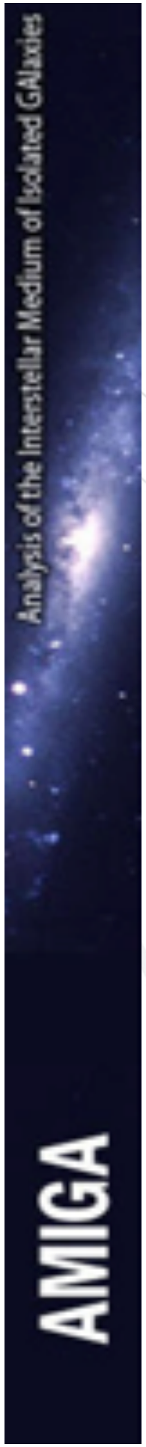


Digital Science

Reproducibility and Visibility in Astronomy

José Enrique Ruiz on behalf of the Wf4Ever Team

SCIOPS 2013
ESAC, FRIDAY 13th SEPTEMBER 2013

Wf4Ever
Advanced Workflow Preservation Technologies for Enhanced Science

2011 - 2013

1. Intelligent Software Components (ISOCO, Spain)
2. University of Manchester (UNIMAN, UK)
3. Universidad Politécnica de Madrid (UPM, Spain)
4. Poznan Supercomputing and Networking Centre (Poland)
5. University of Oxford and OeRC (OXF, UK)

6. Instituto Astrofísica Andalucía (IAA-CSIC, Sp
7. Leiden University Medical Centre (LUMC

Reproducible Science

Astronomy Research Lifecycle

Astronomy research lifecycle is **entirely digital**

- Observation proposals
- Data reduction pipelines
- Analysis of science ready data
- Catalogs of objects and data archives
- Publish process
  - Final data results
  - Experiment in DL

    ADS/arXiv

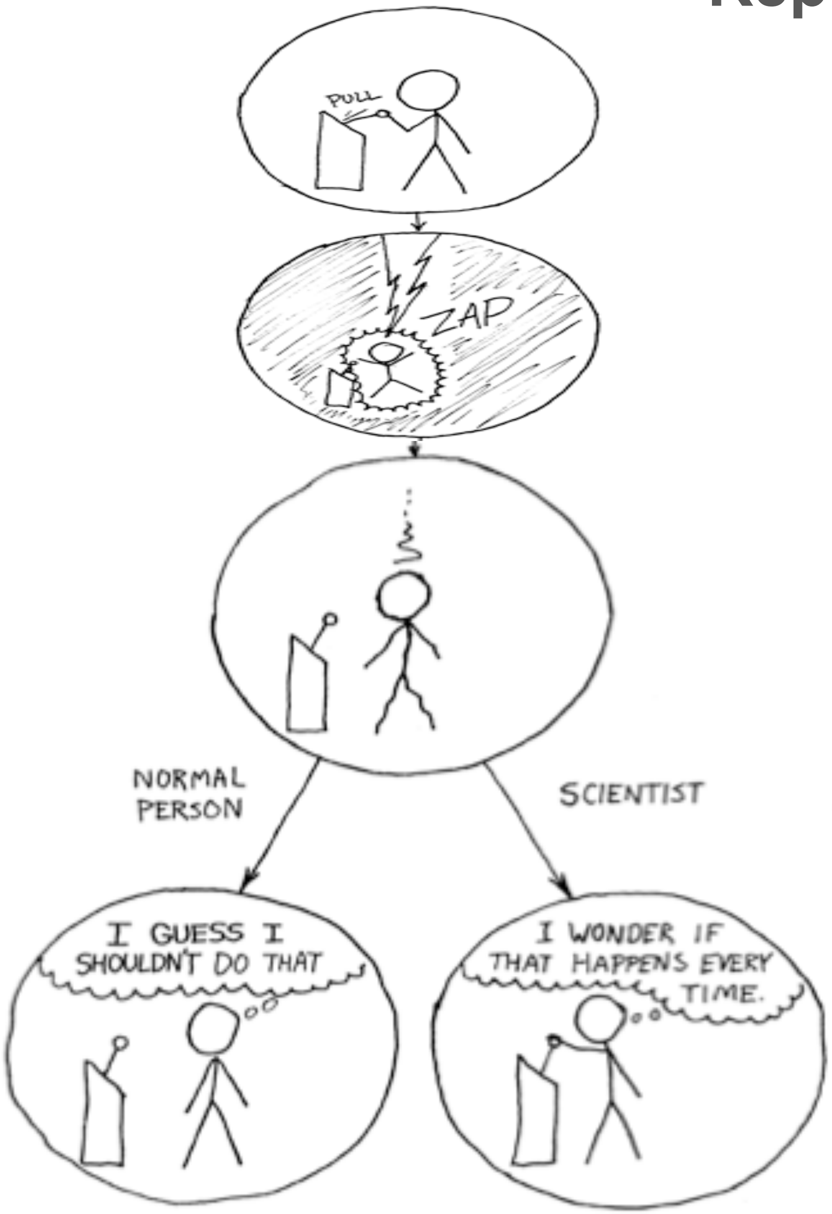
Reproducible research is still not possible in a digital world

A rich infrastructure of data is not efficiently used

A normalized preservation of methodology is needed

Tools

Reproducibility and The Scientific Method


PULL
ZAP
NORMAL PERSON
SCIENTIST
I GUESS I SHOULDN'T DO THAT
I WONDER IF THAT HAPPENS EVERY TIME.

http://xkcd.com/242/

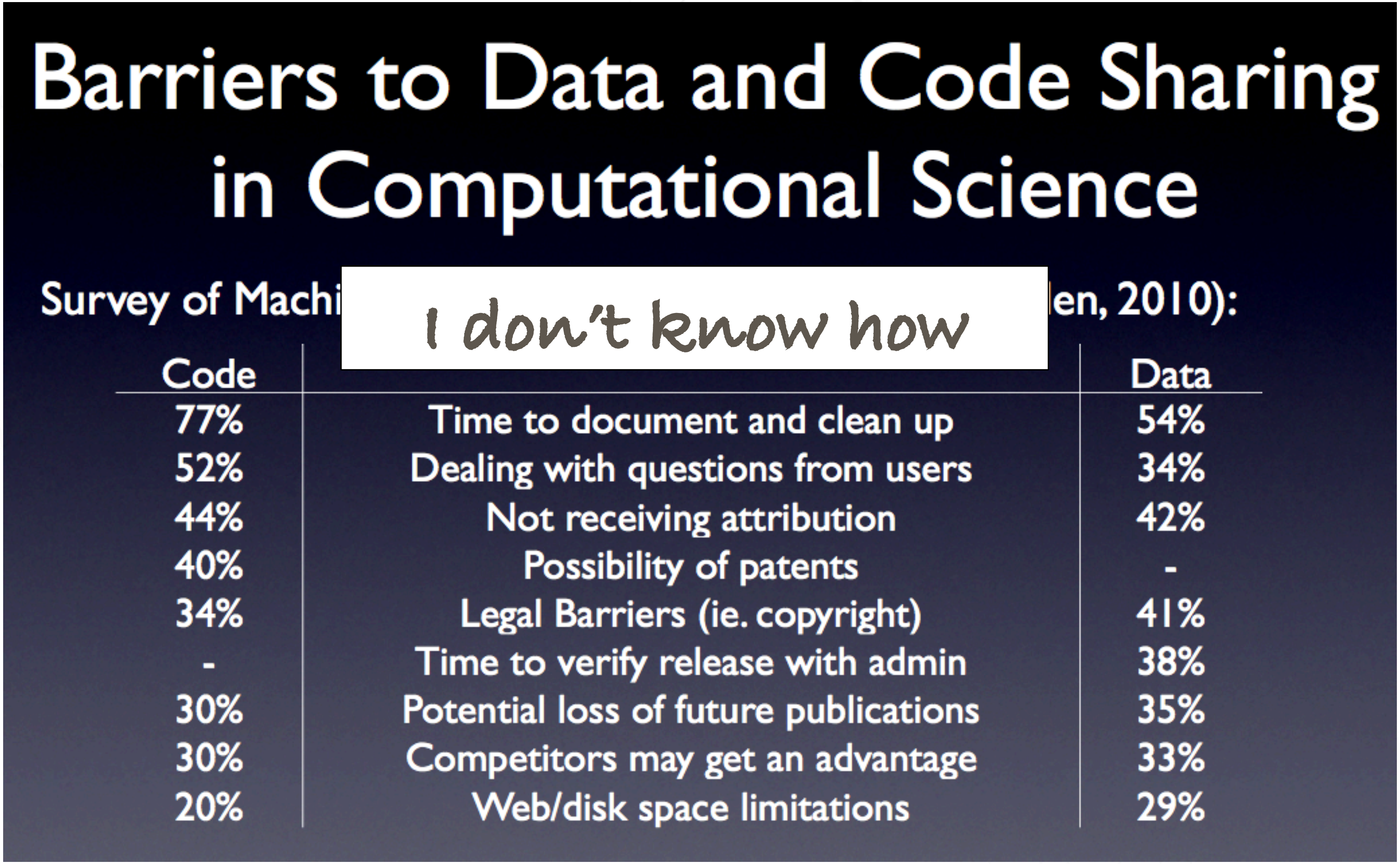
Benefits

- Publishing knowledge, not advertising
- The author, the referee, the re-user
- Reputation, prestige and respect
- Higher quality of publications
  - Authors will be more careful
  - Many eyes to check results

Challenges

- Hard and time consuming
- Need incentives – not rewarded now

Reproducibility and The Scientific Method



Barriers to Data and Code Sharing in Computational Science

Survey of Machi

I don't know how

en, 2010):

Code		Data
77%	Time to document and clean up	54%
52%	Dealing with questions from users	34%
44%	Not receiving attribution	42%
40%	Possibility of patents	-
34%	Legal Barriers (ie. copyright)	41%
-	Time to verify release with admin	38%
30%	Potential loss of future publications	35%
30%	Competitors may get an advantage	33%
20%	Web/disk space limitations	29%

Digital Science - Reproducibility and Visibility in Astronomy

Visibility, Efficiency and Reuse

Optimize return on investments made on big facilities

» Avoid duplication of efforts and reinvention

» How to discover and not duplicate ?

» How to re-use and not duplicate ?

» How to make use of best practices ?

» How to use the rich infrastructure of data ?

» **Intellectual contribs are encoded in software**

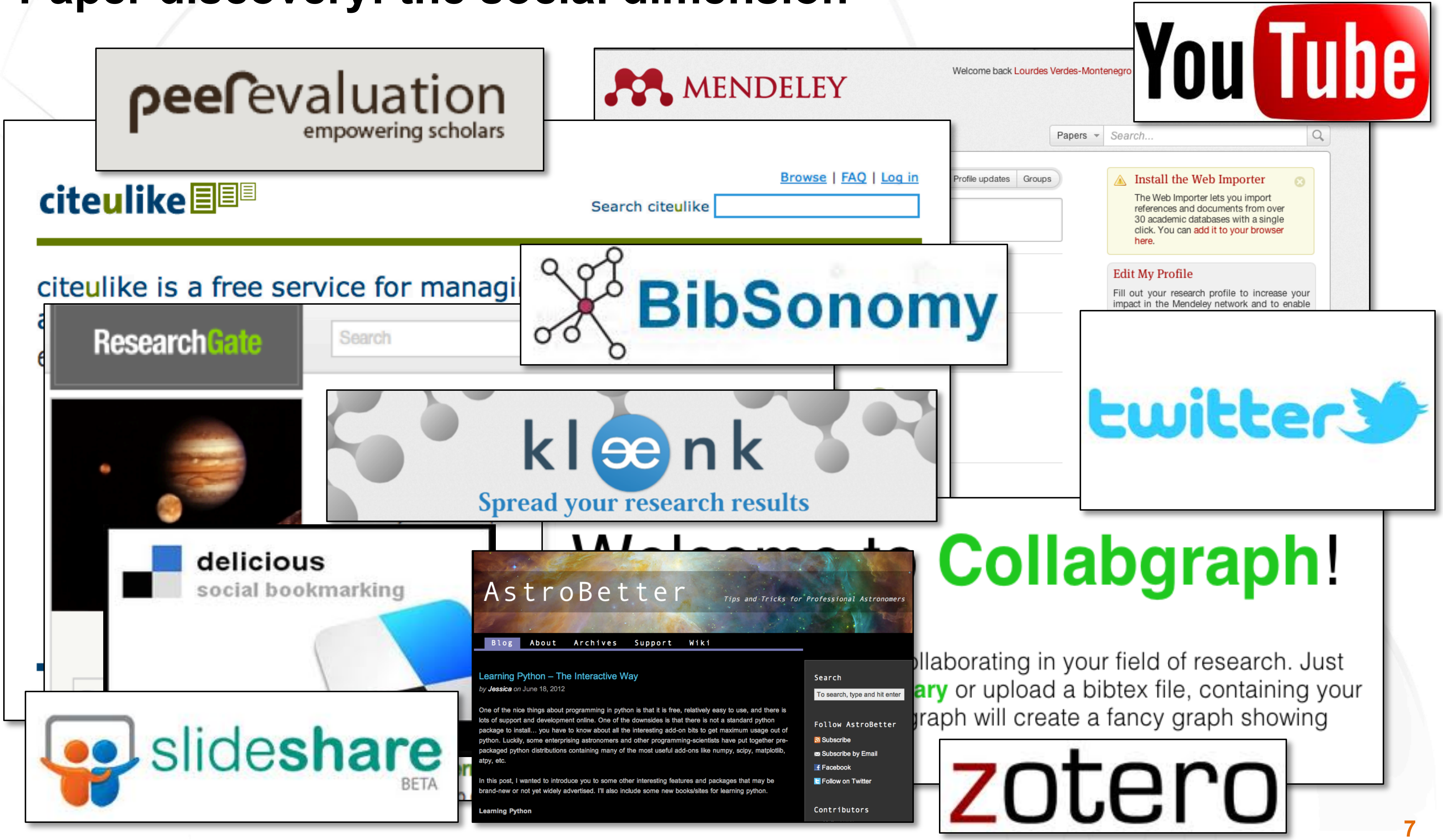
More data in archives does not imply more knowledge

» Expose **complete scientific record**, not the story

» Allow easy **discovery** of methods and tools

PDF
Adobe
IDL
FORTRAN
I R A F
Image Reduction and Analysis Facility
VOSPEC
esa
EXTRAGALACTIC DATABASE
NED
NASA IPAC
python™
IVOA

Paper discovery: the social dimension



Welcome back Lourdes Verdes-Montenegro

Install the Web Importer

The Web Importer lets you import references and documents from over 30 academic databases with a single click. You can add it to your browser here.

Edit My Profile

Fill out your research profile to increase your impact in the Mendeley network and to enable

Learning Python – The Interactive Way

by ***Jessica*** *on* June 18, 2012

One of the nice things about programming in python is that it is free, relatively easy to use, and there is lots of support and development online. One of the downsides is that there is not a standard python package to install… you have to know about all the interesting add-on bits to get maximum usage out of python. Luckily, some enterprising astronomers and other programming-scientists have put together pre-packaged python distributions containing many of the most useful add-ons like numpy, scipy, matplotlib, atpy, etc.

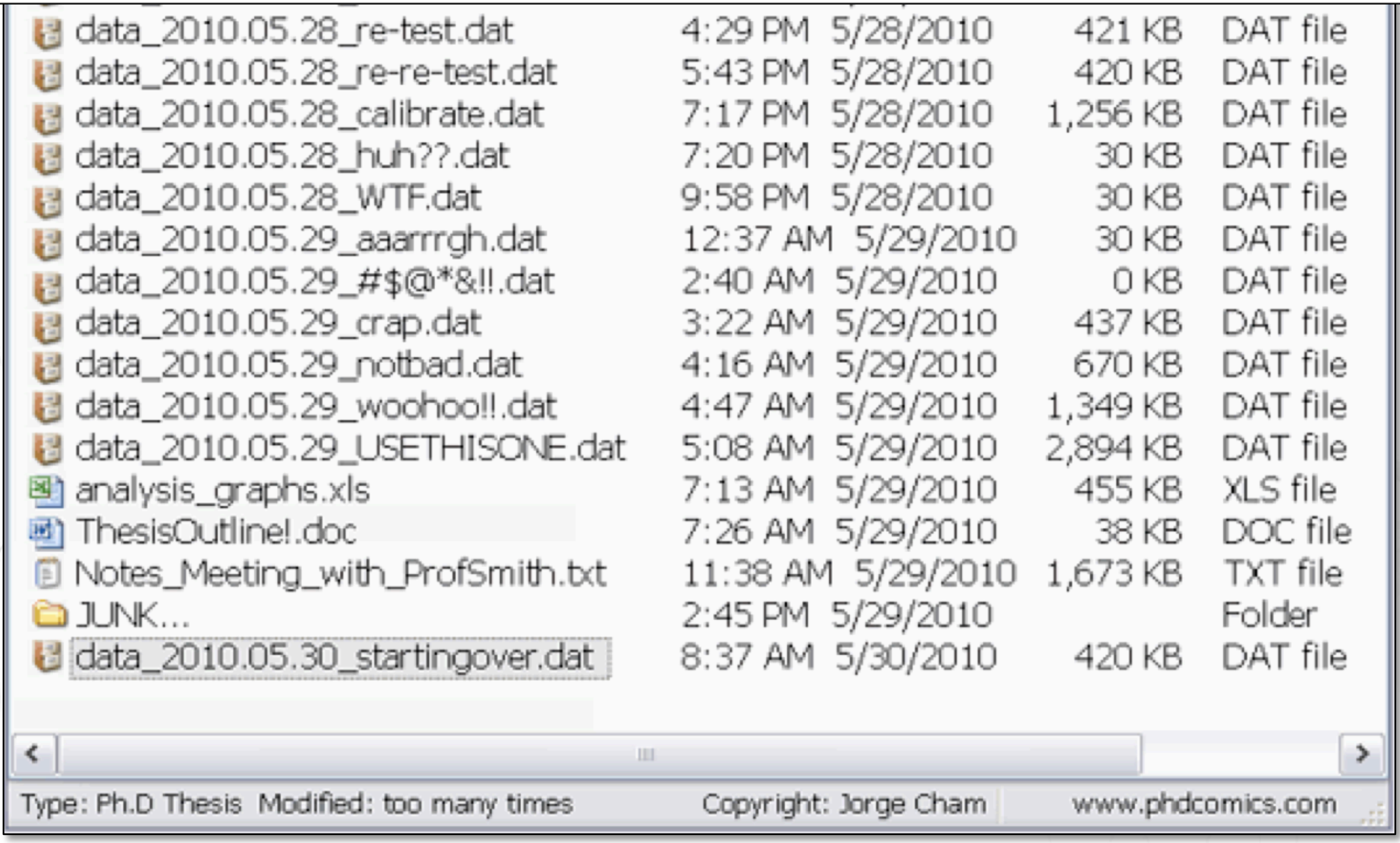
In this post, I wanted to introduce you to some other interesting features and packages that may be brand-new or not yet widely advertised. I'll also include some new books/sites for learning python.

Learning Python

llaborating in your field of research. Just ary or upload a bibtex file, containing your raph will create a fancy graph showing

Time has come to go beyond the PDF

Going beyond automation
Organization

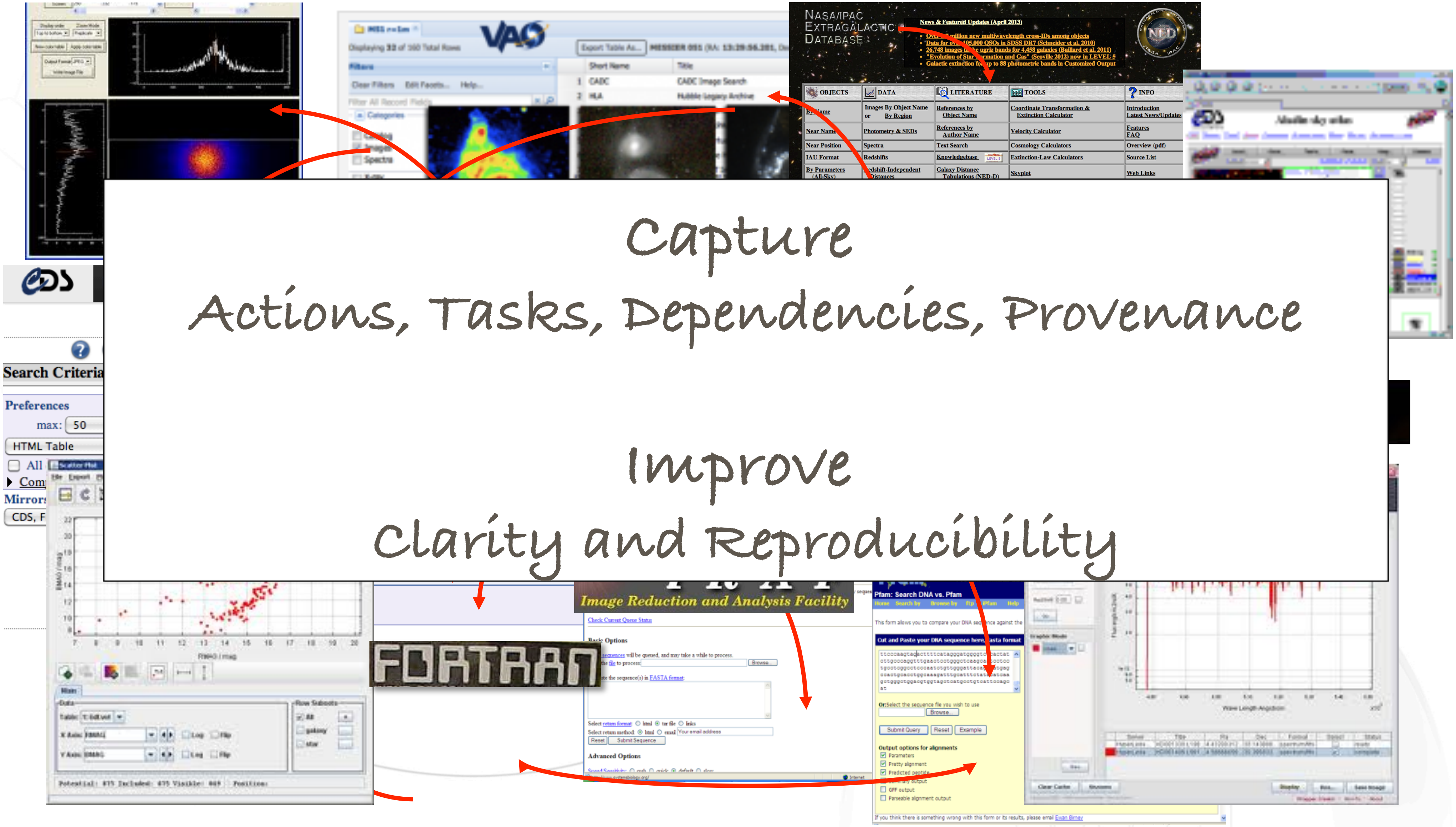


data_2010.05.28_re-test.dat	4:29 PM	5/28/2010	421 KB	DAT file
data_2010.05.28_re-re-test.dat	5:43 PM	5/28/2010	420 KB	DAT file
data_2010.05.28_calibrate.dat	7:17 PM	5/28/2010	1,256 KB	DAT file
data_2010.05.28_huh??.dat	7:20 PM	5/28/2010	30 KB	DAT file
data_2010.05.28_WTF.dat	9:58 PM	5/28/2010	30 KB	DAT file
data_2010.05.29_aaarrrgh.dat	12:37 AM	5/29/2010	30 KB	DAT file
data_2010.05.29_#$@*&!!.dat	2:40 AM	5/29/2010	0 KB	DAT file
data_2010.05.29_crap.dat	3:22 AM	5/29/2010	437 KB	DAT file
data_2010.05.29_notbad.dat	4:16 AM	5/29/2010	670 KB	DAT file
data_2010.05.29_woohoo!!.dat	4:47 AM	5/29/2010	1,349 KB	DAT file
data_2010.05.29_USETHISONE.dat	5:08 AM	5/29/2010	2,894 KB	DAT file
analysis_graphs.xls	7:13 AM	5/29/2010	455 KB	XLS file
ThesisOutline!.doc	7:26 AM	5/29/2010	38 KB	DOC file
Notes_Meeting_with_ProfSmith.txt	11:38 AM	5/29/2010	1,673 KB	TXT file
JUNK...	2:45 PM	5/29/2010		Folder
data_2010.05.30_startingover.dat	8:37 AM	5/30/2010	420 KB	DAT file

Type: Ph.D Thesis Modified: too many times Copyright: Jorge Cham www.phdcomics.com

Workflows to Access and Massage VO Data

Digital Astronomy in the Local Desktop


VAO
NASA/IPAC EXTRAGALACTIC DATABASE
NED
OBJECTS
DATA
LITERATURE
TOOLS
INFO
CDS
Search Criteria
Preferences
max: 50
HTML Table
Mirrors
FORTRAN
IRAF
Image Reduction and Analysis Facility
Pfam: Search DNA vs. Pfam
Cut and Paste your DNA sequence here, fasta format
Submit Query
Reset
Example
Output options for alignments
Basic Options
Advanced Options

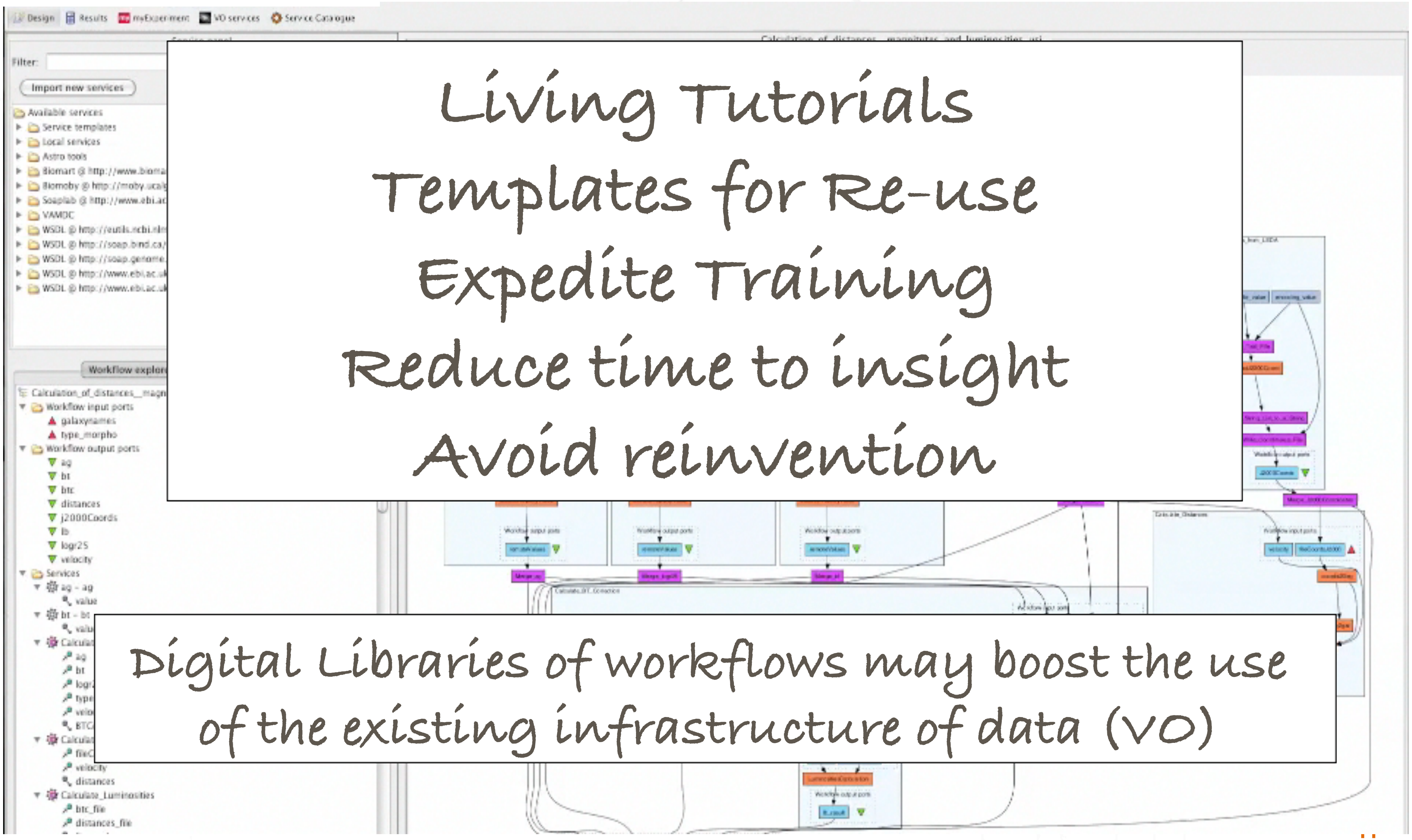
Capture

Actions, Tasks, Dependencies, Provenance

Improve

Clarity and Reproducibility

Scientific Workflows



Living Tutorials

Templates for Re-use

Expedite Training

Reduce time to insight

Avoid reinvention

Digital Libraries of workflows may boost the use of the existing infrastructure of data (VO)

Scientific Workflows

Related Initiatives

- ER-Flow
- VAMDC
- **HELIO**
- Cyber-SKA
- IceCore
- Montage
- **Astro-WISE**
- AstroGrid

Software

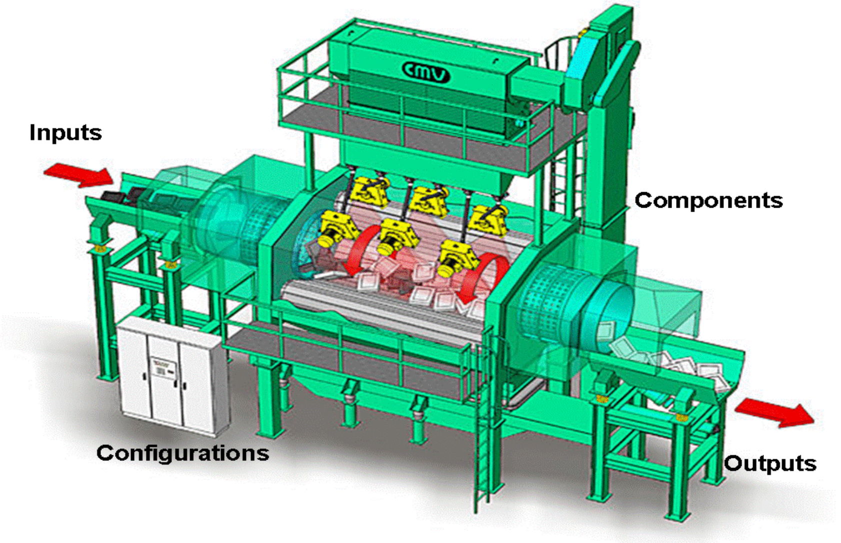
- Taverna
- Kepler
- Pegasus
- Triana
- **ESO Reflex**

IVOA

- AstroGrid
- Grid&WS WG
- VO France Wf WG

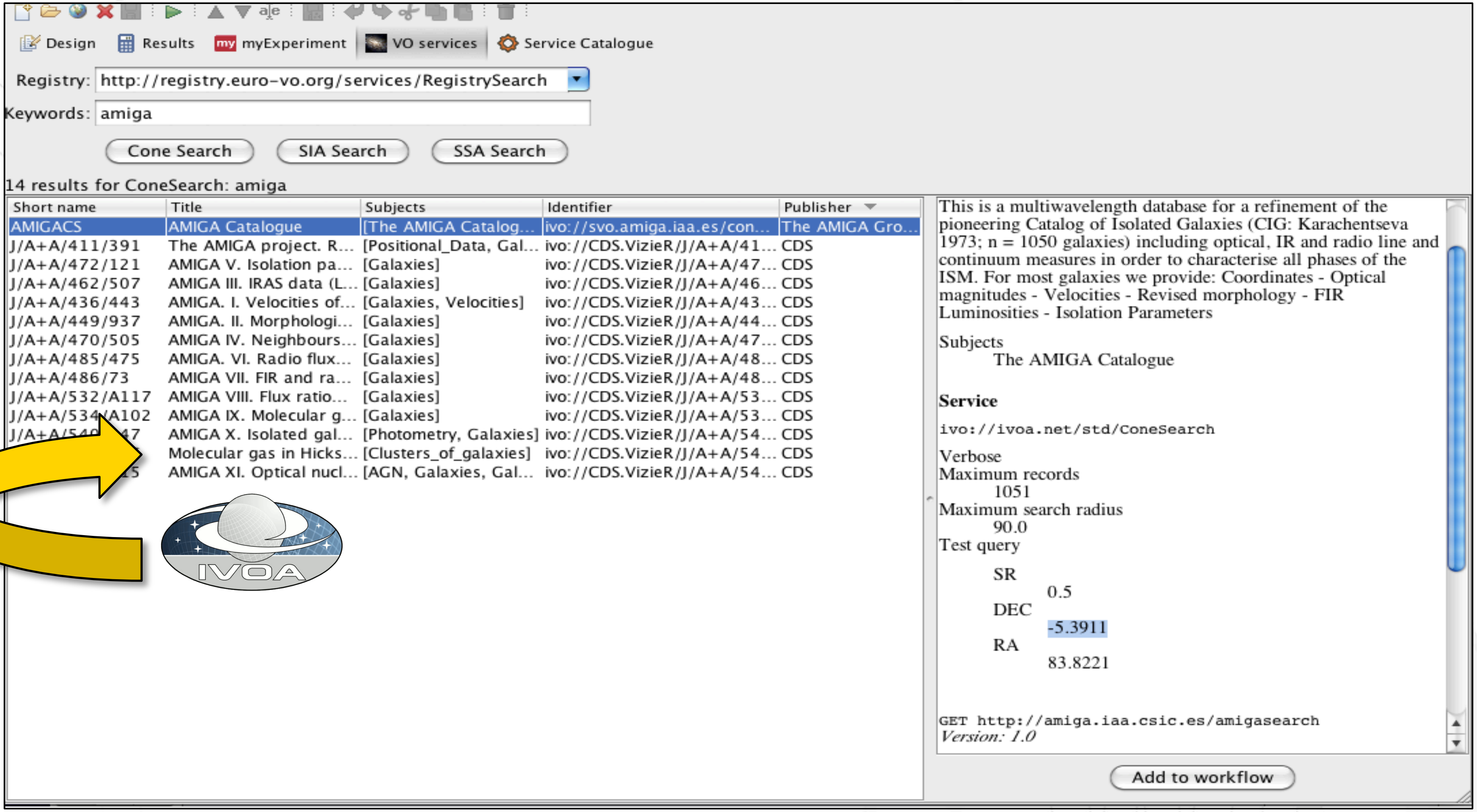
Self descriptive WS

- PDL
- SimDAL, S3



Interoperability
Standards

AstroTaverna: Create, annotate and run a workflow



Registry: http://registry.euro-vo.org/services/RegistrySearch

Keywords: amiga

14 results for ConeSearch: amiga

Short name	Title	Subjects	Identifier	Publisher
AMIGACS	AMIGA Catalogue	[The AMIGA Catalog...	ivo://svo.amiga.iaa.es/con...	The AMIGA Gro...
J/A+A/411/391	The AMIGA project. R...	[Positional_Data, Gal...	ivo://CDS.VizieR/J/A+A/41...	CDS
J/A+A/472/121	AMIGA V. Isolation pa...	[Galaxies]	ivo://CDS.VizieR/J/A+A/47...	CDS
J/A+A/462/507	AMIGA III. IRAS data (L...	[Galaxies]	ivo://CDS.VizieR/J/A+A/46...	CDS
J/A+A/436/443	AMIGA. I. Velocities of...	[Galaxies, Velocities]	ivo://CDS.VizieR/J/A+A/43...	CDS
J/A+A/449/937	AMIGA. II. Morphologi...	[Galaxies]	ivo://CDS.VizieR/J/A+A/44...	CDS
J/A+A/470/505	AMIGA IV. Neighbours...	[Galaxies]	ivo://CDS.VizieR/J/A+A/47...	CDS
J/A+A/485/475	AMIGA. VI. Radio flux...	[Galaxies]	ivo://CDS.VizieR/J/A+A/48...	CDS
J/A+A/486/73	AMIGA VII. FIR and ra...	[Galaxies]	ivo://CDS.VizieR/J/A+A/48...	CDS
J/A+A/532/A117	AMIGA VIII. Flux ratio...	[Galaxies]	ivo://CDS.VizieR/J/A+A/53...	CDS
J/A+A/534/A102	AMIGA IX. Molecular g...	[Galaxies]	ivo://CDS.VizieR/J/A+A/53...	CDS
J/A+A/54[illegible]47	AMIGA X. Isolated gal...	[Photometry, Galaxies]	ivo://CDS.VizieR/J/A+A/54...	CDS
[illegible]	Molecular gas in Hicks...	[Clusters_of_galaxies]	ivo://CDS.VizieR/J/A+A/54...	CDS
[illegible]5	AMIGA XI. Optical nucl...	[AGN, Galaxies, Gal...	ivo://CDS.VizieR/J/A+A/54...	CDS

This is a multiwavelength database for a refinement of the pioneering Catalog of Isolated Galaxies (CIG: Karachentseva 1973; n = 1050 galaxies) including optical, IR and radio line and continuum measures in order to characterise all phases of the ISM. For most galaxies we provide: Coordinates - Optical magnitudes - Velocities - Revised morphology - FIR Luminosities - Isolation Parameters

Subjects
The AMIGA Catalogue

Service

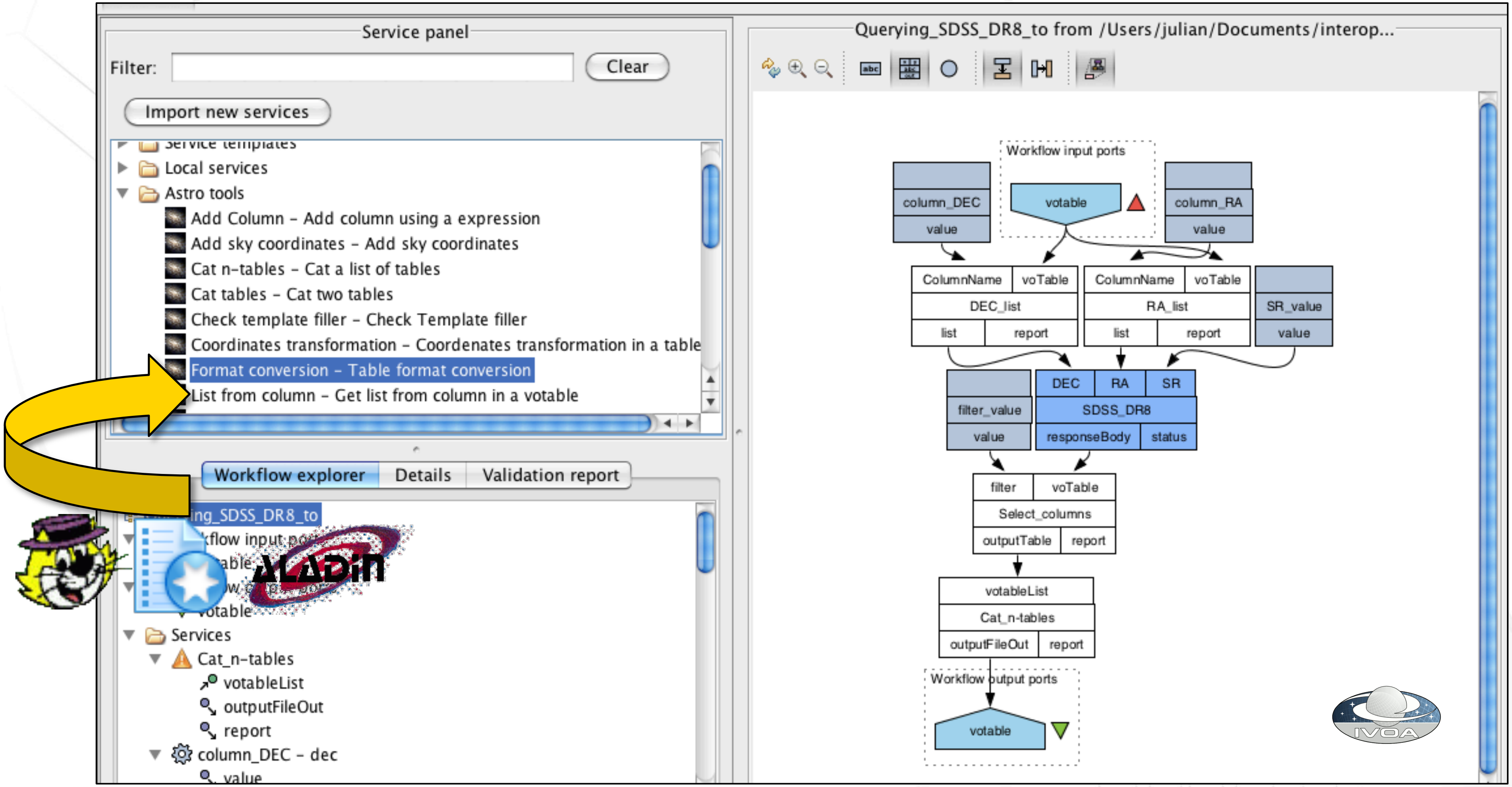
ivo://ivoa.net/std/ConeSearch

Verbose
Maximum records
1051
Maximum search radius
90.0
Test query
SR
0.5
DEC
-5.3911
RA
83.8221

GET http://amiga.iaa.csic.es/amigasearch
Version: 1.0

http://amiga.iaa.es/p/290-astrotaverna.htm

AstroTaverna: Create, annotate and run a workflow



Service panel

Filter: Clear

Import new services

- Service templates
- Local services
- Astro tools
  - Add Column - Add column using a expression
  - Add sky coordinates - Add sky coordinates
  - Cat n-tables - Cat a list of tables
  - Cat tables - Cat two tables
  - Check template filler - Check Template filler
  - Coordinates transformation - Coordenates transformation in a table
  - Format conversion - Table format conversion
  - List from column - Get list from column in a votable

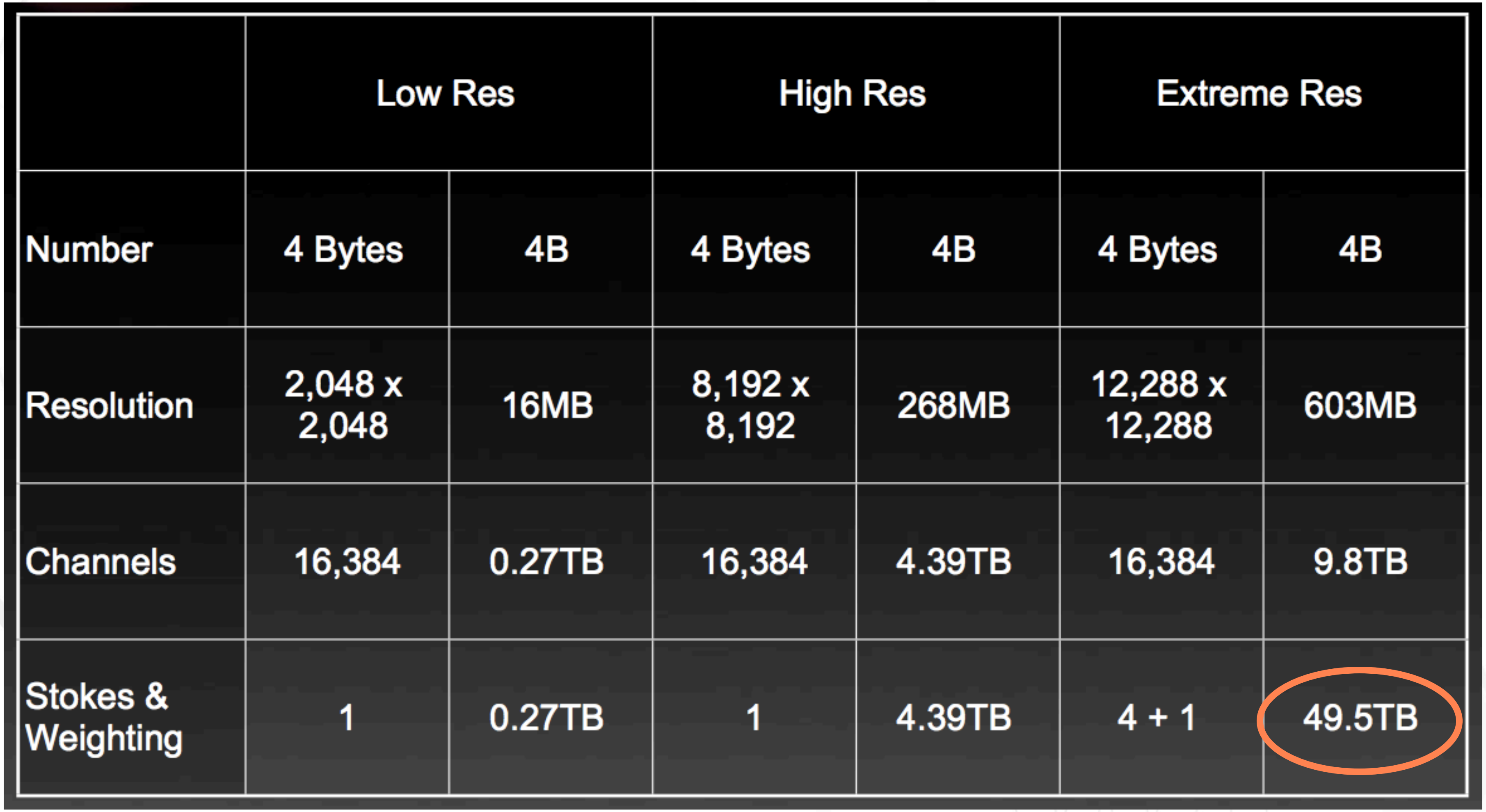
Workflow explorer | Details | Validation report

- ing_SDSS_DR8_to
  - kflow input po
    - able
  - w
    - votable
  - Services
    - Cat_n-tables
      - votableList
      - outputFileOut
      - report
    - column_DEC - dec
      - value

Querying_SDSS_DR8_to from /Users/julian/Documents/interop...

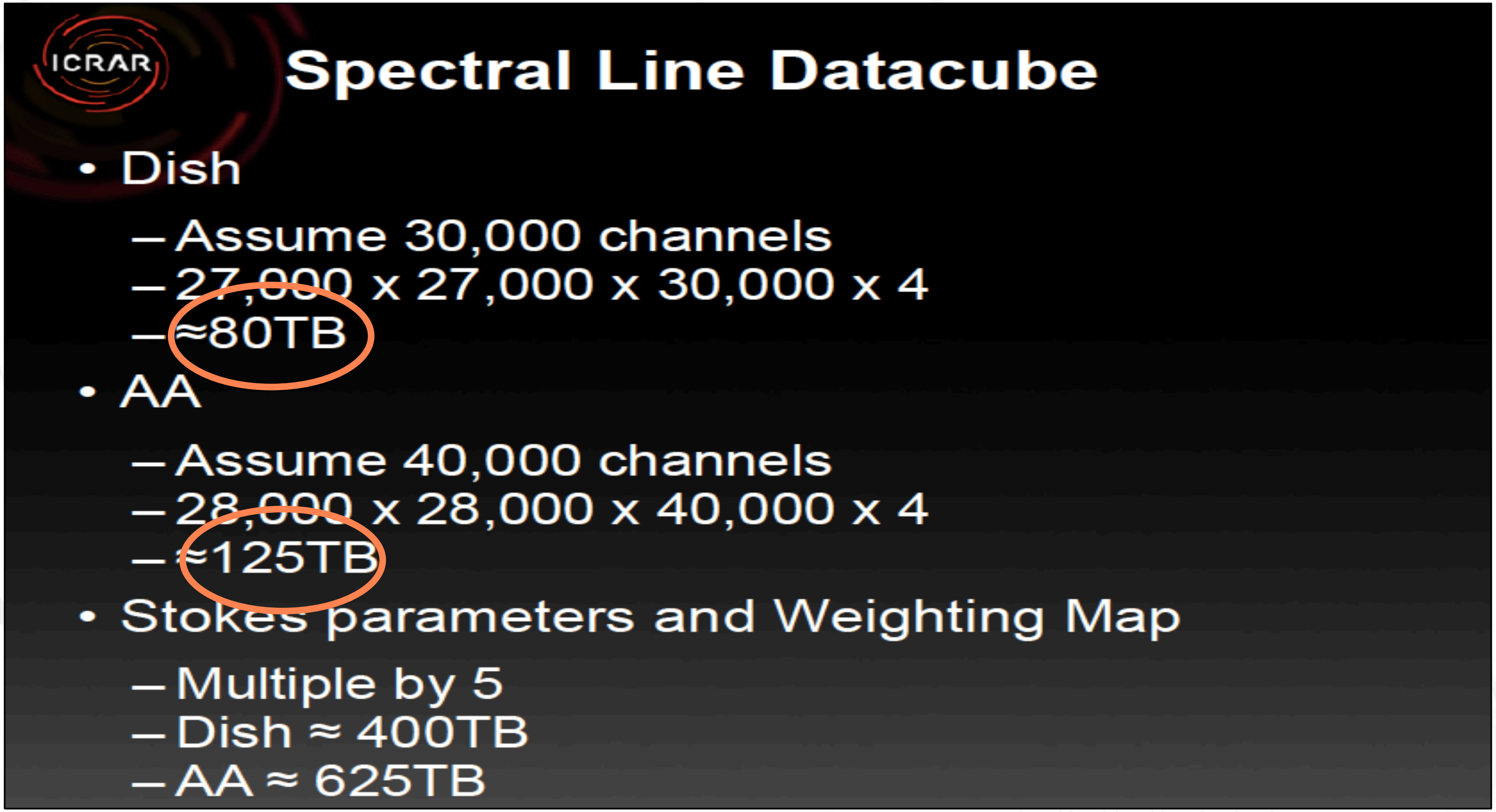
http://amiga.iaa.es/p/290-astrotaverna.htm

ASKAP Datacubes



	Low Res		High Res		Extreme Res	
Number	4 Bytes	4B	4 Bytes	4B	4 Bytes	4B
Resolution	2,048 x 2,048	16MB	8,192 x 8,192	268MB	12,288 x 12,288	603MB
Channels	16,384	0.27TB	16,384	4.39TB	16,384	9.8TB
Stokes & Weighting	1	0.27TB	1	4.39TB	4 + 1	49.5TB

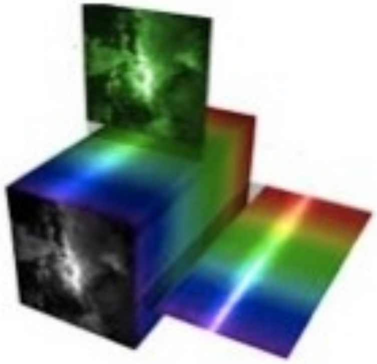
SKA Datacubes



Spectral Line Datacube

- Dish
  - Assume 30,000 channels
  - 27,000 x 27,000 x 30,000 x 4
  - ≈80TB
- AA
  - Assume 40,000 channels
  - 28,000 x 28,000 x 40,000 x 4
  - ≈125TB
- Stokes parameters and Weighting Map
  - Multiple by 5
  - Dish ≈ 400TB
  - AA ≈ 625TB

The next generation of archives

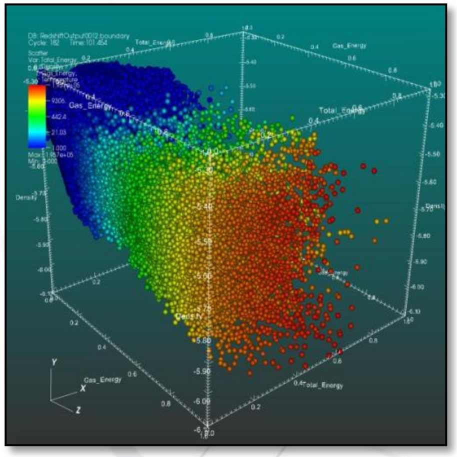


Much wider FoV and spectral coverage

- Large volumes for a single observed dataset

Automated surveys

- Huge amounts of tabular data



Extraction of scientifically relevant info from a multiD param. space

- Exploration services
- Anomaly detection
- Cross-matching data
- Dimensionality reduction

Detailed inspection and subset

- Filtering
- Extraction
- Re-Projection
- Analysis services

We are moving into a world where

- computing and storage are cheap
- **data movement is death**

The *move computing to data* parad

- » A cloud of Web Services

Archives should evolve from nto

» Virtual Data provider

» Software Tasks p

- » Archives speaking W

Astronomy s/facilities/wavelength

Interco eroperable archives

» bservatory

» sks

Web Services based
Scientific Workflows

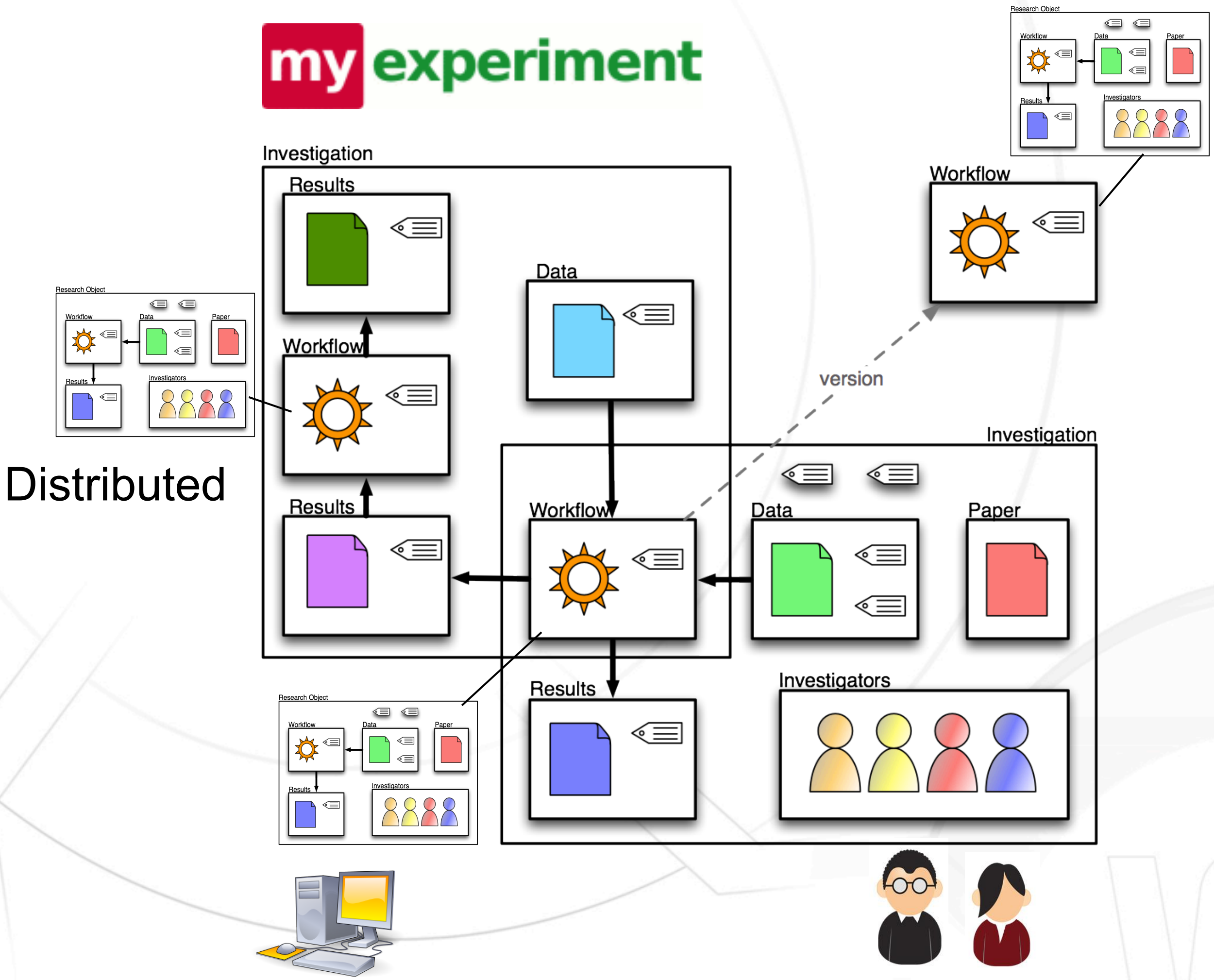
Preservation

Process should enefit of the same privileges acquired by data

Preserving the method ensures replication of final results at any moment

Research Objects

Expose experimental context in a structured way in order to be understood



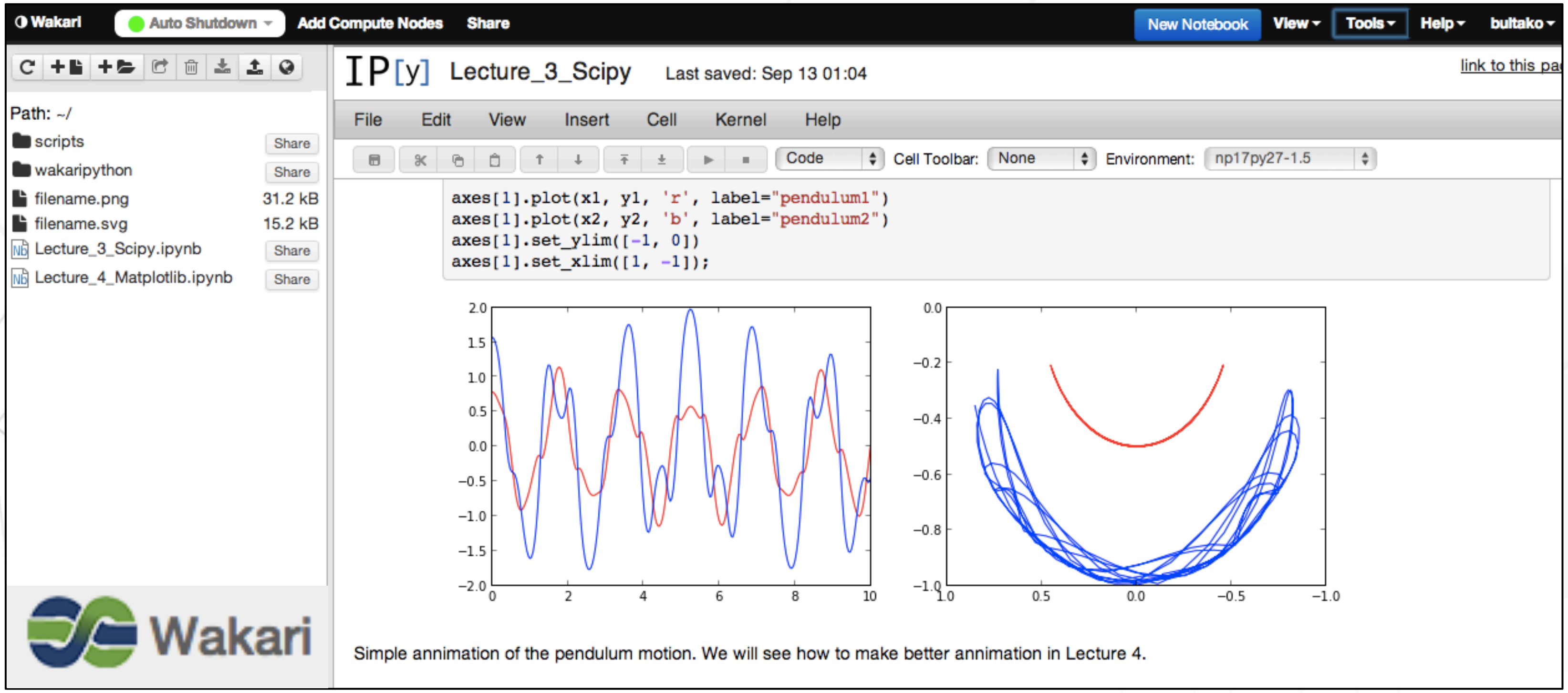
Distributed

Technical Objects

Social Objects

IPython Notebook solutions

- » Web-browser as the working desktop
- » Python code, plots and data, living with rich-text documentation
- » Cloud-based adaptive scalable computing environment
- » Fully shareable, re-usable and executable wikis
- » Social platform and Git versioning



```
axes[1].plot(x1, y1, 'r', label="pendulum1")
axes[1].plot(x2, y2, 'b', label="pendulum2")
axes[1].set_ylim([-1, 0])
axes[1].set_xlim([1, -1]);
```

Simple annimation of the pendulum motion. We will see how to make better annimation in Lecture 4.

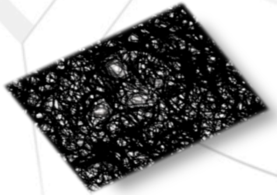
Research Objects

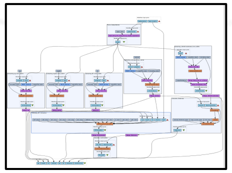
Similar initiative to ESO Telbib

ADSLabs

ADO Linked Components

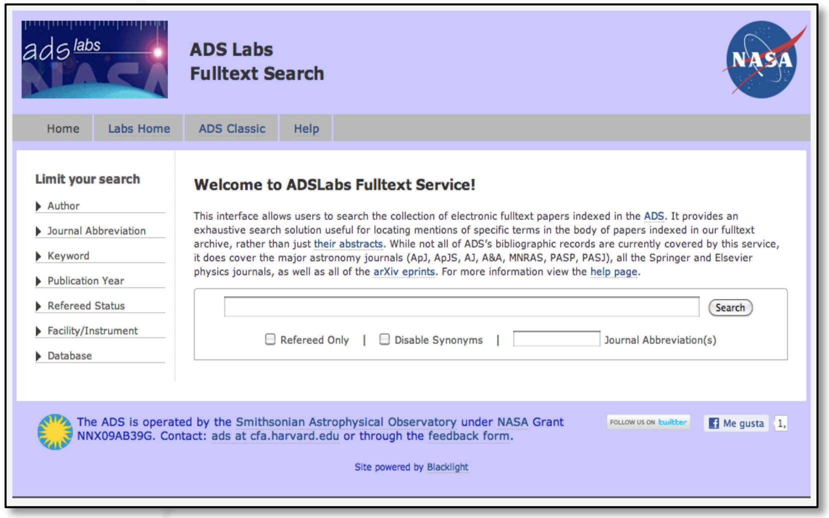
- » Authors
- » Publications
- » Journals
- » Objects SIMBAD
- » Tabular data behind the plots CDS
- » ASCL reference of used software
- » Observing time Proposals
- » Used facilities, surveys or missions





Incentives

http://labs.adsabs.harvard.edu/



ADS Labs
Fulltext Search

Limit your search

- Author
- Journal Abbreviation
- Keyword
- Publication Year
- Refereed Status
- Facility/Instrument
- Database

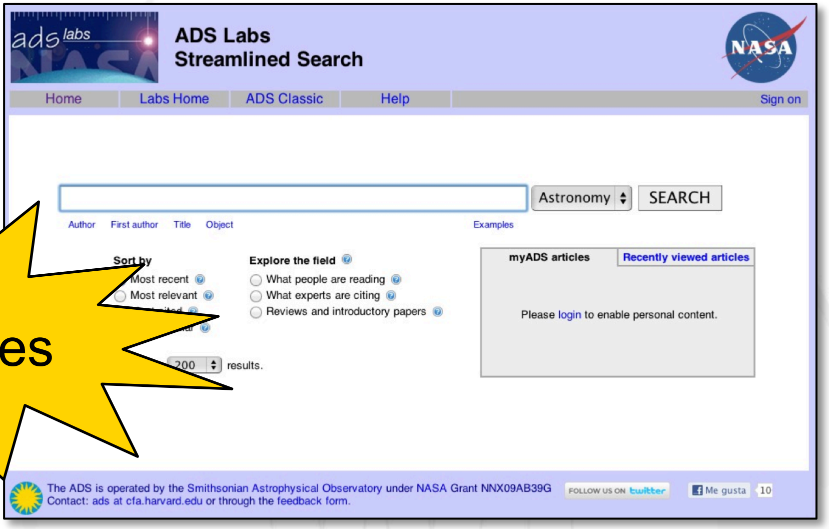
Welcome to ADSLabs Fulltext Service!

This interface allows users to search the collection of electronic fulltext papers indexed in the ADS. It provides an exhaustive search solution useful for locating mentions of specific terms in the body of papers indexed in our fulltext archive, rather than just their abstracts. While not all of ADS's bibliographic records are currently covered by this service, it does cover the major astronomy journals (ApJ, ApJS, AJ, A&A, MNRAS, PASP, PASJ), all the Springer and Elsevier physics journals, as well as all of the arXiv eprints. For more information view the help page.

Search
☐ Refereed Only | ☐ Disable Synonyms | Journal Abbreviation(s)

The ADS is operated by the Smithsonian Astrophysical Observatory under NASA Grant NNX09AB39G. Contact: ads at cfa.harvard.edu or through the feedback form.

Site powered by Blacklight



ADS Labs
Streamlined Search

Sort by

- ○ Most recent
- ○ Most relevant

200 results.

Explore the field

- ○ What people are reading
- ○ What experts are citing
- ○ Reviews and introductory papers

Please login to enable personal content.

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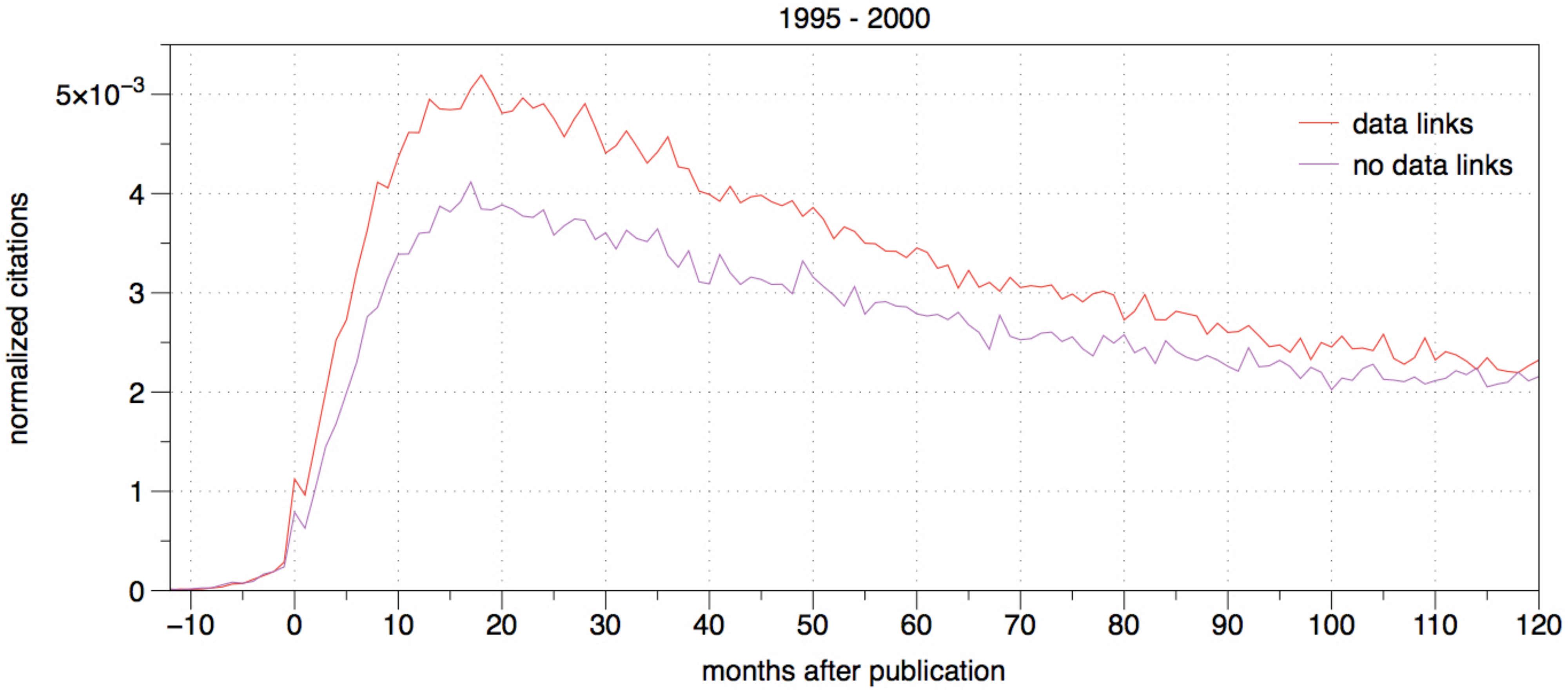
Contact: ads at cfa.harvard.edu or through the feedback form.

The Incentive

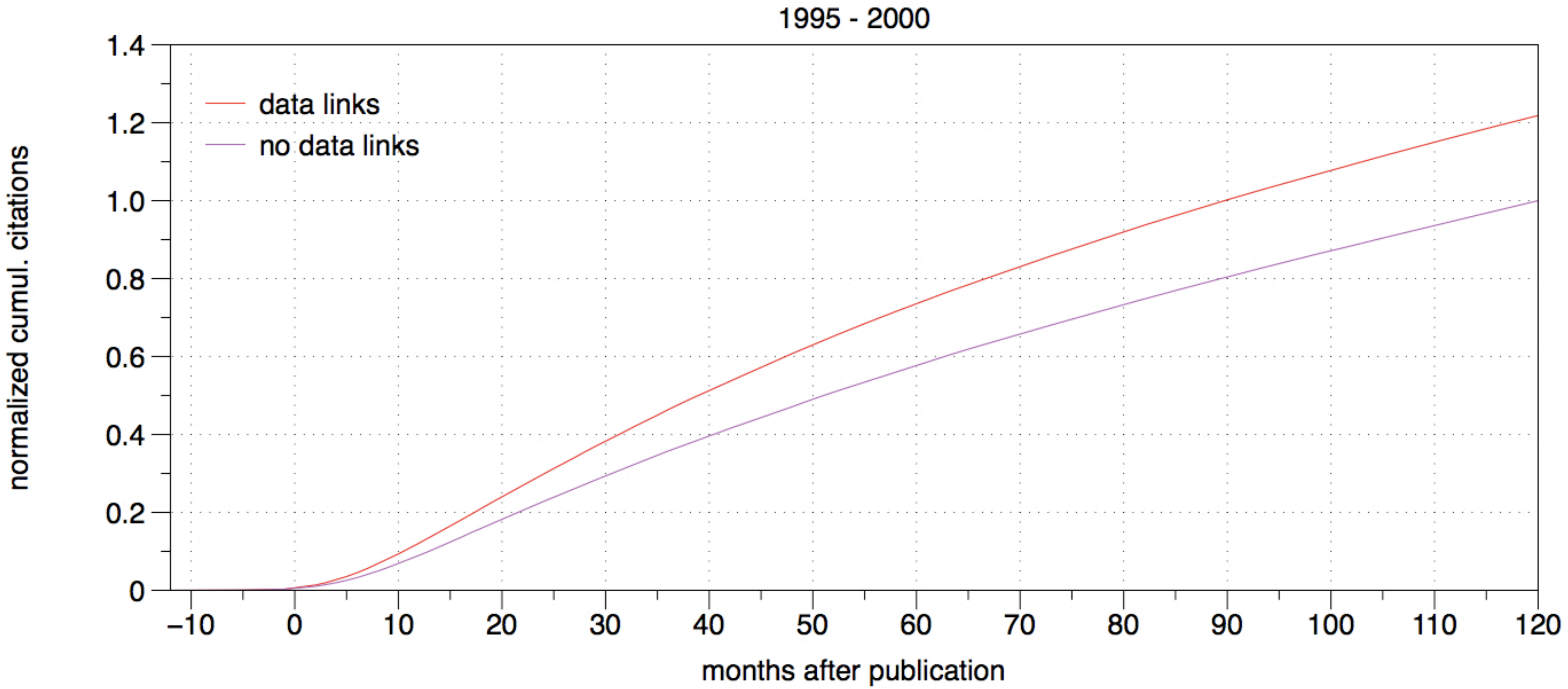
Papers with data links are cited more than those without



Effect of E-printing on Citation Rates in Astronomy and Physics
2006. Edwin A. Henneken et al.

The Incentive

Papers with data links are cited more than those without



Effect of E-printing on Citation Rates in Astronomy and Physics 2006. Edwin A. Henneken et al.

Digital Science - Reproducibility and Visibility in Astronomy

Conclusions

- Reproducibility is at the very heart of the scientific method
- Improving visibility is key in order to avoid reinvention
- Social dimension of science stressed in the discovery process
- Highly specialized science needs re-use to achieve efficiency
- In a digital world, publish decomposable executable papers
- Capture provenance and structure in the local desktop
- Scientific workflows go beyond automation: provide clarity and structure
- Transfer rate is more than an issue for next generation of archives
- The move computing to data paradigm -> back to old terminals
- Process should benefit of the same privileges acquired by data
- Digital libraries of web-services-based workflows
- The distributed digital workflow-centric Research Object
- Preserving knowledge - not only data or advertising

jer@iaa.es