

# Digital Science

## Towards the Executable Paper

José Enrique Ruiz on behalf of the Wf4Ever and CANUBE Teams

IAA Seminars

IAA - CSIC, THURSDAY 31st OCTOBER 2013



### Wf4Ever

### Advanced Workflow Preservation Technologies for Enhanced Science

### 2011 – 2013 EU FP7



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, Spain)
7. Leiden University Medical Centre (LUMC, The Netherlands)

Reproducible  
Science



### IAA – CSIC contribution through AMIGA Group

- **User Functional Requirements**
  - BioGenomics /BioInformaticians
  - Astronomers /AstroInformaticians
  - Publishers /Librarians
  - Computer Scientists
- **Software Development**
  - AstroTaverna Plugin
  - AstroTaverna Starter Pack and Workflows
- **Community Engagement and Collaborations**
  - Spanish Virtual Observatory
  - International Virtual Observatory Alliance
  - Action Spécifique Observatoires Virtuels France
  - Observatoire de Paris-Meudon
  - EU FP7 Projects : Er-Flow and VAMDC
  - SAO NASA /ADS Digital Library



Reproducible  
Science





## CANube Ciencia Abierta en la Nube

Mars – Dec 2013

Open Science Project granted by the Second Call for Proposals of the **Bio-TIC Campus of International Excellence** of the University of Granada.

- Universidad de Granada
- Instituto Astrofísica Andalucía - CSIC
- Campus CEI-BioTic
  
- Red del Sur
- Fidesol
- Intelify
- Grupo Trevenque





Open Science



# Digital Science - Towards the Executable Paper

## Digital Astronomy

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**



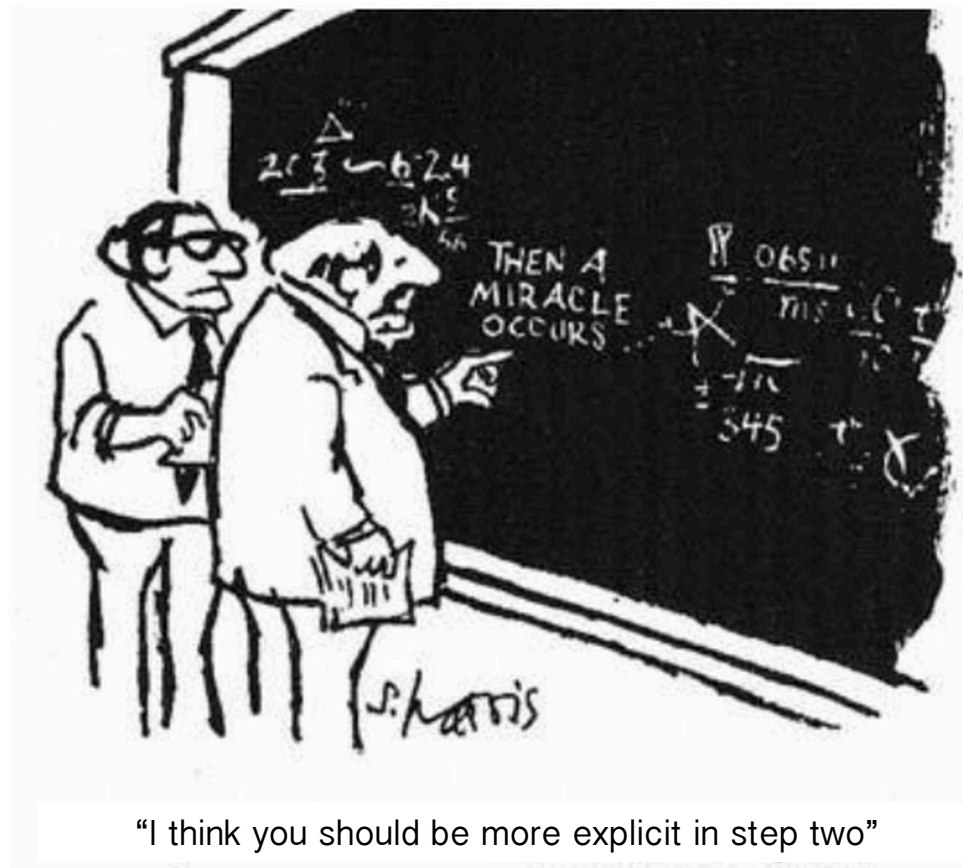
**A normalized preservation of methodology is needed**

**Tools**

## Digital Science - Towards the Executable Paper Reproducibility

“... up to 70% of research from academic labs **cannot be reproduced**, representing an enormous waste of money and effort.”

- Elizabeth Iorns, Science Exchange



# Digital Science - Towards the Executable Paper

## Open Science

Reproducibility is achieved when access is granted for all resources

Reproducibility  $\rightleftharpoons$  Open Access

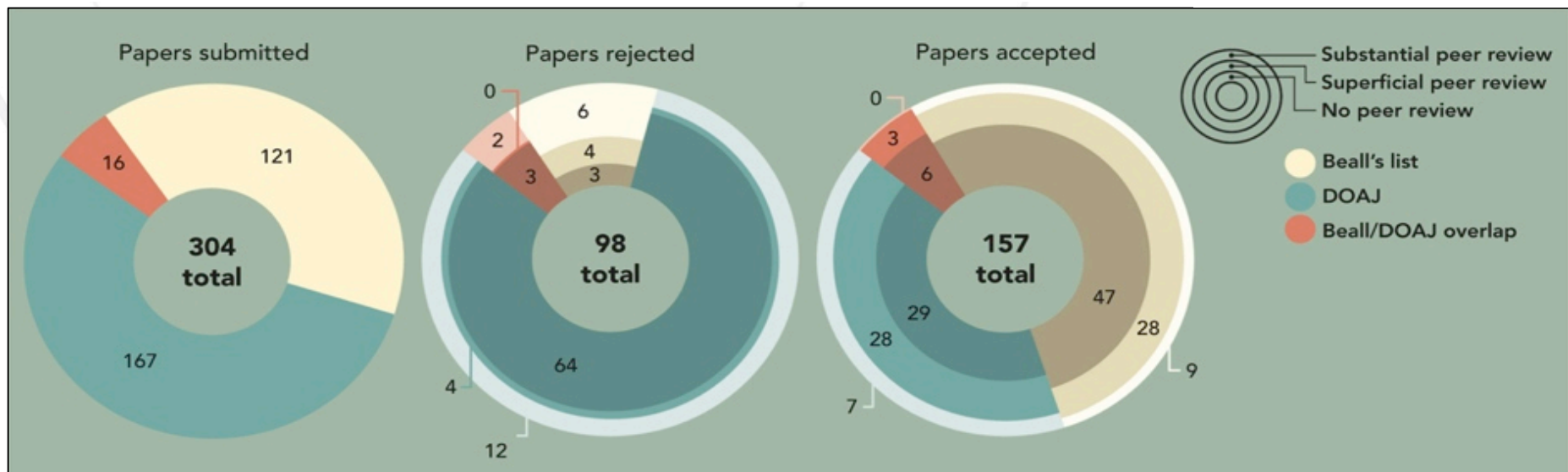
Clamorous fake methods and results published in 157 out of 304 Journals

### Who's Afraid of Peer Review?

John Bohannon

A spoof paper concocted by *Science* reveals little or no scrutiny at many open-access journals.

*Science* 4 October 2013:  
Vol. 342 no. 6154 pp. 60-65  
DOI: 10.1126/science.342.6154.60



# Digital Science - Towards the Executable Paper

## Open Science

### More trial, less error - An effort to improve scientific studies

Recomendar 322 personas recomiendan esto. Sé el primero de tus amigos.



Tweet 84

Share

Share this

+1 15

Email

nature

International weekly journal of science

Home | News & Comment | Research | Careers & Jobs | Current Issue | Archive | Audio & Video | For Authors

Archive > Volume 501 > Issue 7468 > News > Article

NATURE | NEWS



### Mozilla plan seeks to debug scientific code

Software experiment raises prospect of extra peer review.

Erika Check Hayden

24 September 2012

“One worry I have is that, with reviews like this, scientists will be even more **discouraged** from publishing their code [...] We need to get more code out there, **not improve how it looks.**”

By NE (F incorrect claims that a new service has sprung up to fact-check reported findings by repeating the experiments.

A year-old Palo Alto, California, [company](#), Science Exchange, announced on Tuesday its "Reproducibility Initiative," aimed at improving the trustworthiness of published papers. Scientists who want to validate their findings will be able to apply to the initiative, which will choose a lab to redo the study and determine whether the results match.

group Thu, Aug 2 2012

Scientists skeptical as athletes get all taped up Wed, Aug 1 2012

Jon Torrent vies for \$10 million genome prize Tue, Jul 24 2012

Close relationships ..

entered the debate, aiming to discover whether a review process could improve the quality of researcher-built software that is used in myriad fields today, ranging from ecology and biology to social science. In an experiment being run by the Mozilla Science Lab, software engineers have reviewed selected pieces of code from published papers in computational biology. "Scientific code does not have that comprehensive, off-the-shelf nature that we want to be associated with the way science is published and presented, and this is our attempt to poke at that issue," says Mozilla Science Lab director Kaitlin Thaney.

- Cancer institute tackles sloppy data
- Publish your computer code: it is good enough
- Computational science: ...Error

[More related stories](#)



# Barriers to Data and Code Sharing in Computational Science

Survey of Machine Learning Community, NIPS (Stodden, 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%  |

Tools

# Digital Science - Towards the Executable Paper

## Open Science

### Repeatable

The methodology is clearly exposed  
I could repeat the experiment

### Reproducible

Clear methodology and available resources  
I could reproduce the results

### Reusable

I know how it could be useful for my needs  
I could use all or some parts as it is  
I could modify and adapt it even for other purposes





# Digital Science - Towards the Executable Paper

## 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 contributions encoded in software**

**More data in archives do not imply more knowledge**

- » Expose **complete scientific record**, not the story
- » Allow easy **discovery** of methods and tools



# Digital Science - Towards the Executable Paper

## Visibility and Social Discovery

### Paper discovery: the social dimension

The collage features several logos and screenshots of digital science and social discovery tools:

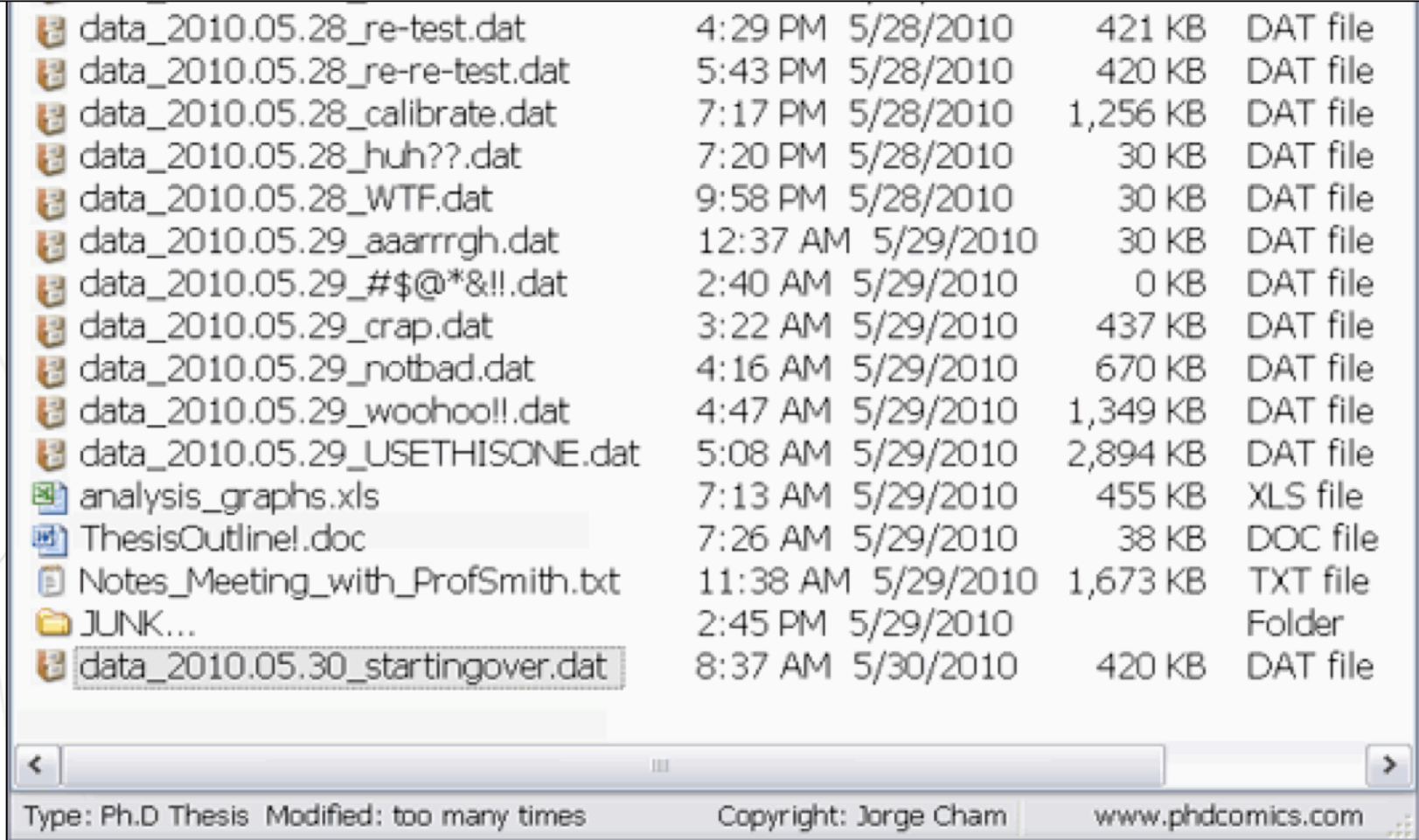
- peerevaluation**: empowering scholars
- MENDELEY**: Welcome back Lourdes Verdes-Montenegro
- YouTube**
- citeulike**: Search citeulike [input field]
- BibSonomy**: Search [input field]
- ResearchGate**: Search [input field]
- klænk**: Spread your research results
- delicious**: social bookmarking
- slideshow**: BETA
- AstroBetter**: Tips and Tricks for Professional Astronomers
- Collabgraph!**: Collaborating in your field of research. Just [input field] or upload a bibtex file, containing your [input field] graph will create a fancy graph showing [input field]
- zotero**

Time has come to go **beyond the PDF**





# Going beyond automation Organization



The screenshot shows a Windows file explorer window with a directory listing. The files and folders are listed with their names, modification times, sizes, and file types. The file 'data\_2010.05.30\_startingover.dat' is selected.

| File Name                        | Modification Time  | Size     | File Type |
|----------------------------------|--------------------|----------|-----------|
| 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_aaarrgh.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

# Digital Science - Towards the Executable Paper

## Digital Astronomy in the Local Desktop

**Capture**  
Actions, Tasks, Dependencies, Provenance

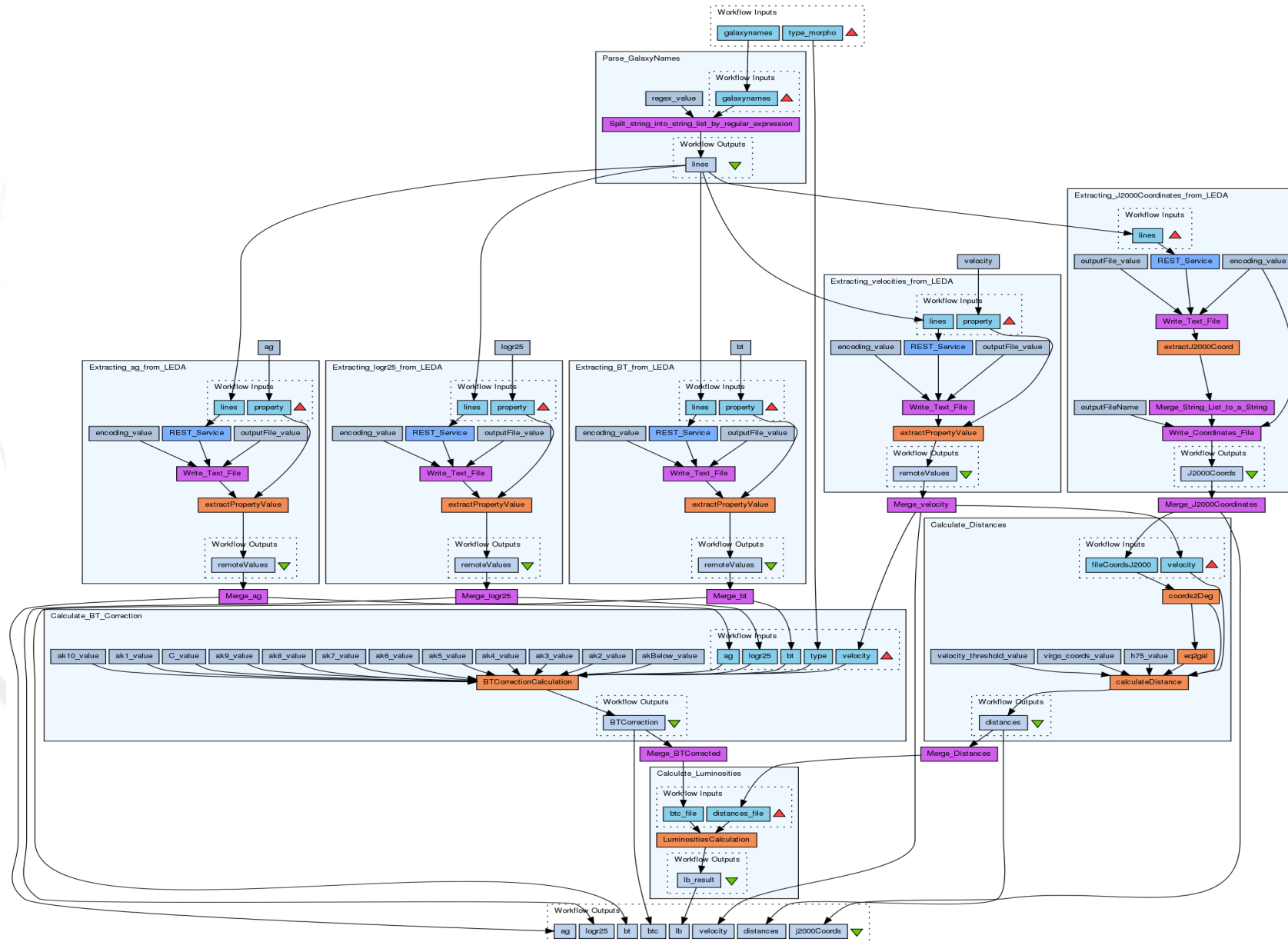
**Improve**  
Clarity and Reproducibility

**FORTRAN**

The collage includes several software interfaces:

- VAO (Virtual Astronomy Observing):** A web-based interface for astronomical data analysis, showing a table of objects and various analysis tools.
- NASA/IPAC Extragalactic Database (NED):** A database interface for extragalactic objects, featuring a table of objects and various analysis tools.
- CDS (Centre for Data Services):** A web-based interface for astronomical data, showing search criteria and preferences.
- Image Reduction and Analysis Facility (IRAF):** A software package for astronomical image reduction and analysis, showing a command-line interface with various options.

# Digital Science - Towards the Executable Paper Scientific Workflows

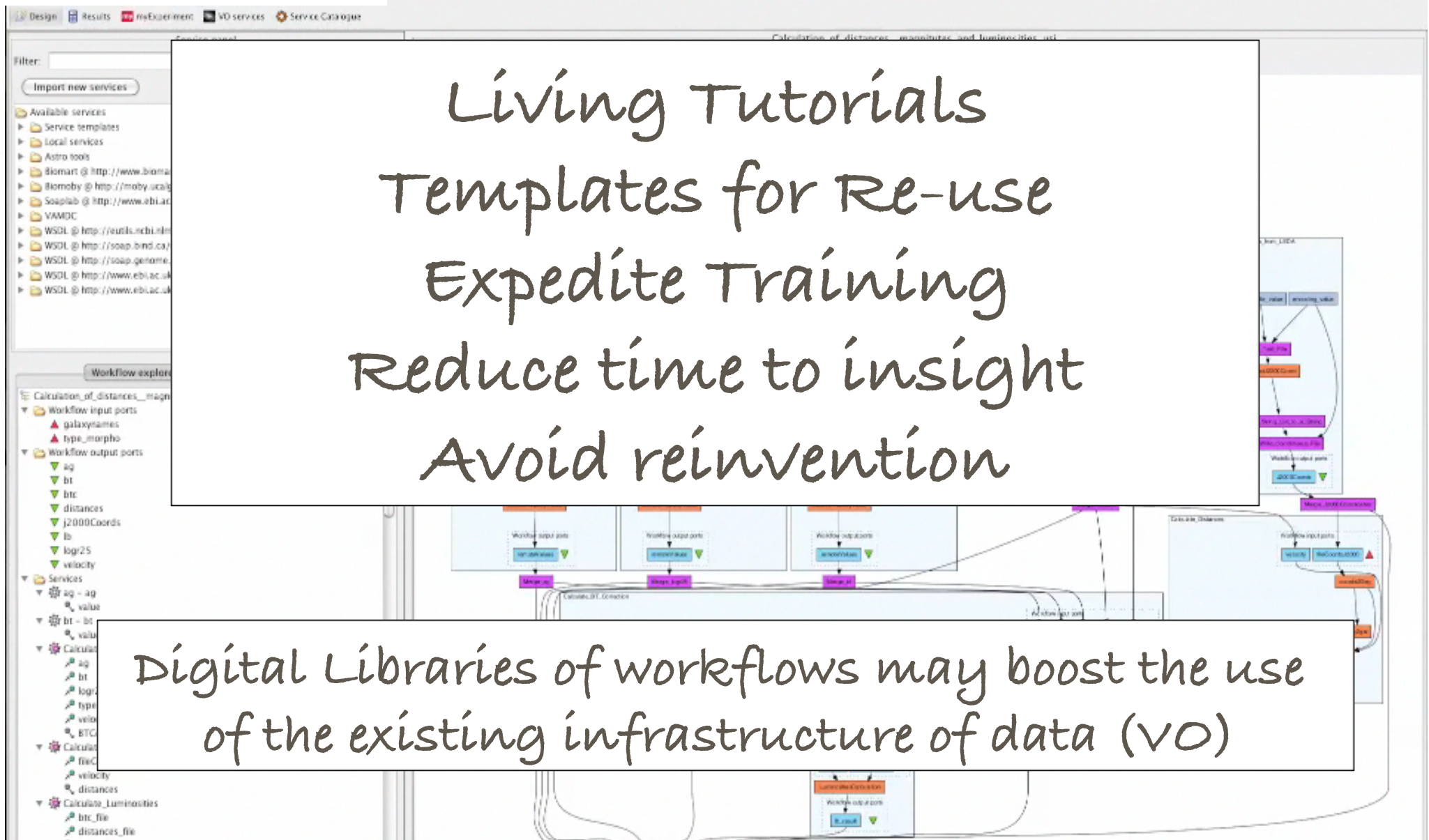




# Digital Science - Towards the Executable Paper Scientific Workflows

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)



# Digital Science - Towards the Executable Paper Scientific Workflows

## Related Initiatives

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

## Software

- › Taverna
- › Kepler
- › Pegasus
- › Triana
- › ESO Reflex

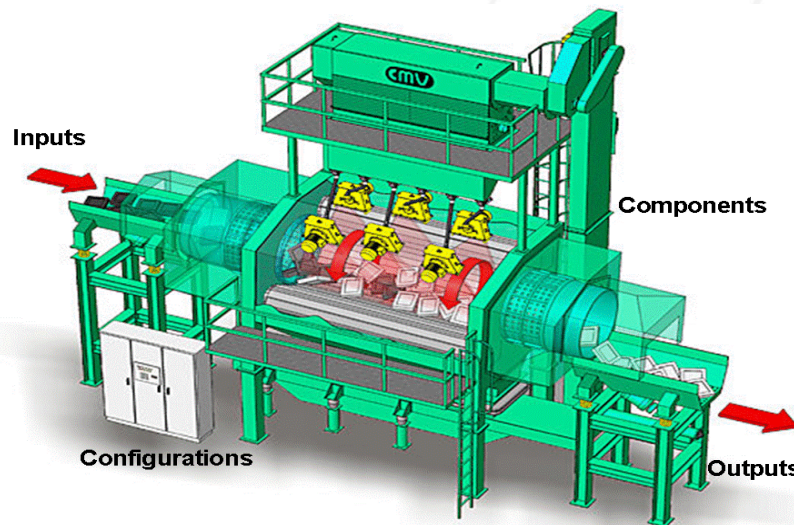
## IVOA



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

## Self descriptive WS

- › PDL
- › SimDAL, S3

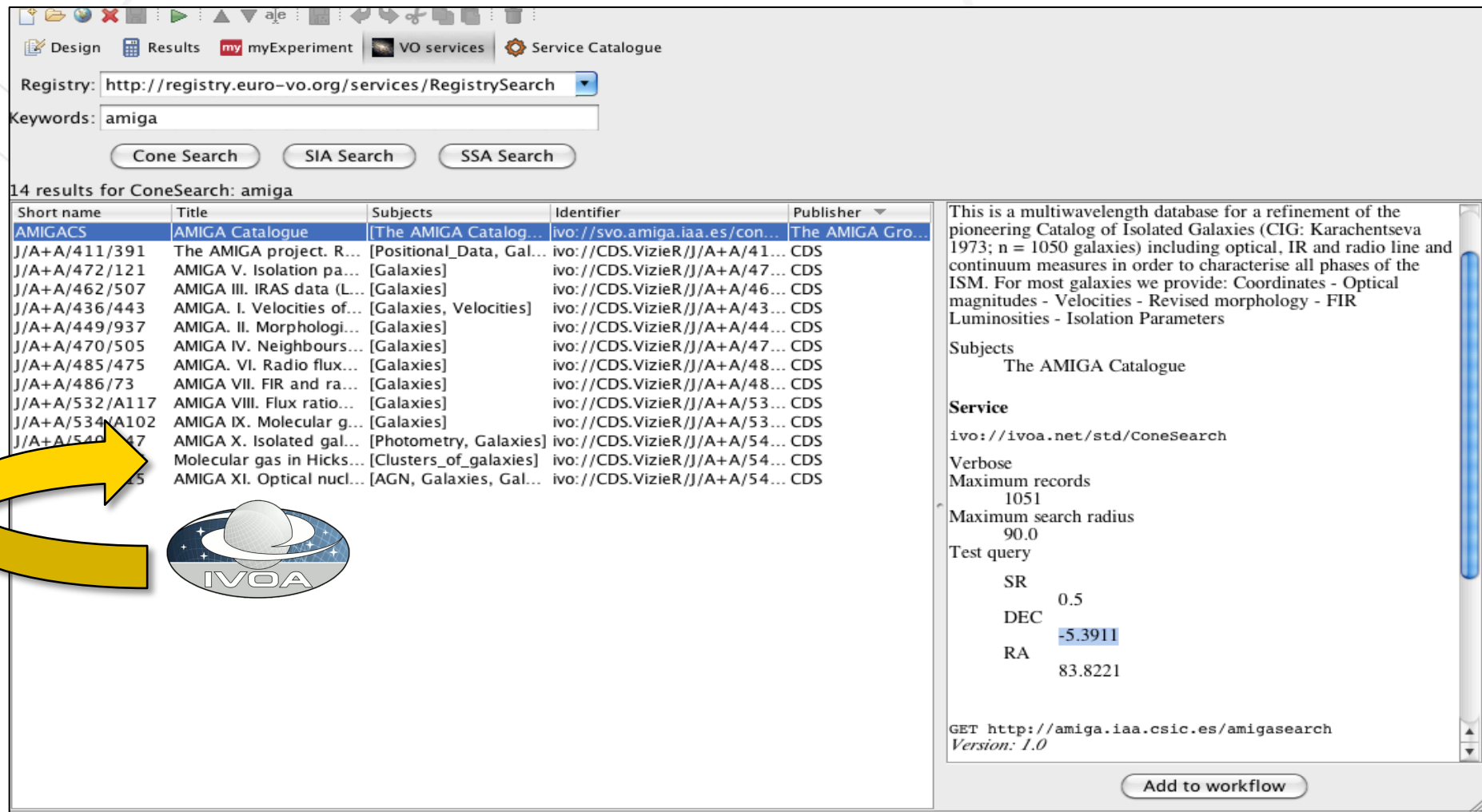


Interoperability  
Standards

# Digital Science - Towards the Executable Paper

## Astronomical Research Objects in Action

### AstroTaverna: Create, annotate and run a workflow



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

Keywords: amiga

Cone Search SIA Search SSA Search

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/540/47   | AMIGA X. Isolated gal...   | [Photometry, Galaxies]   | ivo://CDS.VizieR/J/A+A/54...  | CDS              |
| J/A+A/540/47   | Molecular gas in Hicks...  | [Clusters_of_galaxies]   | ivo://CDS.VizieR/J/A+A/54...  | CDS              |
| J/A+A/540/47   | 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  
DEC 0.5  
RA -5.3911  
83.8221

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

Add to workflow



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

# Digital Science - Towards the Executable Paper Astronomical Research Objects in Action

## AstroTaverna: Create, annotate and run a workflow

The screenshot displays the AstroTaverna interface. On the left, the 'Service panel' shows a list of services under 'Astro tools', with 'List from column - Get list from column in a votable' highlighted. A yellow arrow points from this service to the workflow diagram on the right. The workflow diagram, titled 'Querying\_SDSS\_DR8\_to from /Users/julian/Documents/interop...', illustrates the process of querying SDSS DR8 data. It starts with 'Workflow input ports' including 'column\_DEC' and 'column\_RA'. These feed into a 'votable' service, which then feeds into a 'Select\_columns' service. The 'Select\_columns' service outputs a 'filter' and a 'voTable', which are used by the 'Cat\_n-tables' service to produce a 'votableList'. Finally, the 'votableList' feeds into another 'votable' service, which produces the 'Workflow output ports'.

**Workflow Diagram Details:**

- Workflow input ports:** column\_DEC (value), column\_RA (value), votable.
- Select\_columns Service:** Inputs: ColumnName, voTable. Outputs: filter\_value, value, filter, voTable, Select\_columns, outputTable, report.
- Cat\_n-tables Service:** Inputs: filter\_value, value, filter, voTable. Outputs: votableList, Cat\_n-tables, outputFileOut, report.
- Workflow output ports:** votable.

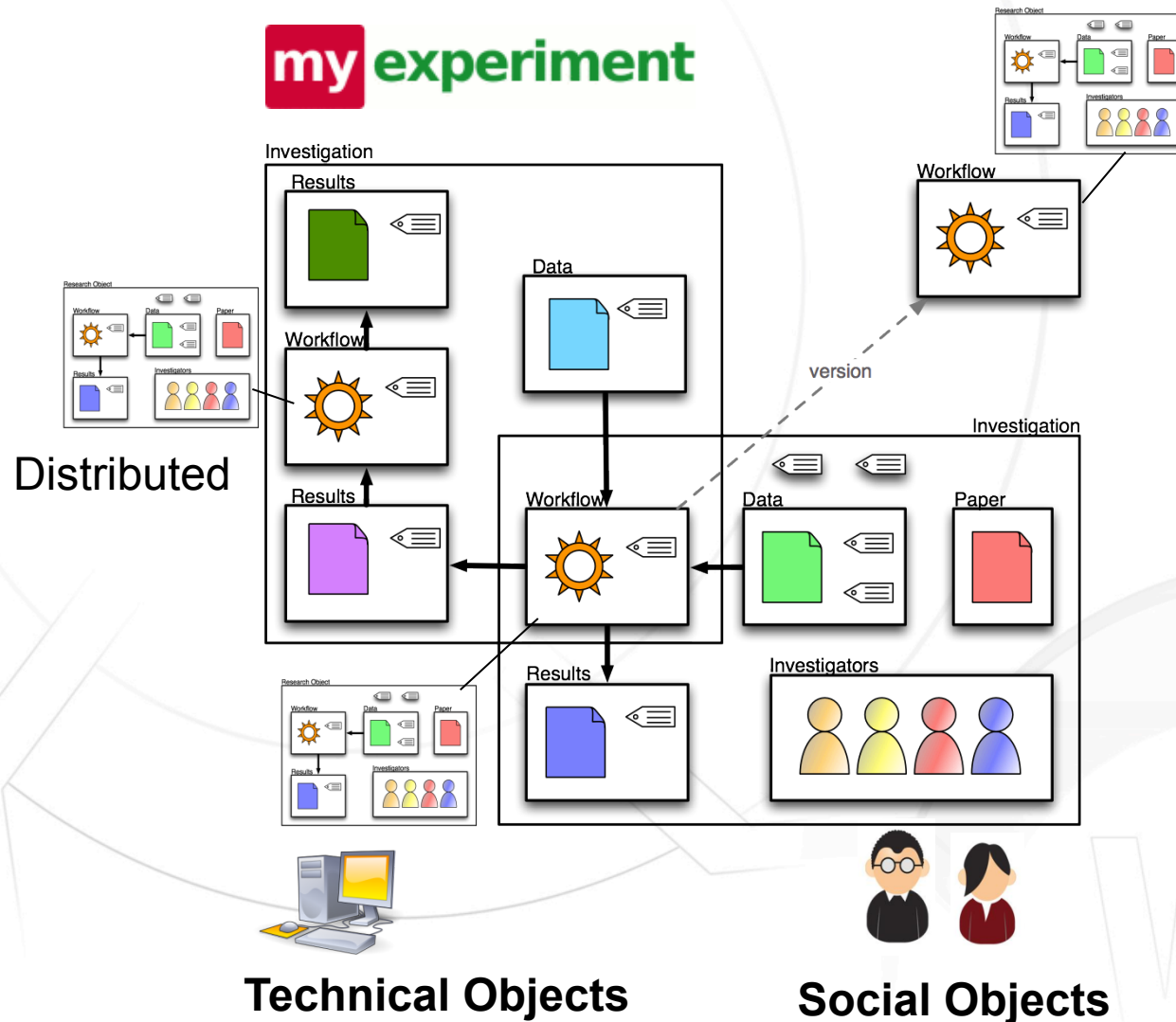
**Service Panel Details:**

- 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

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

# Digital Science - Towards the Executable Paper Research Objects

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





## The IPython Notebook

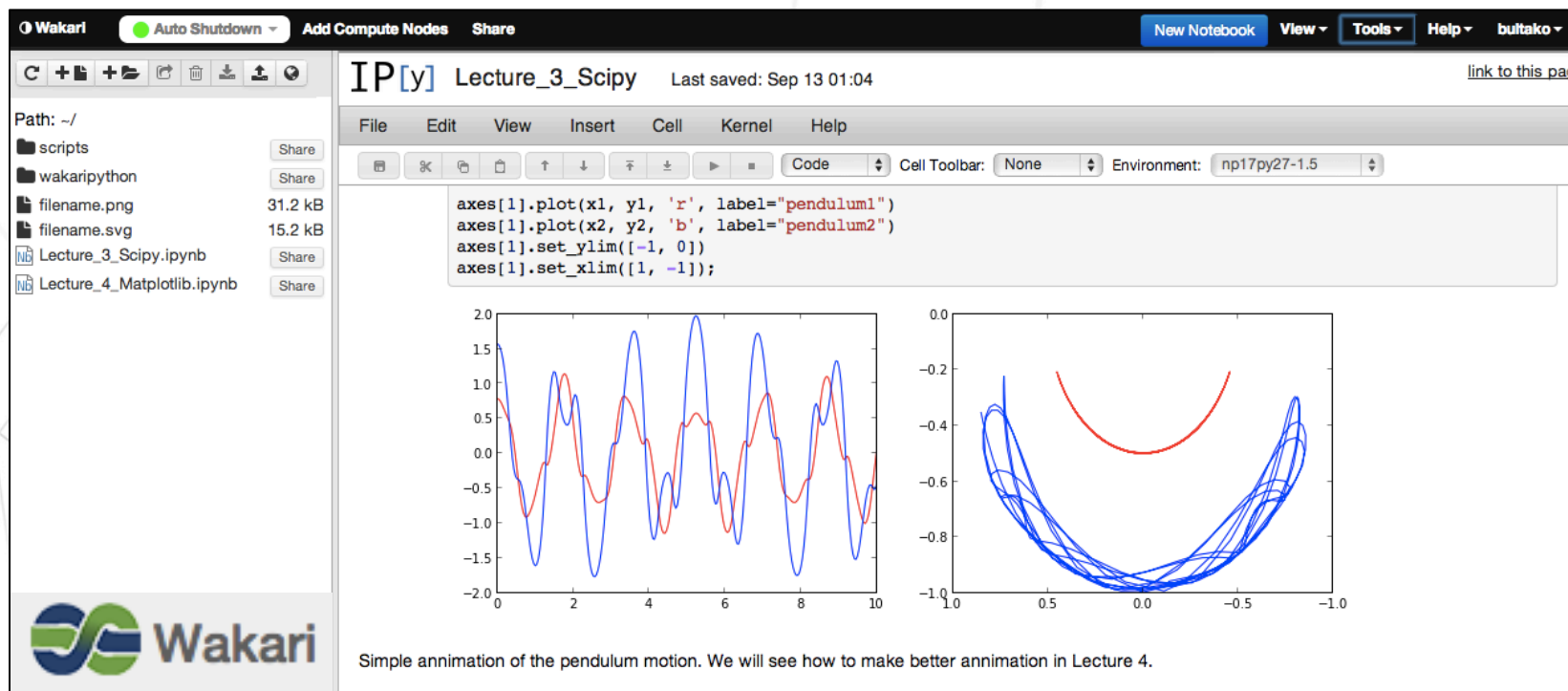
Hands On!

WF



## IPython Notebook solutions

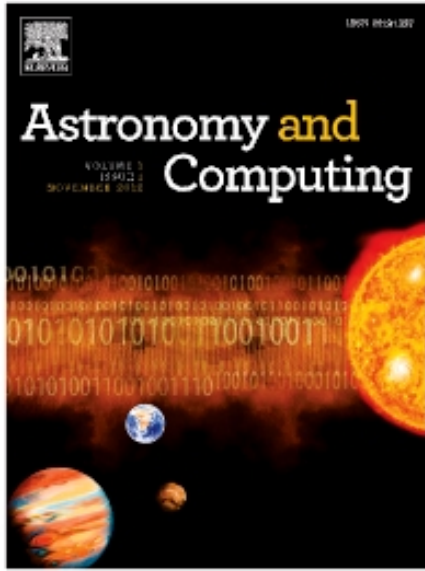
- » **Web-browser** as the working desktop
- » Python code, plots and data, living with **rich-text documentation**
- » Cloud-based adaptive **scalable computing environment**
- » Fully **shareable**, re-usable and **executable wikis**
- » **Social** platform and Git **versioning**





article of the future

# Digital Science - Towards the Executable Paper Research Objects



## Graphical abstract

### Source code repositories

The journal strongly encourages authors to make source code available where appropriate, especially in the case

### Video data

Elsevier accepts video material and animation sequences to support and enhance your scientific research. Authors who have video or animation files that they wish to submit with their article are strongly encouraged to include links to these within the body of the article. This can be done in the same way as a figure or table by referring to the video or animation content and noting in the body text where it should be placed. All submitted files should be properly labeled so that they directly relate to the video file's content. In order to ensure that your video or animation material is directly usable, please provide the files in one of our recommended file formats with a preferred maximum size of 50 MB. Video and animation files supplied will be published online in the electronic version of your article in Elsevier Web products, including ScienceDirect: <http://www.sciencedirect.com>. Please supply 'stills' with your files: you can choose any frame from the video or animation or make a separate image. These will be used instead of standard icons and will personalize the link to your video data. For more detailed instructions please visit our video instruction pages at <http://www.elsevier.com/artworkinstructions>. Note: since video and animation cannot be electronic and the print version for the

## AudioSlides

### MATLAB FIG files

#### \*NEW\* Inline supplementary computer code

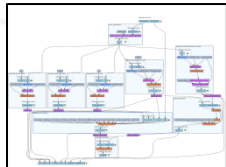
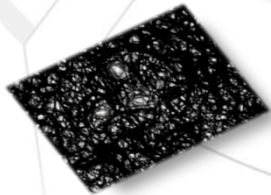
Elsevier now offers you the possibility to place supplementary computer code, data snippets, algorithms and other machine readable structures at the right place in your online article in reusable .txt format. This will allow readers to easily view this material in the appropriate context, and to directly copy it to the clipboard or download the original source file for testing or re-use. If you would like to have reusable "computer code" inserted into the body of your online article please indicate in your manuscript where they should be placed and number them in order of appearance, e.g. "Insert Inline Supplementary Computer Code 1 here". To support discoverability and reusability please submit these items in \*.txt format and make sure to include a descriptive title and caption that references the characteristics and the appropriate environment of this material, e.g. 'An algorithm for filtering text files in R'. For more information please visit <http://www.elsevier.com/ism>.

# Digital Science - Towards the Executable Paper Research Objects

## ADSLabs

### ADO Linked Components

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



Incentives



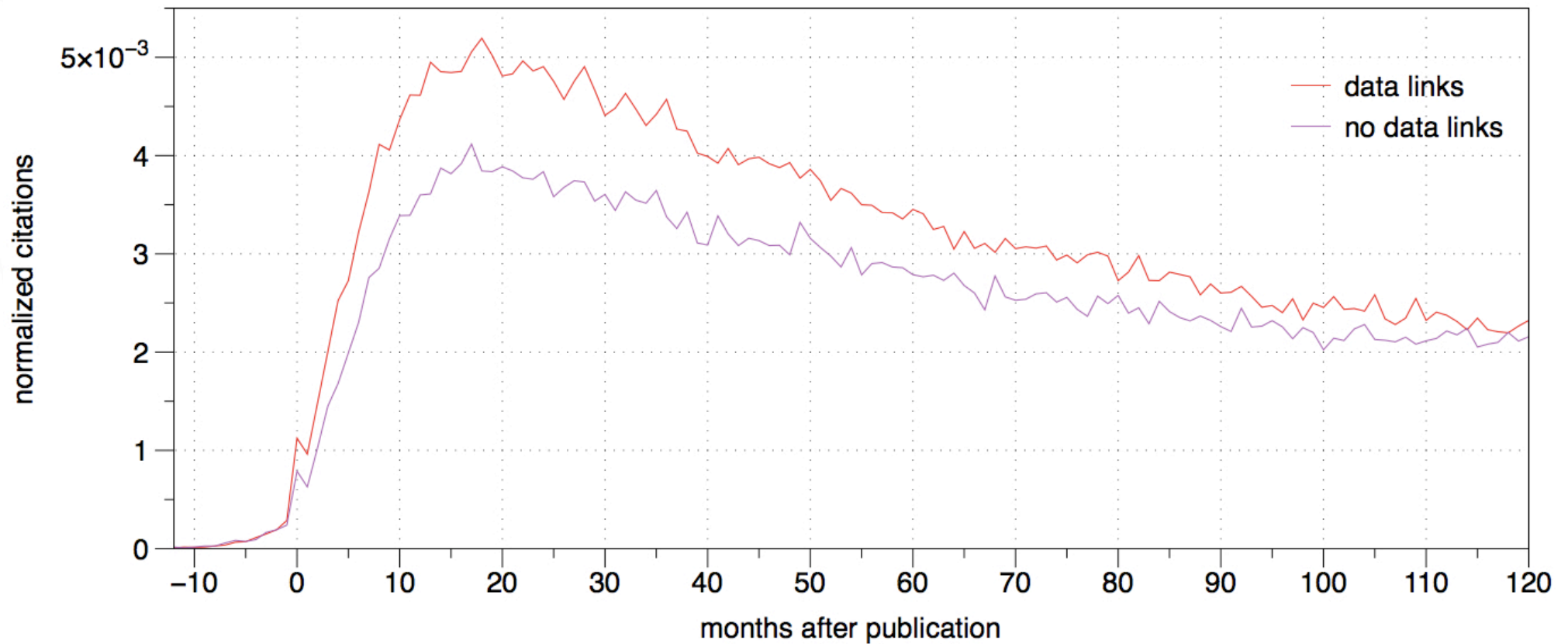
<http://labs.adsabs.harvard.edu/>

The screenshot shows the ADS 2 search interface. At the top, there's a navigation bar with 'Home', 'Search', 'Feedback', 'Help', and 'Work for us'. Below that, a search bar contains 'isolated galaxies' and a 'Search' button. To the left, there's a 'Limit your search' sidebar with various filters like 'Top papers', 'Authors', 'Database', etc. The main content area displays a list of search results, including titles like 'Broadband Imaging of Isolated and Interacting Seyfert Galaxies' and 'Statistical study of isolated and non-isolated AGNs in the Local Universe'. Each result includes the author's name, publication date, and a brief abstract snippet.

## The Incentive

Papers with data links are cited more than those without

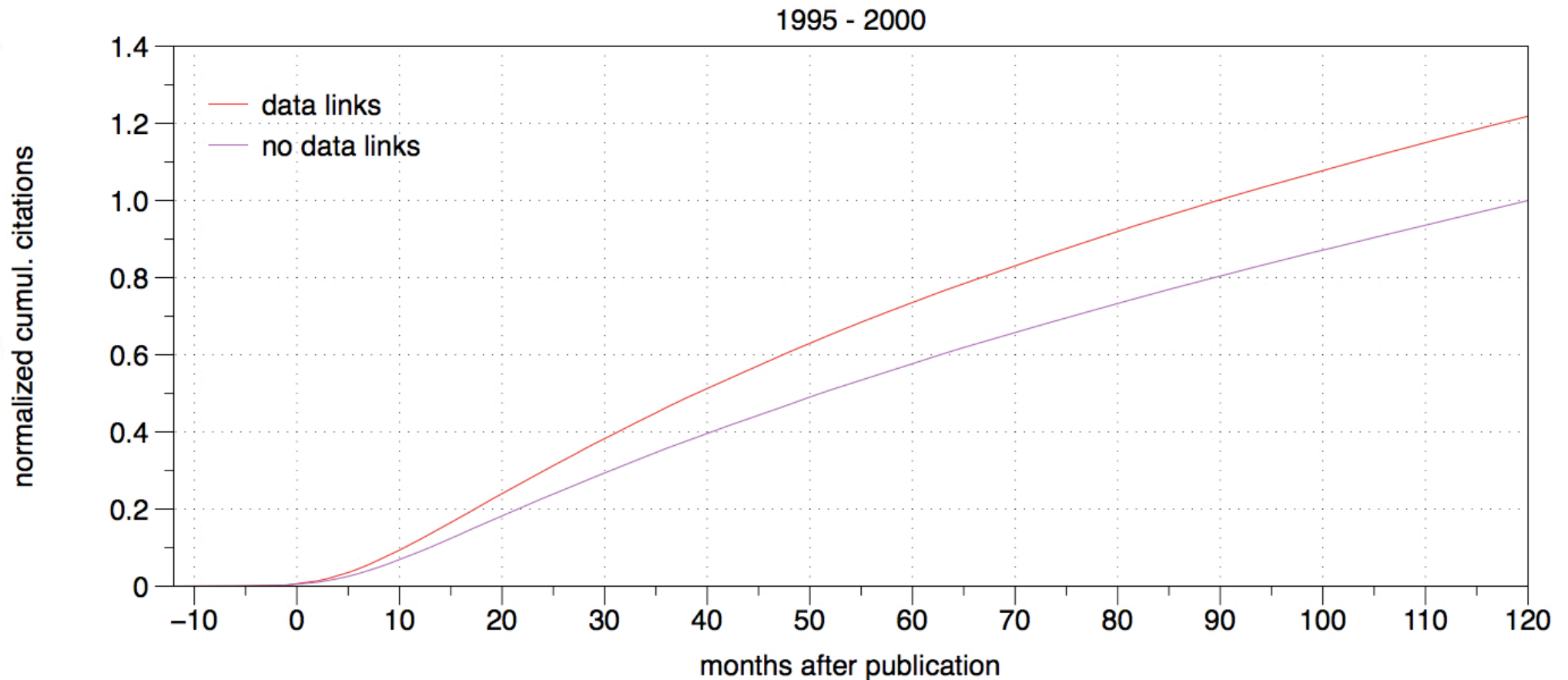
1995 - 2000



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 - Towards the Executable Paper

## Conclusions

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- » **AMIGA** group invested in reproducible science projects
- » **Reproducibility** is at the very heart of the scientific method
- » **Open data** – access to all resources involved must be granted
- » **Re-use** needed in highly specialized science to achieve efficiency
- » Improving **visibility** is key in order to avoid reinvention
- » **Social dimension of science** stressed in the discovery process
- » Time has come to go **Beyond the PDF**
- » Capture provenance and structure in the **local desktop**
- » Scientific workflows **go beyond automation** – provide clarity and structure
- » **Research Object**
  - › Modular distributed aggregation of digital resources
  - › Executable, re-usable, documented, socially curated and inspected..
- » **Other initiatives**
  - › IPython notebooks-based solutions
  - › Elsevier Paper of the Future
  - › ADSLabs, ..




## How NOT to be a good Astronomer in XXI Century

- » In marketing just advertise your results – do not say how to reproduce them
- » Do things quickly and forget about them once you've submitted the paper
- » Be untidy – spread your code and data in a variety of formats, folders and disks
- » Do not provide data results – including the plots is just fine
- » Practise the “data mine-ing” – input data and/or results are mine
- » Practise the “data flirting” – please call me, if you want to know more
- » Always cite the same authors and papers or those that cite you
- » Do not reference other resources than published papers – never provide URL links
- » Do not search info on Internet with other tools than ADS or arXiv
- » Do not contact others if you re-use – duplicate and reinvent for your own

 <http://amiga.iaa.es/p/212-workflows.htm>

 <http://www.wf4ever-project.org>

 <http://canu.be>

 [jer@iaa.es](mailto:jer@iaa.es)