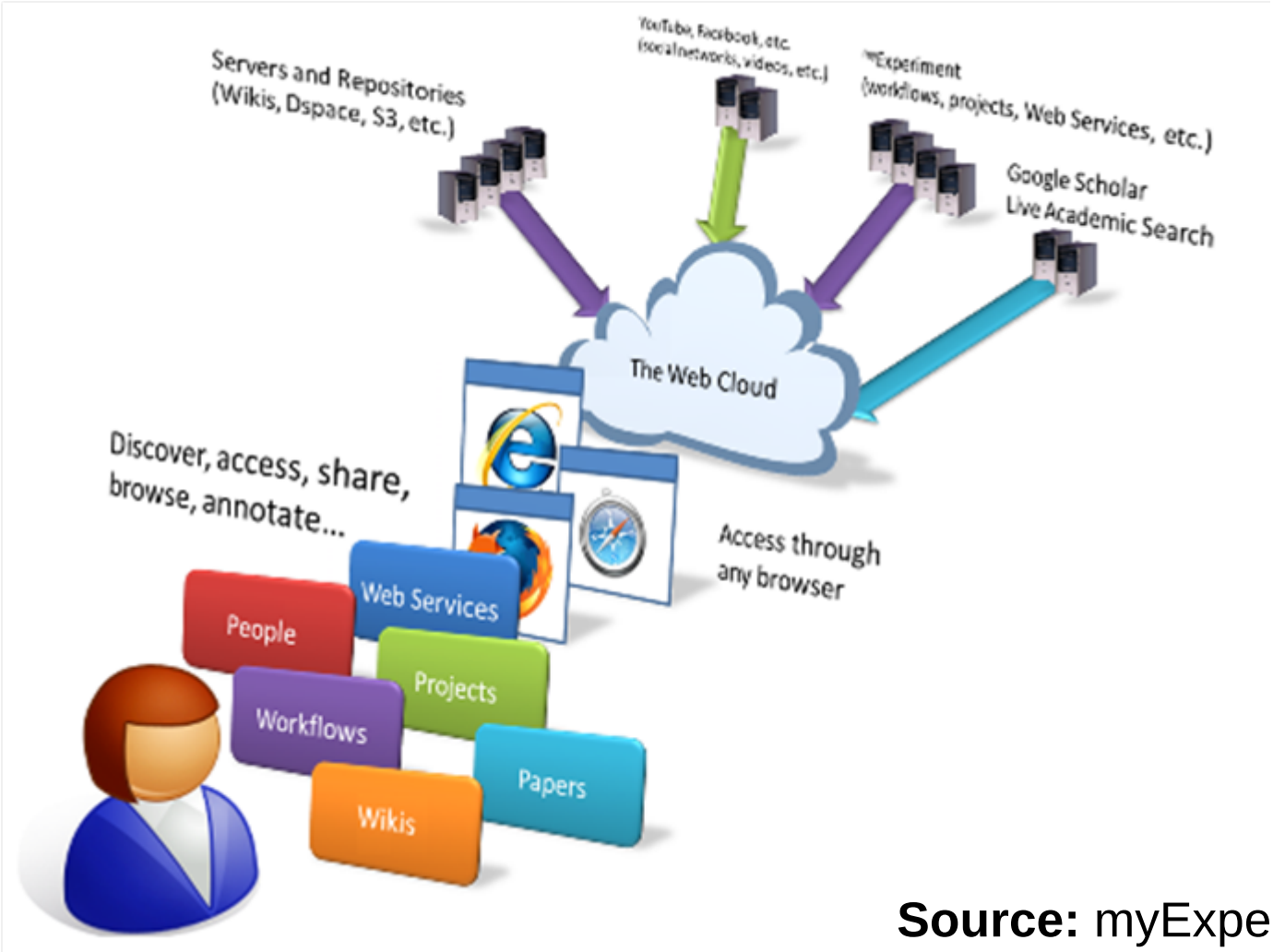
XSTAR workflow implemented with TAVERNA



Spectral modeling workflow presents problems: XSPEC is an interactive application

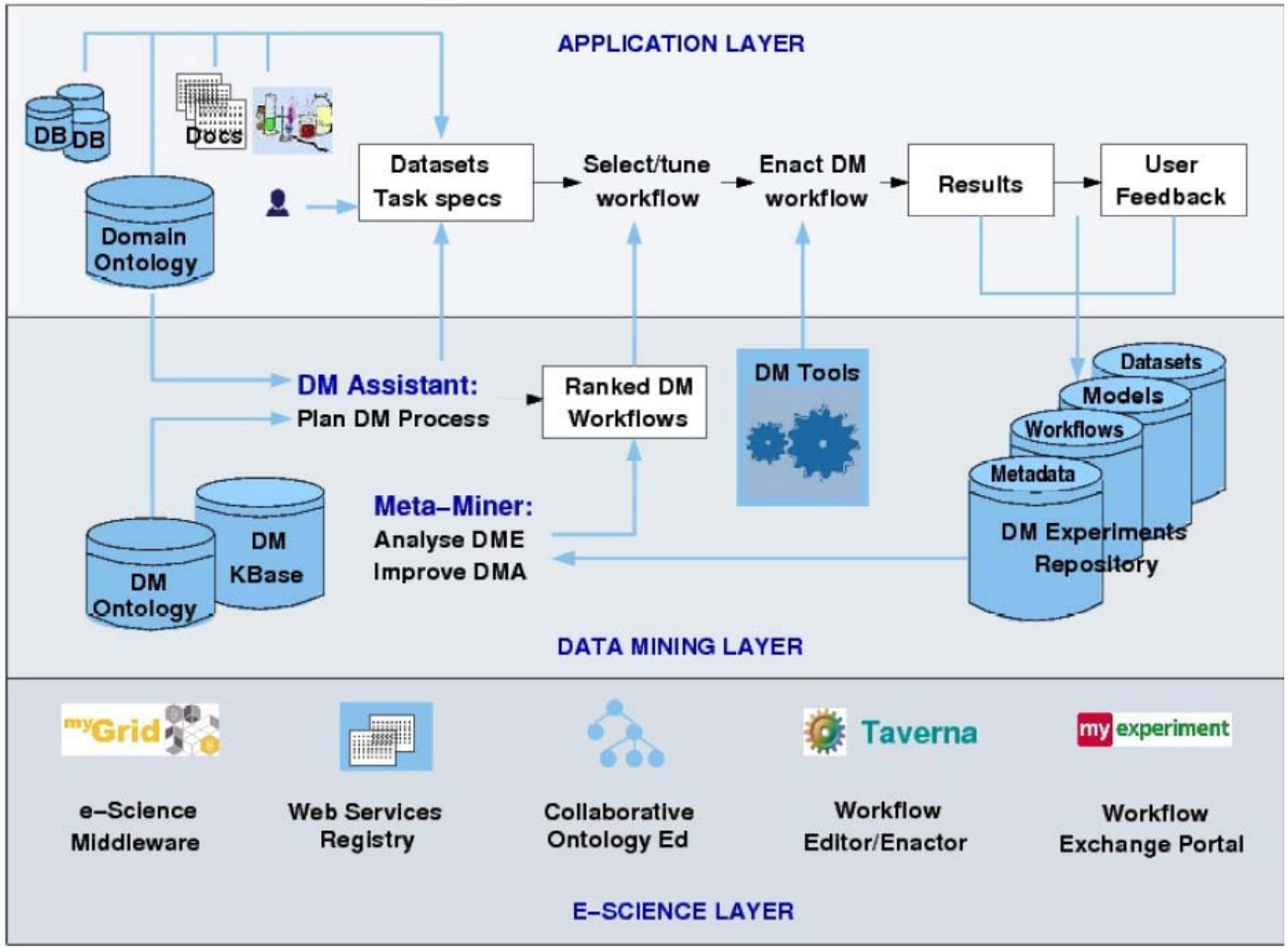


Develop user communities with myVAMDC



Source: myExperiment

Scale VAMDC to a virtual laboratory for interdisciplinary collaborative A&M data mining with e-lico



Source: e-lico

In conclusion…

- ✓XSTAR deployment for data-intensive applications has allowed us to test possible approaches and methods for VAMDC
- ✓VAMDC needs not to develop fancy new tools as they can be usually found in other current e-science initiatives
- ✓User community developments can be carried out within the social-network paradigm
- ✓Can we scale VAMDC up to a virtual laboratory for interdisciplinary collaborative A&M data mining?