

# Workflows Access and Massage VO Data

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on behalf of the Wf4Ever Team

IVOA INTEROP SPRING MEETING 2013  
HEIDELBERG, MAY16th 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 (PSCN, Poland)
5. University of Oxford and OeRC (OXF, UK)
6. Instituto Astrofísica Andalucía (IAA-CSIC, Spain)
7. Leiden University Medical Centre (LUMC, Netherlands)

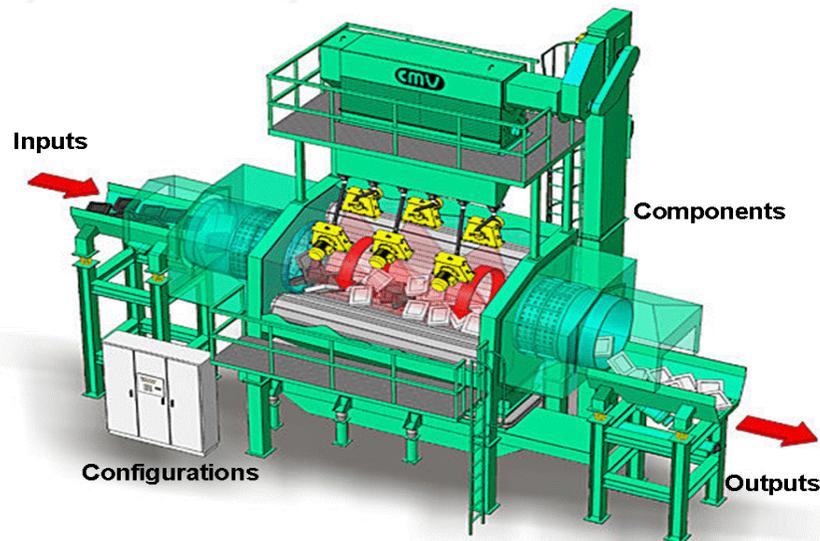
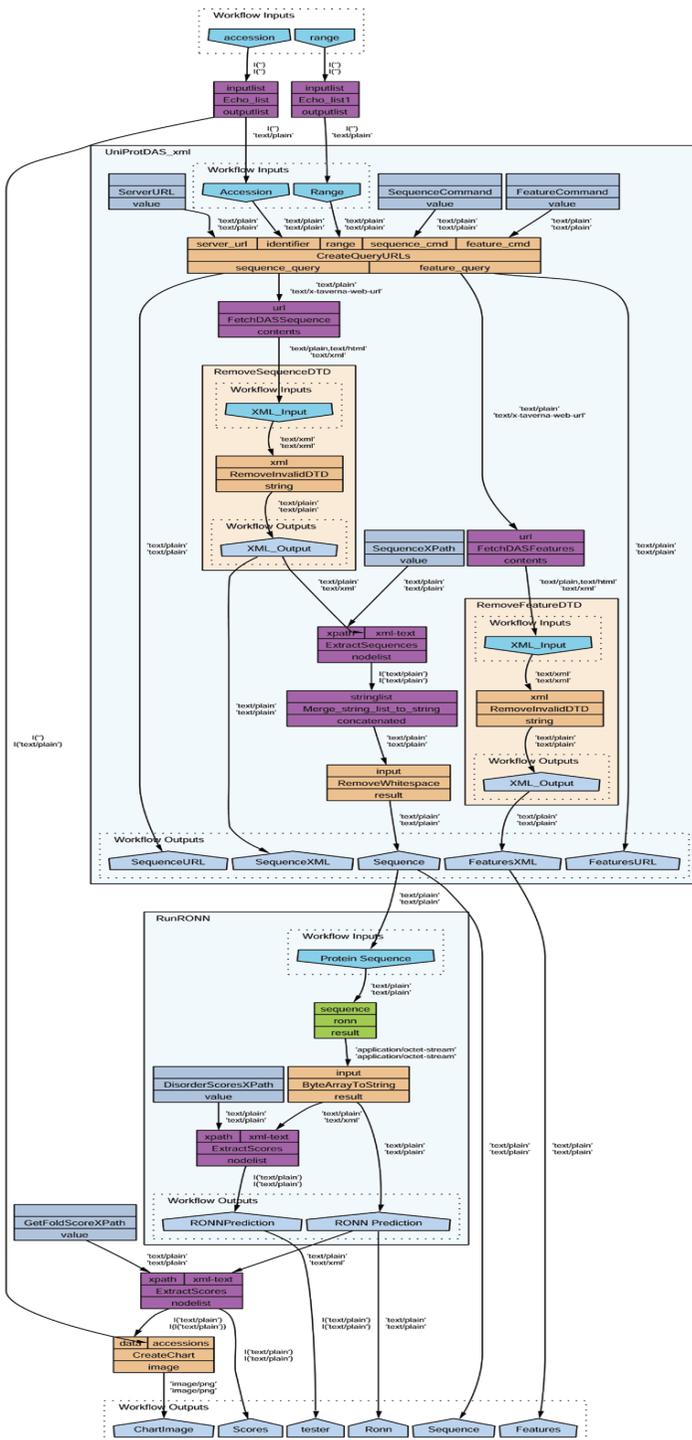
Reproducible  
Science



# Workflows to Access and Massage VO Data

## What is a Scientific Workflow?

- » A mechanism for coordinating the execution of **services** and **codes**, and linking together **resources**.
- » The combination of **data** and **processes** into a configurable, modular, **structured** set of steps that implement **semi-automated** computational solutions in scientific problem-solving.
- » The **implementation** of a scientific method.



### » IVOA Note Definition

*These are networks of analytical steps that may involve, e.g., database access and querying steps, data analysis and mining steps, and many other steps including computationally intensive jobs on high performance cluster computers.*

### » Wf Software

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

### Related Initiatives

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

### In the VO

- › GWS WG
- › VO France WF WG
- › VAMDC
- › AstroGrid

# Workflows to Access and Massage VO Data Digital Astronomy

**Capturing Actions  
Reproducibility**

4	2310.0	1.0	3	31.9	3.0	1.5	0	1	12.818	0.424	0.252	0.863	0.017	11.685
5	7865.0	10.0	3	105.9	0.0	1.5	0	1	15.602	0.364	0.225	0.131	0.118	15.128
72	5164.0	9.0	2	68.5	5.0	1.5	1	1	14.445	0.325	0.315	0.367	0.028	13.735

**IRAF**  
Image Reduction and Analysis Facility

**FORTRAN**

**IDL**

**VOSPEC**

**NASA/IPAC EXTRAGALACTIC DATABASE**

**Python**

**VizieR**

**CDSD**

**Portal**

**Sirius**

**Aladin**

**Search Criteria**

**Find catalogs among**

**Preferences**

**max:** 50

**HTML Table**

**All**

**Com**

**Mirrors**

**CDS, F**

**700 tables**

**or Position:**

**J2000**

**Submit Query**

**Reset**

**Example**

**Output options for alignments**

Parameters

Pretty alignment

Predicted catalog

GFF output

Possible alignment output

**Display**

**Print**

**Save Image**

**News & Feature Updates (April 2013)**

- Over 1 million new multiwavelength cross-IDs among objects
- Data for over 16,000 QSOs in SDSS P17 (Schneider et al. 2010)
- 26,748 image fitting results for 4,488 galaxies (Hallard et al. 2011)
- Evolution of Star formation and Gal. Growth (Seymour 2012) now in IAS 12.2
- Galactic extinction maps to 88 photometric bands in Customized Output

**OBJECTS**

**DATA**

**LITERATURE**

**TOOLS**

**INFO**

**Introduction**

**Latest News/Updates**

**Features**

**EAD**

**Overview (pdf)**

**Source List**

**Web Links**

**Glossary & Lesson**

**Team**

**Contact Us or Comment**

**Coordinate Transformation & Extinction Calculator**

**Velocity Calculator**

**Cosmology Calculators**

**Extinction-Law Calculators**

**Skyplot**

**XY offset to RA/DEC**

**Batch Job Submission**

**Pick Up Results**

**Build Data Table from Input List**

**By Name**

**Near Name/Position (Cross-Matching)**

**References by Object Name**

**References by Author Name**

**Text Search**

**Knowledgbase**

**Galaxy Distance Tabulations (NED-D)**

**Abstracts**

**Thesis Abstracts**

**Images By Object Name or By Region**

**Photometry & SEDs**

**Redshifts**

**Redshift/Independent Distances**

**Classifications by Object Name**

**Polishes**

**Diameters**

## Workflows to Access and Massage VO Data

# Digital Astronomy

A STORY TOLD IN FILE NAMES:

Location: C:\user\research\data

Filename	Date Modified	Size	Type
data_2010.05.28_test.dat	3:37 PM 5/28/2010	420 KB	DAT file
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_20			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

Going beyond Automation  
Improving Documentation and  
Readability

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

### AstroTaverna Workflows

Retrieving and Manipulating VO Data + Catalogs + HTML Pages

- ConeSearch
- SIA
- SSA
- TAP coming soon...

- Tabular Data (VOTables) + Access to JDBC databases
- Images, but not yet Spectra

- Crossmatching, File Resolving, Coordinates and reference system transformation.. (**STILTS**)

- Overplotting sources on Images and filtering, overplot circles, ellipses, etc. as a function of physical magnitude. Resampling, crops, blinks, mosaics, motion blinks, RGBs, fusion, diff.. (**ALADIN**)

- **SAMP** for final inspection

+ Advanced Analysis using Scripts

*No interactive actions and decisions based on visual inspection*

### VOData Access: VO Services Discovery

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/547/A47	AMIGA X. Isolated gal...	[Photometry, Galaxies]	ivo://CDS.VizieR/J/A+A/54...	CDS
J/A+A/547/A96	Molecular gas in Hicks...	[Clusters_of_galaxies]	ivo://CDS.VizieR/J/A+A/54...	CDS
J/A+A/547/A96	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

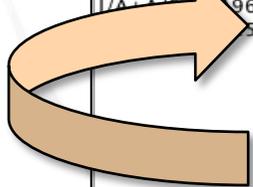
Subjects  
The AMIGA Catalogue

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

Add to workflow



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

# Workflows to Access and Massage VO Data AstroTaverna

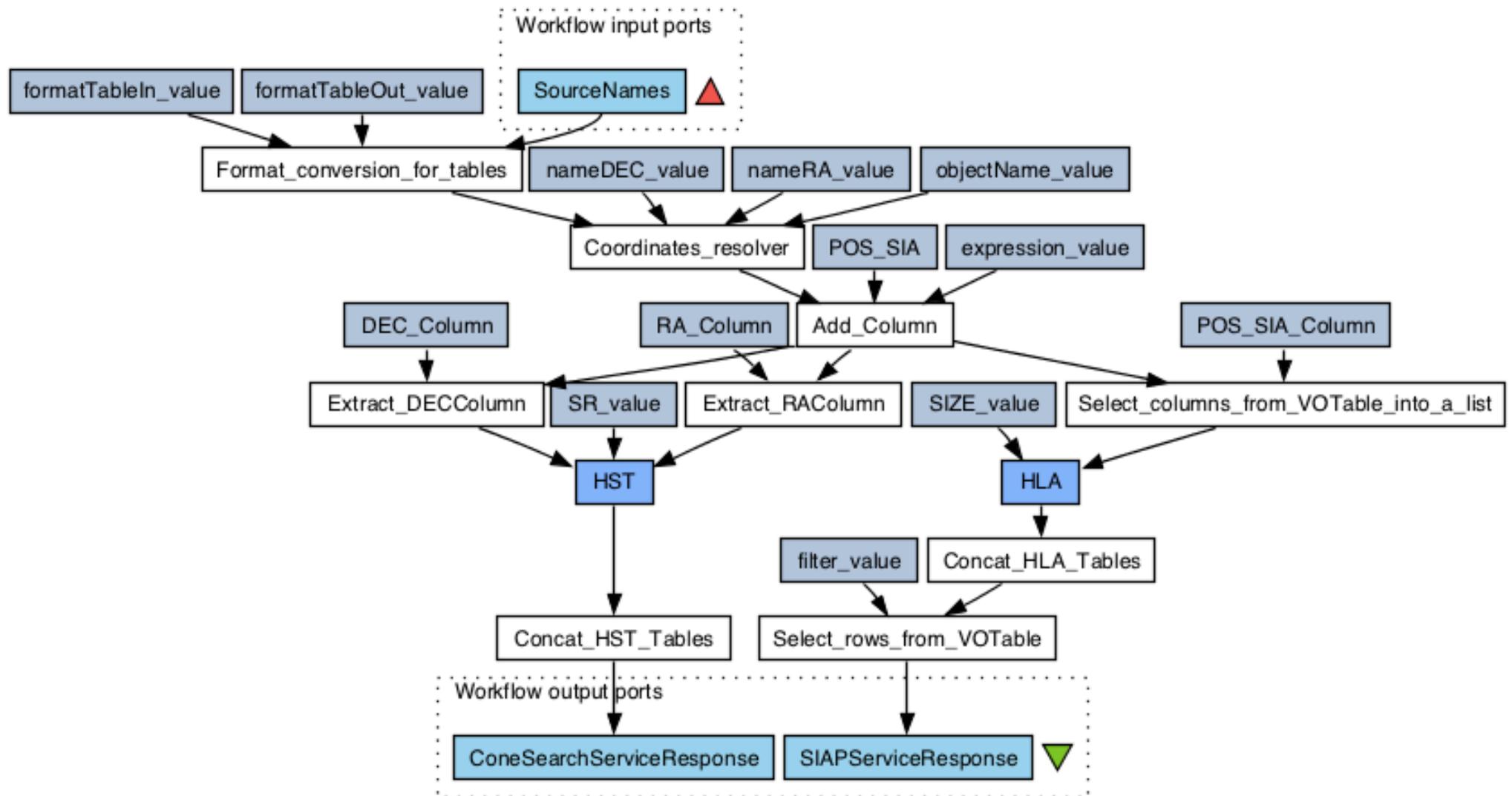
## VOData Massage: VOTables, STILTS, Aladin, TerminalSim

The screenshot displays the AstroTaverna interface. On the left, the 'Service panel' shows a list of services under 'Astro tools', with 'Format conversion - Table format conversion' highlighted. Below the list are tabs for 'Workflow explorer', 'Details', and 'Validation report'. The main area on the right shows a workflow diagram titled 'Querying\_SDSS\_DR8\_to from /Users/julian/Documents/interop...'. The diagram illustrates the flow of data through several steps: 'Workflow input ports' (column\_DEC, votable, column\_RA), 'Select\_columns' (DEC\_list, RA\_list, SR\_value), 'filter' (filter\_value, SDSS\_DR8), 'Cat\_n-tables' (votableList, Cat\_n-tables), and 'Workflow output ports' (votable). A large orange arrow points from the highlighted service in the panel to the workflow diagram.

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

# Workflows to Access and Massage VO Data

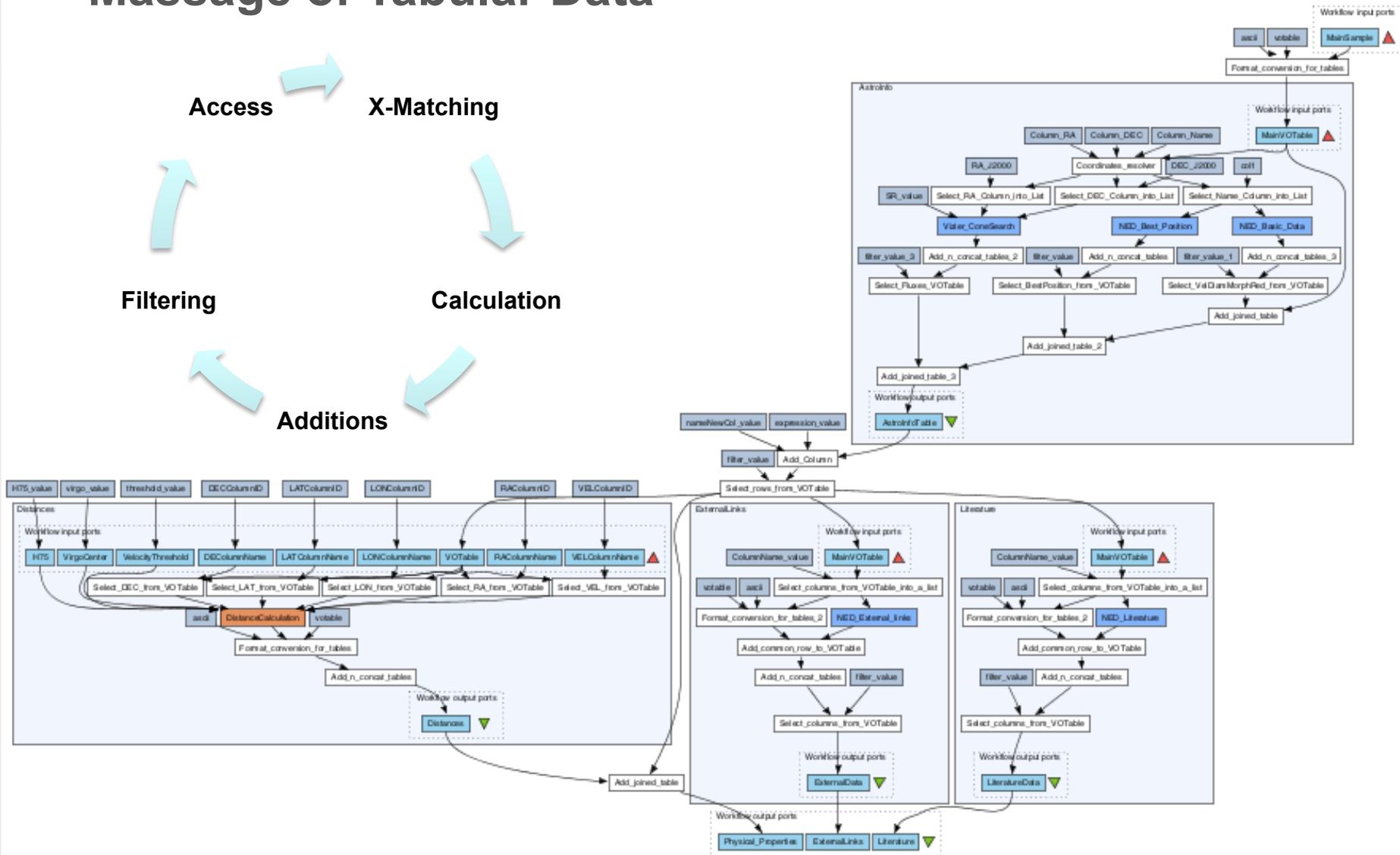
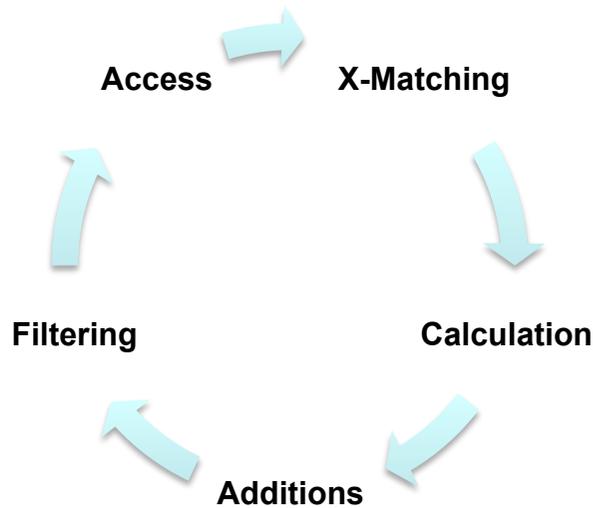
## VOData Consumers



# Workflows to Access and Massage VO Data

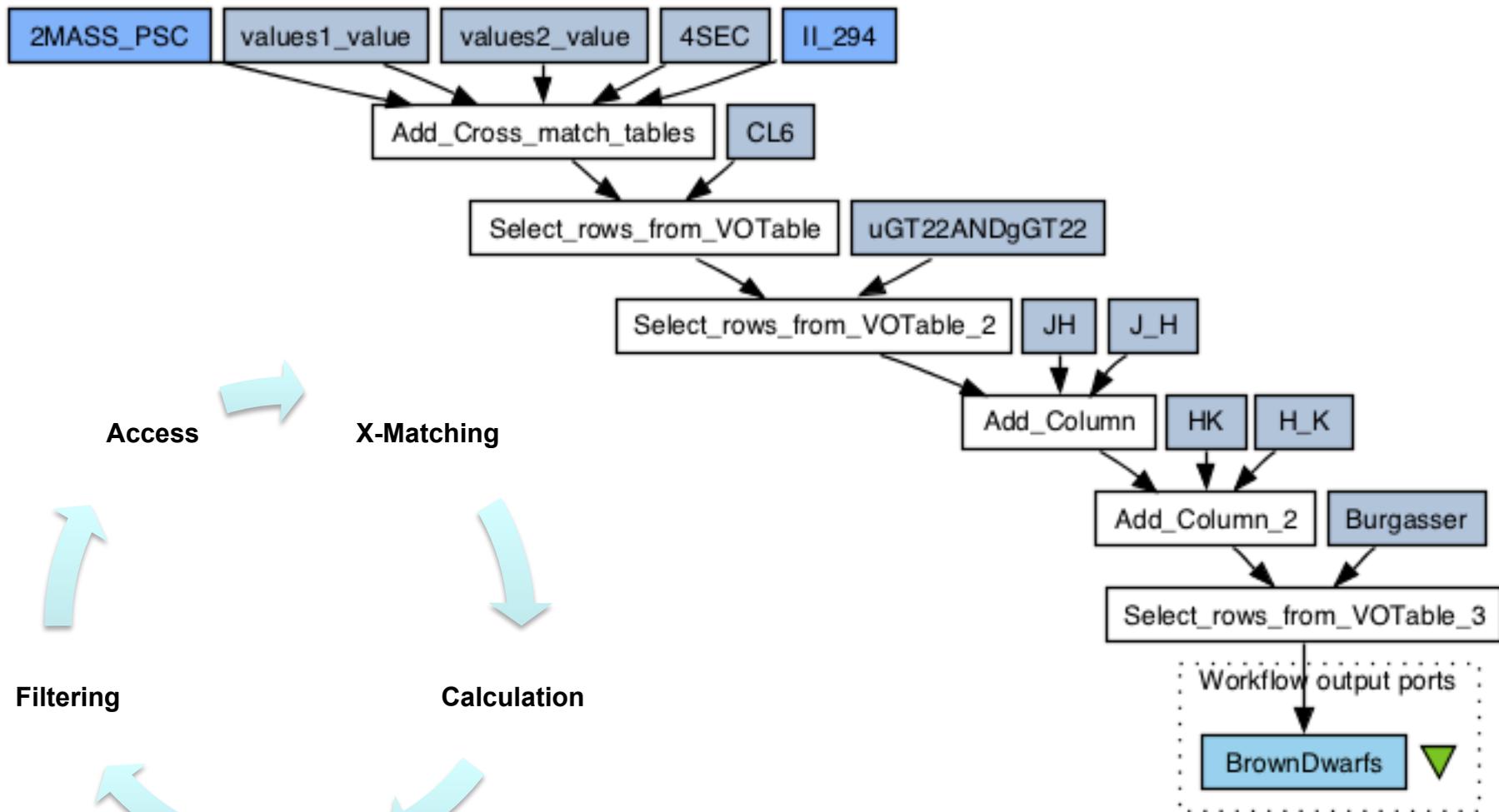
## VOData Manipulation

### Massage of Tabular Data



# Workflows to Access and Massage VO Data

## VOData Manipulation



Access

X-Matching

Filtering

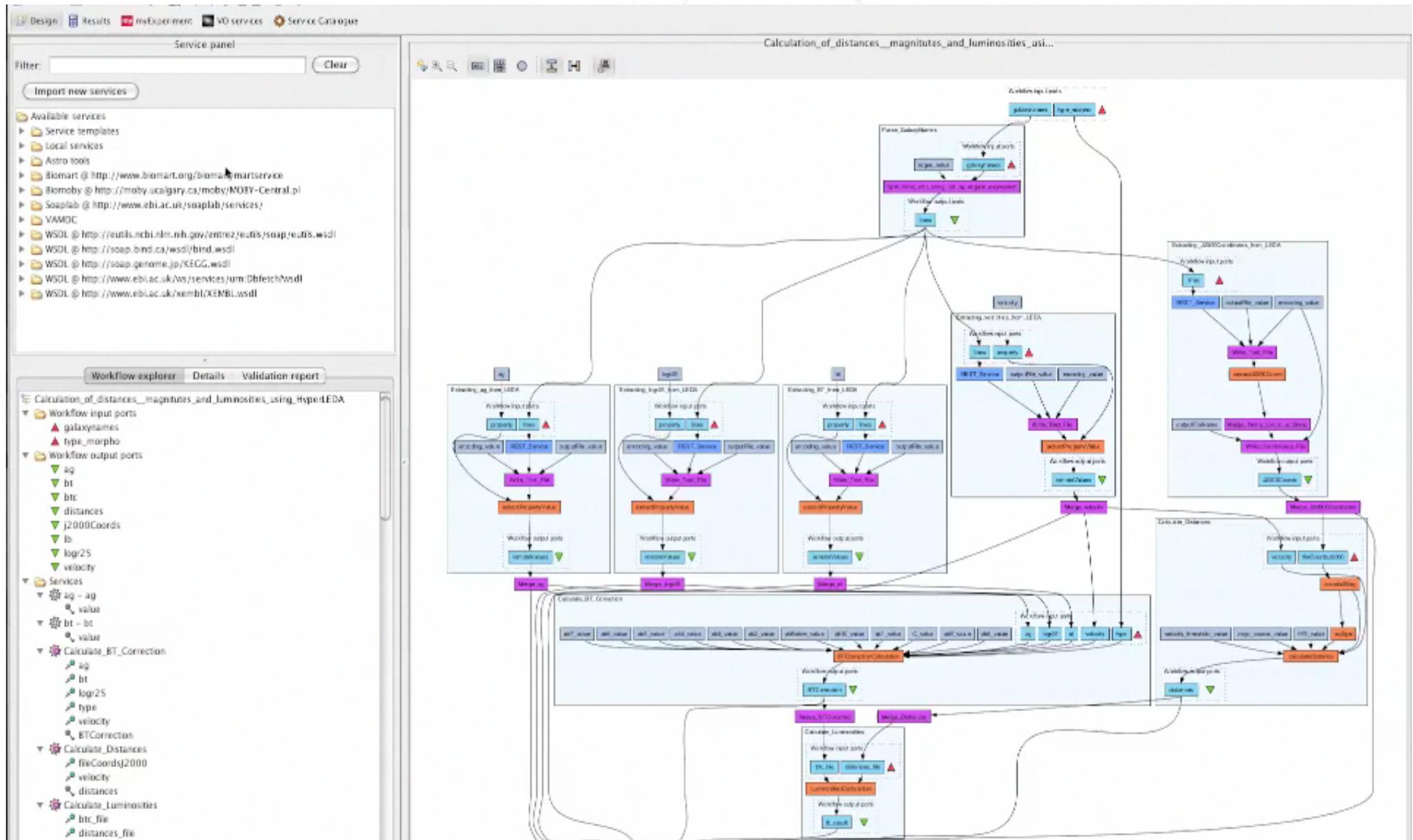
Calculation

Additions



# Workflows to Access and Massage VO Data

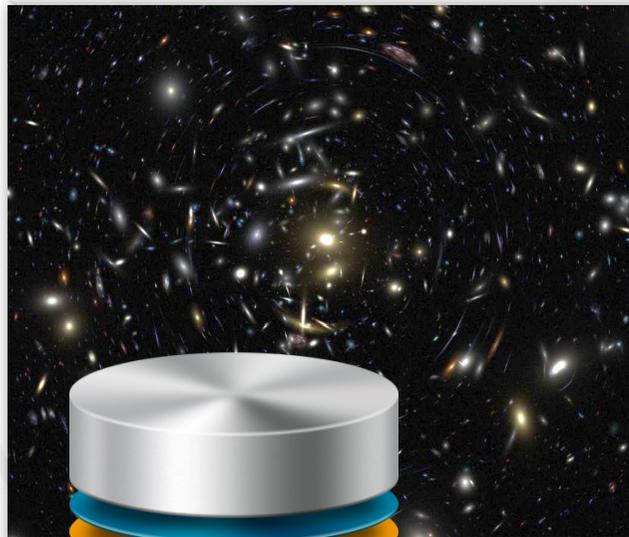
## VOData Curation



# Workflows to Access and Massage VO Data

## VOTable Format Interoperability

### Calculation of **Luminosity Profiles** for a **Sample of Galaxies** extracted from SDSS DR8

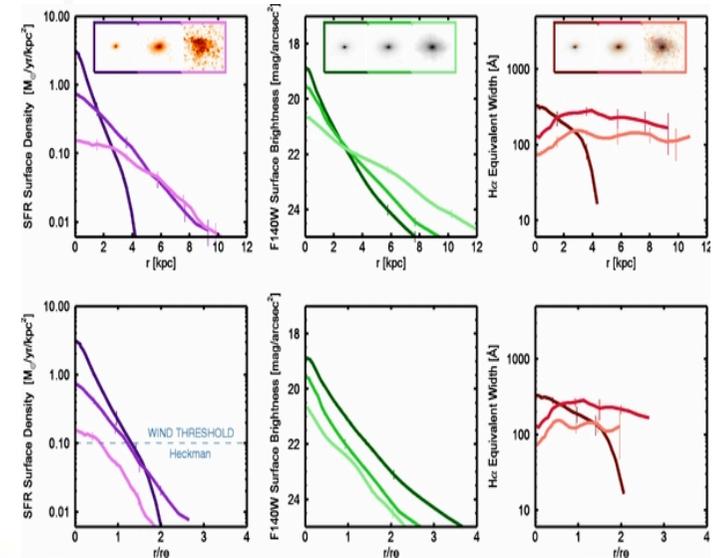


**IRAF**  
Image Reduction and Analysis Facility



**SEtractor**

**GALFIT**



90 galaxies observed in 3 bands

# Workflows to Access and Massage VO Data

## Method Inspection

### Aladin Scripts and Macro executing in GUI/noGUI mode

The screenshot shows the Aladin GUI interface. A window titled "Annotation" is open, displaying a description and an example of Aladin scripts. Below the window, a workflow explorer shows a workflow named "rkflow52" with input and output ports. A diagram on the right illustrates the workflow structure, showing a "Script" input port leading to a "Use\_Aladin\_scripts" process block, which then outputs to a "Use\_Aladin\_scripts\_VOTable" output port.

**Annotation Window Content:**

Description  
Very simple execution of Aladin scripts

Example

```
get Skyview(600,Default,"DSS2 Red",Tan,J2000,0,NN) 13 29 52.70 +47 11 42.9
get Skyview(600,Default,"DSS2 Blue",Tan,J2000,0,NN) 13 29 52.75 +47 11 42.4
RGB @1 @2
get NVSS(0.25,15.0,"Stokes I",Sine) M51
cview NVSS
contour 4
cview "RGB img"
backup /Users/jer/Desktop/Aladin.aj
```

**Workflow Diagram:**

Workflow input ports: Script (blue trapezoid with red triangle)

Process block: Use\_Aladin\_scripts (rectangle with three output ports: ERROR\_OUTPUT, STD\_OUTPUT, VOTable)

Workflow output ports: Use\_Aladin\_scripts\_VOTable (blue trapezoid with green triangle)

# Workflows to Access and Massage VO Data

## VOData Inspection

Taverna Workbench 2.4.0

Design Results myExperiment VO services Service Catalogue

Workflow runs Remove

Click on a run to see its values  
Click on a service in the diagram to see intermediate values (if available)

Retrieve\_physical\_pr 2013-05-16 00:33:55  
Retrieving information 2013-05-16 00:31:36  
Workflow52 2013-05-16 00:28:57  
Workflow7 2013-05-16 00:20:16  
Workflow6 2013-05-15 22:30:53  
Workflow52 2013-05-15 19:27:28  
Workflow52 2013-05-15 19:26:36  
Workflow52 2013-05-15 19:20:16

Graph Progress report

Workflow output ports: Distances

Finished Pause Cancel Edit executed workflow Refresh intermediate values Show workflow results

Intermediate values for the service **Select\_columns\_from\_VOTable\_into\_a\_list** Invocation started 2013-05-16 00:34:24, ended 2013-05-16 00:34:24 (99 ms) Save iteration values

View all

Invocation

Value type: VOTable Refresh Save value

VOTable Metadata SAMP

pos_dec_equ_J2000_s	pos_lon_ecl_J2000_d	pos_lat_ecl_J2000_d	pos_lon_gal_d	pos_lat_gal_d	pos_lon_sup_gal_d	pos_lat_sup_gal_d	e_fks	logLks	e_logLks	f_logLks
+29d47m50.3s	13.55959	26.80127	110.63356	-31.92316	323.17406	18.74751	0.002	11.23	0.02	
+30d46m54.8s	14.06032	27.67947	110.89036	-30.96325	324.20576	18.84756	0.001	10.41	0.05	
+30d14m45.3s	20.68785	34.26096	114.85982	-23.02275	333.30611	17.88005	0.00053			1

SAMP

# Workflows to Access and Massage VO Data

## Learning by the example

Pack: AstroTaverna Starter Pack

Creator: [Jose Enrique Ruiz](#)  
Created at: Fri Apr 12 18:10:31 CEST 2013  
Last updated at: Tue Apr 23 19:41:01 CEST 2013

This is a set of small snippets using AstroTaverna plugin, developed in the Wf4Ever project. The purpose of this pack is to make the design and development of astrond Virtual Observatory workflows easier, learning by the example.

AstroTaverna may be installed on Taverna 2.4 Workbench

<http://wf4ever.github.io/astrotaverna/>

Pack Items (28) Tags (5) Comments (0)

- ⚙️ [Add a common row to a VOTable](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-22 15:15:42 +0000]
- ⚙️ [Adding a column to a VOTable using a mathematical expression](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 19:08:32 +0000]
- ⚙️ [Cocatenates several VOTables into one](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 20:04:14 +0000]
- ⚙️ [Concatenates two VOTables with the same number of columns into a single one](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 19:22:47 +0000]
- ⚙️ [Coordinate units conversion](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 18:15:12 +0000]
- ⚙️ [Crossmatching VOTables](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 17:21:39 +0000]
- ⚙️ [Discovery of Brown Dwarfs mining the 2MASS and SDSS databases](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 16:38:32 +0000]
- ⚙️ [Executes Python script](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-22 14:55:27 +0000]
- ⚙️ [Extract a column from a VOTable into a List](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 19:41:57 +0000]
- ⚙️ [Joins two VOTables with the same number of rows into a single one](#)  
Added by [Jose Enrique Ruiz](#) [2013-04-12 19:23:00 +0000]

Workflow Entry: **Perform Multi-ConeSearch queries to a VO Service (version 1)**

Type: Taverna 2

Uploader: [Jose Enrique Ruiz](#)  
Created at: Mon Apr 22 21:43:39 CEST 2013  
License: [Creative Commons Attribution-Share Alike 3.0 License](#)

```
graph TD
    subgraph Workflow_Inputs
        RA_J2000[RA_J2000]
        VOTable[VOTable]
        DEC_J2000[DEC_J2000]
    end
    RA_J2000 --> S1[Select_columns_from_VOTable_into_a_list]
    VOTable --> S1
    DEC_J2000 --> S2[Select_columns_from_VOTable_into_a_list_2]
    S1 --> AMIGACS[AMIGACS]
    S2 --> AMIGACS
    AMIGACS --> A[Add_n_concat_tables]
    A --> subgraph Workflow_Outputs
        FinalOutput[FinalOutput]
    end
```

Snippet showing how to use AstroTaverna "VO service perspective" and other tools for performing Multi-ConeSearch queries to a VO Services. The input is a VOTable with a list of source names and coordinates to perform the multi-query. Please \*note how the AMIGACS block list handling is configured\* with right click -> Configure running -> List Handling. Add\_n\_concat\_tables tool is used to concatenate the list of responses issued from the multiquery. The result is a VOTable that may be rendered properly in the perspective Results, coosing Value Type as VOTable.

### VO compliant data from pipelines

Traditional data processing pipelines, e.g., **instrumental or survey data processing pipelines**, which produce higher, level data products. At present there are many variants of these and they have little or no direct connection to VO, aside from possibly **producing VO-compliant data** or being optionally driven from VO.

It is not clear how much VO mechanisms are needed at this level (VO compliant data and metadata, modelling provenance, etc.)

### Driving Data Processing Pipelines from the VO

In this case we have a traditional data processing pipeline and the remote user or **client software invokes a job to do some pipeline reprocessing**, e.g., to custom reprocess an instrumental dataset to produce a new image, cube, etc. The "workflow" in this case runs at a single site, and VO is used to drive the job remotely (**SSO, UWS**) and manage the results (**VOSpace, VO data services**).

We could think on integrating the traditional data processing pipelines we already have with VO, to allow **VO users to do on-the-fly reprocessing** to generate data products which can be analysed with VO (custom reprocessing of observatory data for example)

Some attempts to integrate general processing applications have been made with CEA and UWS.

### Distributed Data Analysis Workflows

In this case a user or a client defines and executes a distributed workflow, which invokes **services on multiple remote sites via the VO infrastructure**. The workflow would be entirely in VO-space, driving simpler services at the individual sites.

The AstroTaverna developments provide a graphical tool for the composition and design of workflows based on VO services and data from different archives and facilities.

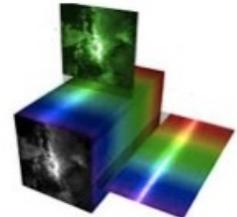
**Self Descriptive Web Services:** S3, SimDAL, PDL, DataLink

# Workflows to Access and Massage VO Data

## The next generation of archives

### Much wider FoV and spectral coverage

- » Large volumes for an observed datacube
- » Subproducts are **Virtual Data** generated on-the-fly



	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

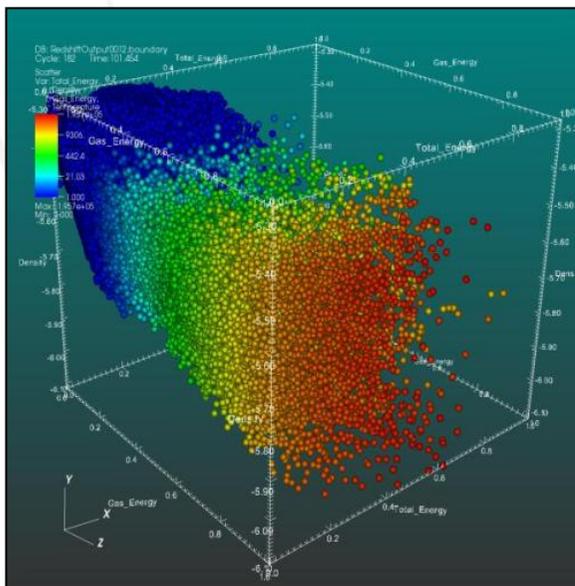
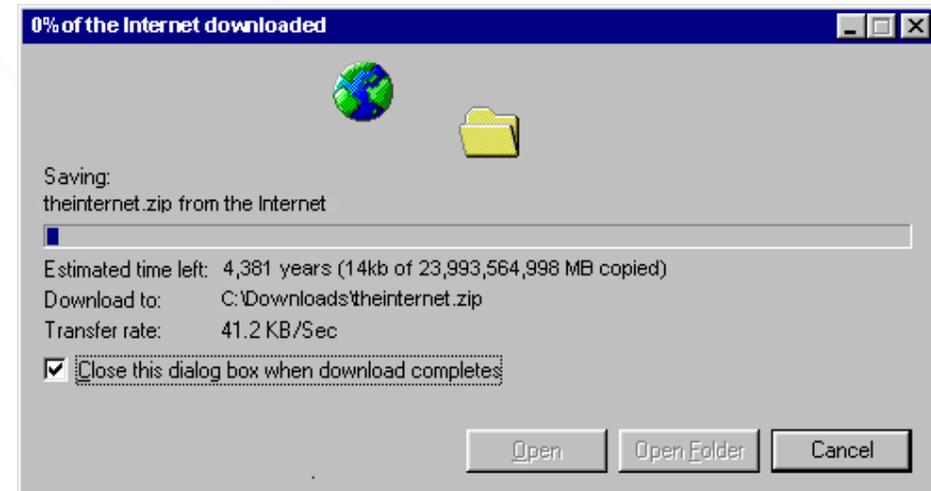
ASKAP Cubes  
Prof. Kevin Vinsen

# Workflows to Access and Massage VO Data

## The next generation of archives

### Automated surveys

- » Huge amounts of tabular data
- » Services for KDD



Extraction of scientifically relevant information from a multidimensional parameter space

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

## Workflows to Access and Massage VO Data

### The next generation of archives

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#### » A cloud of Web Services

Archives should evolve from data providers into

- » Virtual data providers
- » Software tasks providers

#### » Archives speaking Web Services

Astronomy of multi archives/facilities/wavelength

Interconnected and interoperable archives

- » Data -> Virtual Observatory
- » Software Tasks



Preservation

**Process should benefit of the same privileges acquired by data**

Preserving the method ensures replication of final results at any moment