# Building on Existing Communities: the Virtual Astronomical Observatory (and NIST)

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# Data in astronomy

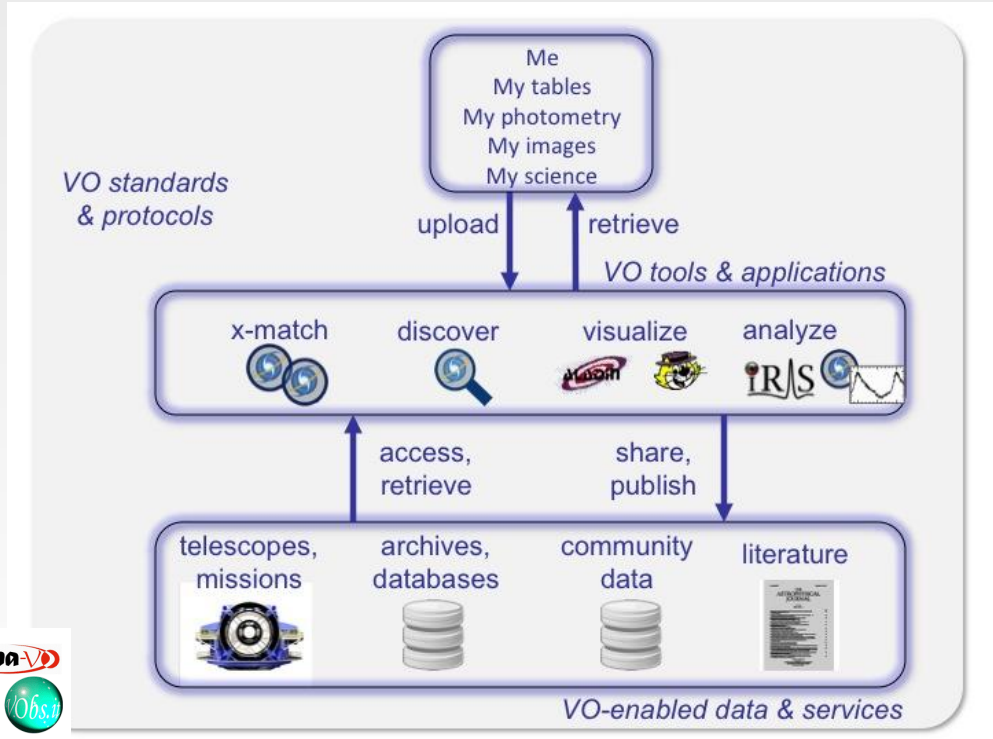
- ~70 major data centers and observatories with substantial on-line data holdings
- ~10,000 data “resources” (catalogs, surveys, archives)
- Data centers host from a few to ~100s TB each, currently at least 2 PB total
- Current growth rate ~0.5 PB/yr, increasing
- Current request rate ~1 PB/yr
- Future surveys will increase data rates to PB/day
  - “For LSST, the telescope is a peripheral to the data system” (T. Tyson)

*How do astronomers navigate through all of this data?*

# The Virtual Observatory

*The VO is a data discovery, access, and integration facility*

- Images, spectra, time series
- Catalogs, databases
- Transient event notices
- Software and services
- Application inter-communication
- Distributed computing
  - authentication, authorization, process management
- International coordination collaboration IVOA W3C)




# Virtual Observatory capabilities

- Data exchange / interoperability / multi-λ (co-observing)

  *Data Access Layer (SIAP, SSAP / time series)*
- Query and cross-match across distributed databases

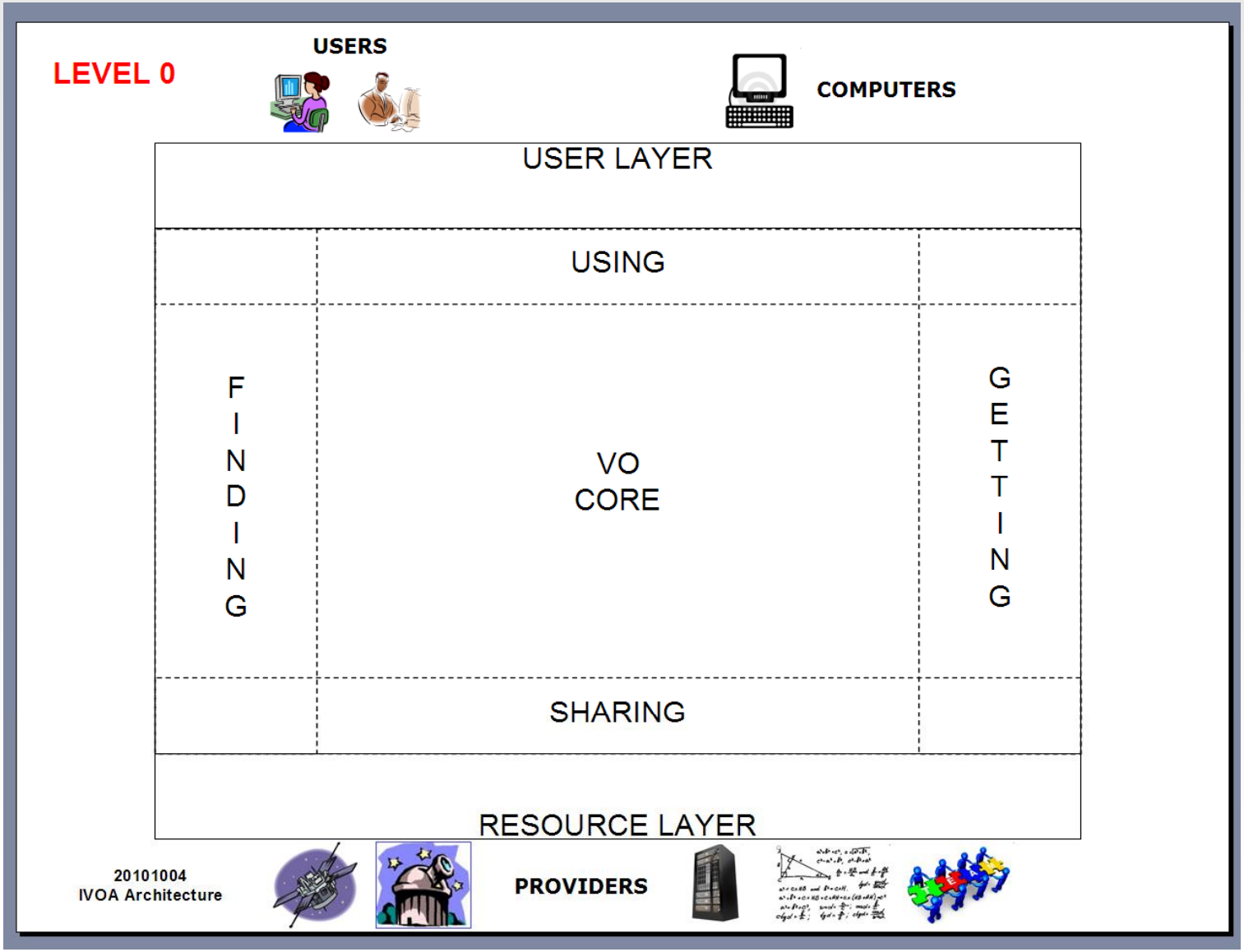
  *Cone Search, Table Access Protocol*
- Remote (but managed) access to centralized computing and data storage resources

  *VOSpace, Single-Sign-On (OpenID), SciDrive*
- Transient event notification, scalable to $10^6$ messages/night

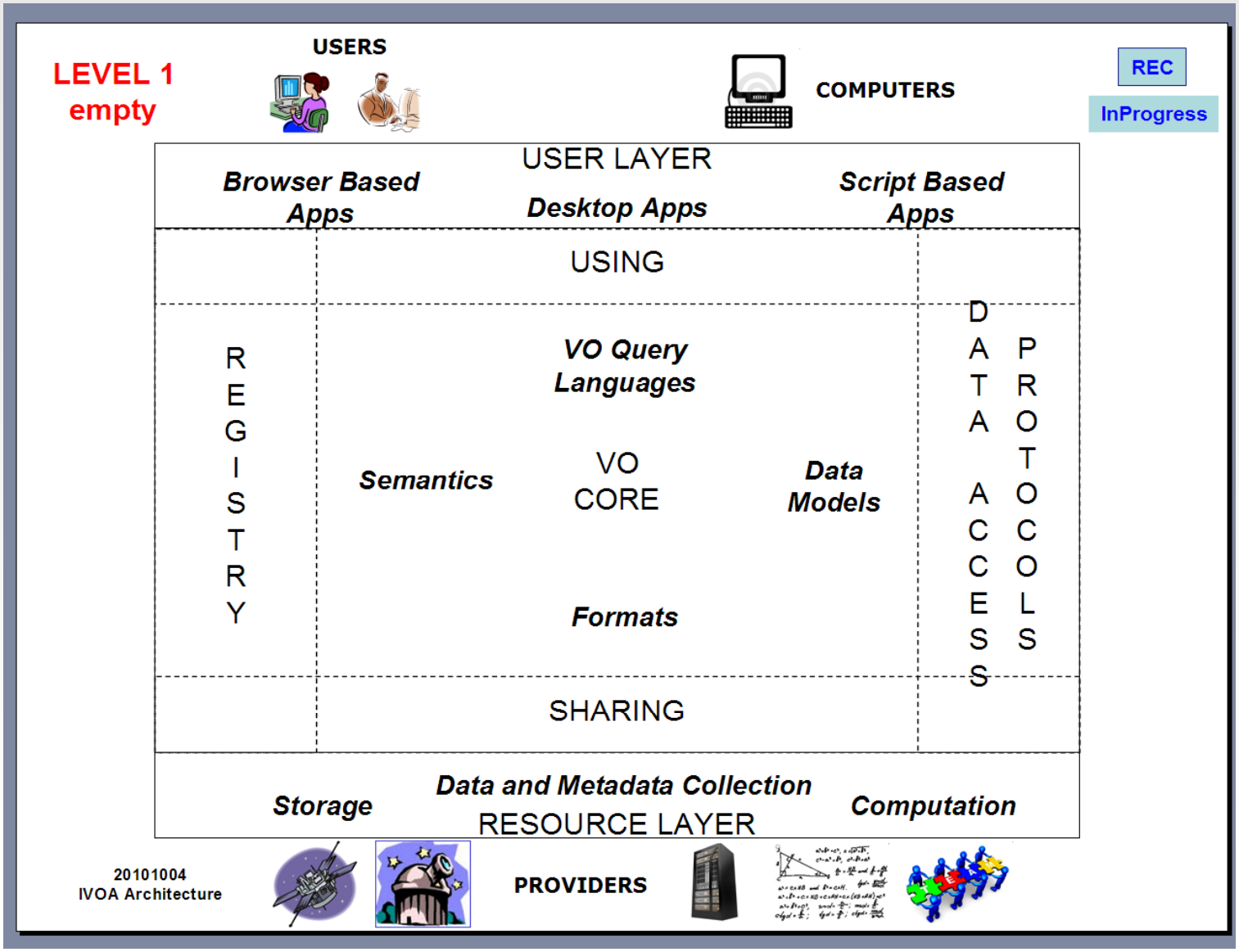
  *VOEvent*
- Data mining, characterization, classification, statistical analysis

  *VOStat, Data Mining and Exploration toolkit*

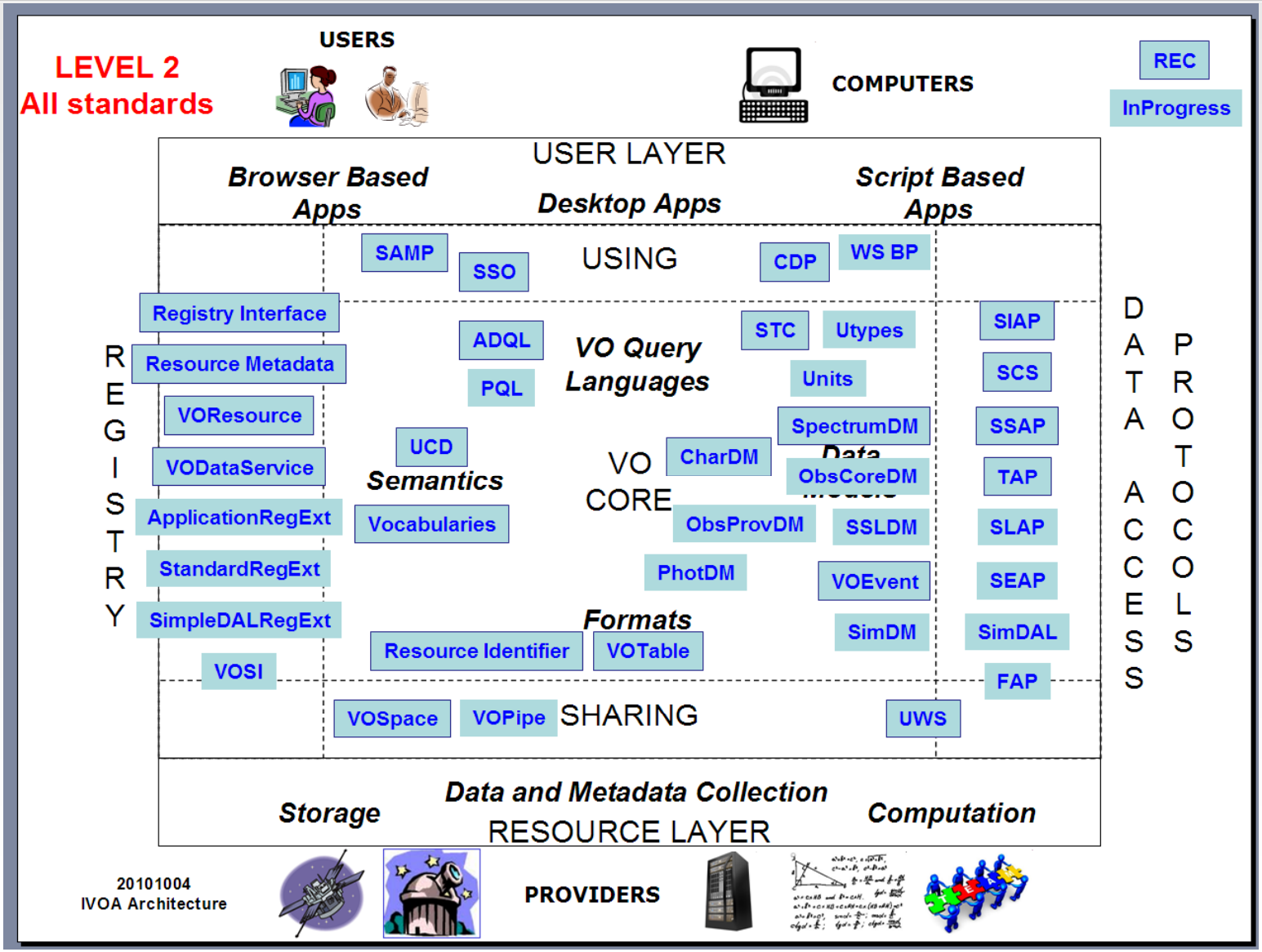
# VO architecture



# VO architecture



# VO architecture



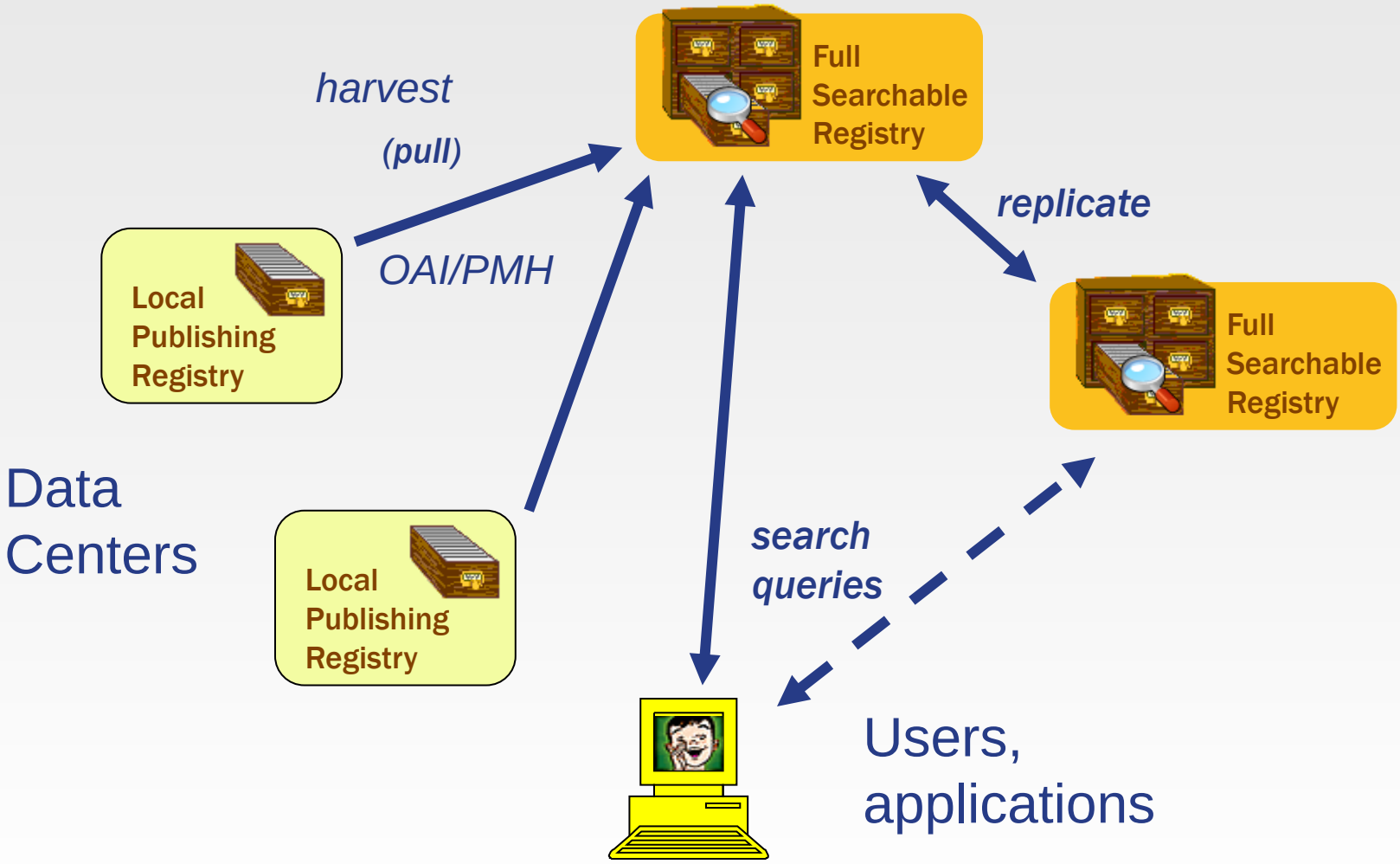
# Key to discovery: Registry

- Used to discover and locate *resources*—data and services—that can be used in a VO application
- Resource: anything that is describable and identifiable.
  - Besides data and services: organizations, projects, software, standards
- Registry: a list of resource descriptions
  - Expressed as structured metadata in XML

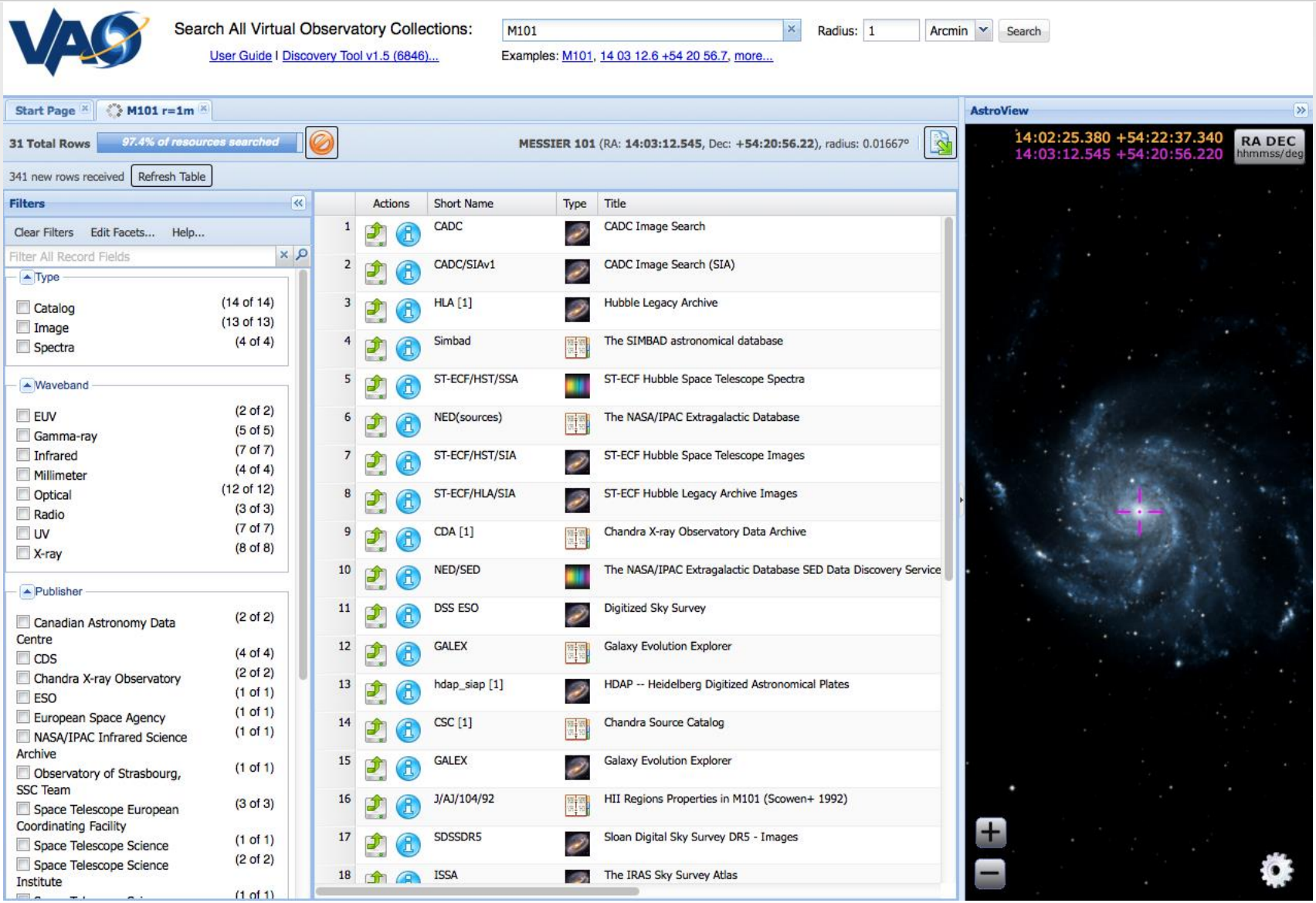
    to enable automated processing and searching

    Metadata based on Dublin Core

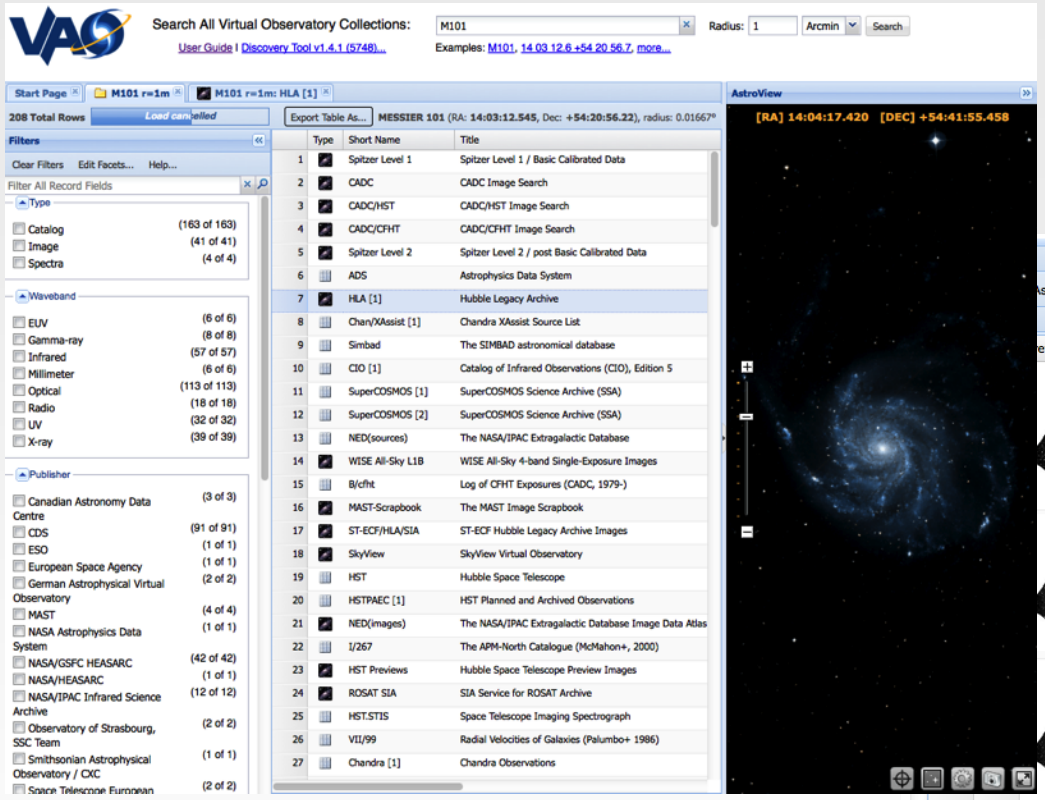
# Registry framework

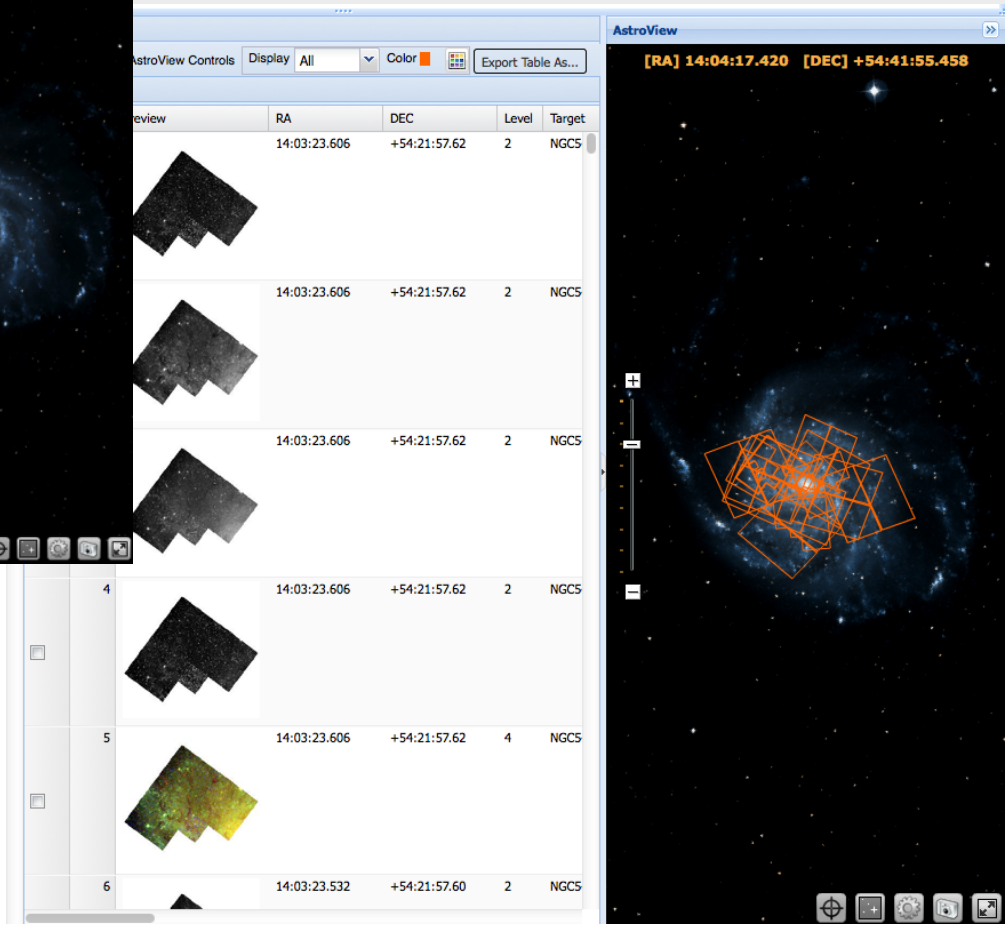


# Data discovery

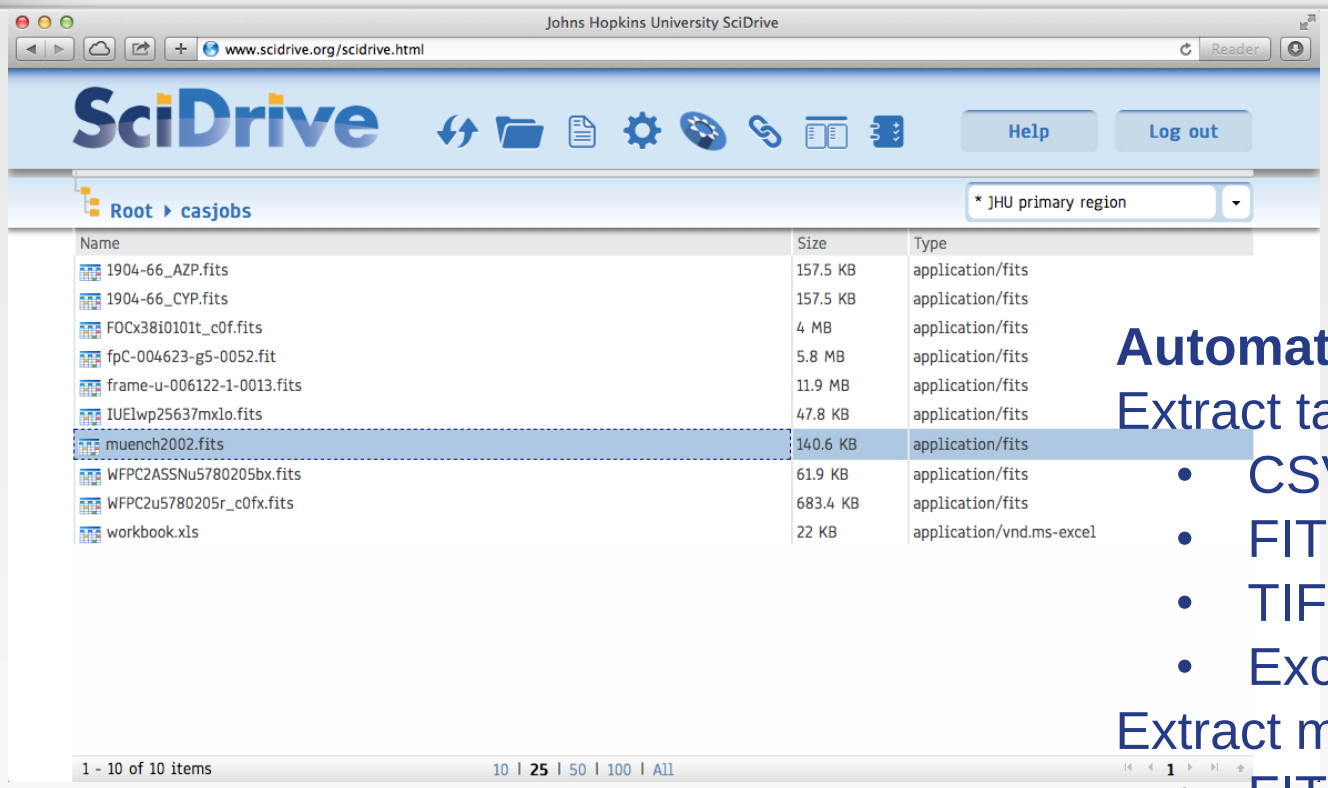


# Data discovery



# SciDrive: astro-centric cloud storage




*Controlled data sharing*
*Single sign-on*
*Deployable as virtual machine*

**Automatic Metadata Extraction**

Extract tabular data from:

- CSV
- FITS
- TIFF
- Excel

Extract metadata from:

- FITS
- Image files (TIFF, JPG)

Automatically upload tables into relational databases:

- CasJobs/MyDB
- SQLShare

# The VO concept elsewhere

- Space Science
  - Virtual Heliophysics Observatory (HELIO)
  - Virtual Radiation Belt Observatory (ViRBO)
  - Virtual Space Physics Observatory (VSPO)
  - Virtual Magnetospheric Observatory (VMO)
  - Virtual Ionosphere Thermosphere Mesosphere Observatory (VITMO)
  - Virtual Solar-Terrestrial Observatory (VSTO)
  - Virtual Sun/Earth Observatory (VSEO)
- Virtual Solar Observatory
- Planetary Science Virtual Observatory
- Deep Carbon Virtual Observatory
- Virtual Brain Observatory

# Data management at NIST

National Institute of Standards and Technology
U.S. Department of Commerce

- I move to NIST 7/28/2014 as Director, Office of Data and Informatics, Material Measurement Laboratory
  - Materials science, chemistry, biology
  - Materials Genome Initiative
- Foster a culture of data management, curation, re-use in a bench-scientist / PI-dominated organization having a strong record of providing “gold standard” data
- Inward-looking challenges
  - Tools, support, advice, common platforms, solution broker
  - Big data, lots of small/medium data
- Outward-looking challenges
  - Service directory
  - Modern web interfaces, APIs, better service integration
  - Get better sense of what communities want from NIST
- Define standards, standard practices
- Collaboration:  other government agencies, universities, domain repositories

Home • Goals of the Materials Genome Initiative

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## Goals of the Materials Genome Initiative

The MGI aims to double the speed at which we discover, develop and manufacture new materials by:

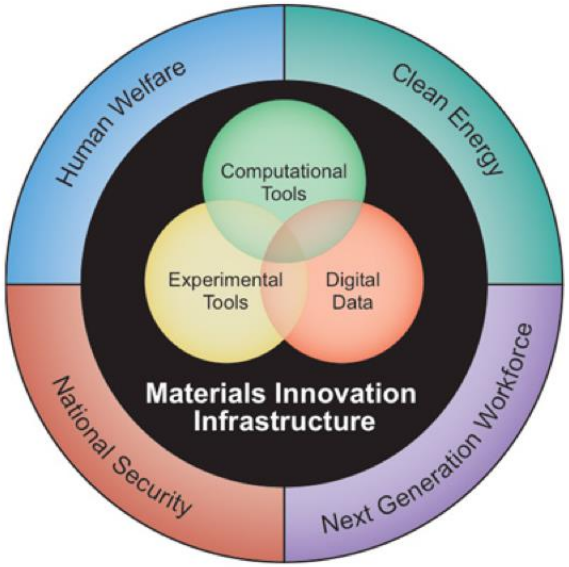
- Developing a "materials innovation infrastructure" that includes:
  - **Computational tools**: software for predictive modeling, simulation, design and exploration
  - **Experimental tools**: synthesis and processing; quantitative characterization and analytic tools; accelerated testing and rapid prototyping; techniques to validate and advance materials theory
  - **Digital data**: data and interoperability standards for material properties; advanced data mining, analytic tools and open/proprietary data warehouses
  - **Collaborative networks**: integrated centers in computation, data informatics and experimentation; sharing of best practices across disparate centers via formal and informal networking; educational materials for the next generation workforce; public/private partnerships
- Building the materials innovation infrastructure while addressing high priority material problems of national importance
- Advancing a culture that supports the use of the materials innovation infrastructure and also embraces a more open, collaborative approach to developing advanced materials

MATERIALS GENOME INITIATIVE

Download the MGI White Paper

Download the MGI Presentation

Download the MGI Fact Sheet




NIST is working to build the materials innovation infrastructure in support of the Administration's Materials Genome Initiative.

http://www.nist.gov/mgi

# NDS and domain repositories

- Domain repositories are discipline-specific
- Various business models in use; long-term sustainability is a major challenge*
- Potential NDS roles
  - Customizable data management and curation tools built on a common substrate
  - Access to cloud-like storage but at non-commercial rates
  - A directory of ontology-building and metadata management tools
  - A directory of domain repositories
  - Accreditation services
  - Advice, referral services, “genius bar”

* “Sustaining Domain Repositories for Digital Data: A White Paper,” C. Ember & R. Hanisch, eds. http://datacommunity.icpsr.umich.edu/sites/default/files/WhitePaper_ICPSR_SDRDD_121113.pdf

# Technologies/standards to build on

- Just use the VO standards!
  - OK, seriously… NIH syndrome
  - Much could be re-used in terms of architecture
  - Generic, collection-level metadata
- Cross-talk with Research Data Alliance (ANDS, EUDAT)
  - Data Citation WG
  - Data Description Registry Interoperability WG
  - Data Type Registries WG
  - Domain Repositories IG
  - Long Tail of Research Data IG
  - Metadata IG
  - Metadata Standards Directory WG
  - Preservation e-Infrastructure WG
  - and others…

*Dataverse, Dryad, iRODS, DSpace, etc.*

# Lessons learned re/ federation

- It takes more time than you think
  - Community consensus requires buy-in early and throughout
- Top-down imposition of standards likely to fail
- Balance requirements coming from a research-oriented community with innovation in IT
- Marketing is very important
  - Managing expectations
  - Build it, and they might come
- Coordination at the international level is essential
  - But takes time and effort
- Data models – sometimes seem obvious, more often not
- Metadata collection and curation are eternal but essential tasks

# Lessons learned re/ federation

- For example, the Cancer Biomedical Informatics Grid (caBIG) [$350M]
  - "…goal was to provide shared computing for biomedical research and to develop software tools and standard formats for information exchange."
  - "The program grew too rapidly without careful prioritization or a cost-effective business model."
  - "…software is overdesigned, difficult to use, or lacking support and documentation."
  - "***The failure to link the mission objectives to the technology shows how important user acceptance and buy-in can be.***" (M. Biddick, Fusion PPT)

J. Foley, *InformationWeek*, 4/8/2011

http://www.informationweek.com/architecture/report-blasts-problem-plagued-cancer-research-grid/d/d-id/1097068?