Workflow systems and VO standards

André Schaaff, Observatoire de Strasbourg
schaaff@astro.u-strasbg.fr

Topics

- Quick introduction to workflows and workflow systems
- VO standards and workflows with a focus on the use of the IVOA Characterization standard

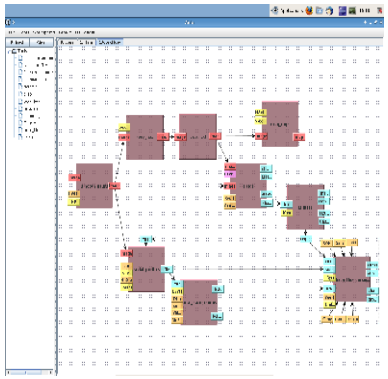
Workflows and workflow systems

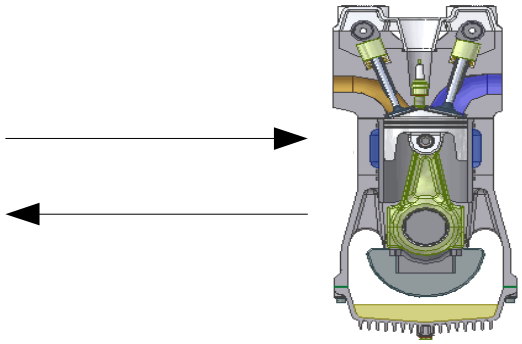
Introduction to workflows / workflow systems

- **A workflow ?**
  - **Different tools executed by hand under shell**
    - Not very efficient but could be a solution if the tools are interactive
  - **Script file**
    - Same as previous but a first step to the formalization
      - easily reusable, ...
    - Involved tools are mainly black boxes (or converted to) with just I/O
    - ...
  - **Description language**
    - The workflow is described in a specific language (often in XML format)
      - not executed like a shell script but interpreted by a workflow engine

Introduction to workflows / workflow systems (2)

- "Sophisticated" workflow system
  - Graphical design tool
  - Workflow description (XML, ...) is sent to an engine who executes the workflow by dispatching the tasks
  - Execution is often visible step by step
  - Possible storage of intermediate data to change some parameters without the re execution of the whole workflow
  - Result(s) can be exploited through tools related to the kind of output data (FITS, ...)





Tasks

Local cluster

Grid

User desktop

Storage (VOSpace, ...)

Local or remote DB

...

Workflow jungle

- **Workflow languages**
  - AGWL, BPEL4WS, BPML, DGL, DPML, GJobDL, GSFL, GFDL, GWorkflowDL, MoML, SWFL, WSCL, WSCI, WSFL, XLANG, YAWL, SCUFL/XScufl, WPDL, PIF, PSL, OWL-S, xWFL, …
- **" language formalisms**
  - Petri net, UML activity diagram, BPMN, DAG, IPO, GPSG, Workflow Patterns, Pi Calculus, Finite-State Machine, Gamma-calculus, ...
- **" engines**
  - BioPipe, BizTalk, BPWS4J, DAGMan, GridAnt, Grid Job Handler, GRMS, GWFE, GWES, IT Innovation Enactment Engine, JIGSA, JOpera, Kepler, Karajan, Moteur, OSWorkflow, Pegasus (uses DAGMan), Platform Process Manager, ScyFLOW, SDSC Matrix, SHOP2, Taverna, Triana, wftk, YAWL Engine, WebAndFlo, WFEE, …
- **" composition/designing tools**
  - ilog's BPMN Modeller, CAT, GWUI, XBaya GUI for Workflow Composition, Taverna, Triana, JOpera, Platform Process Manager, ...
- **" mapping from abstract to concrete workflows**
  - CWG, ACWG, Grid Job Handler, GWES, …

Focus

- **Taverna, Scufl/XScufl**
  - **Developed in the frame of myGrid which is a UK e-Science project**
  - **See Kevin Benson (Taverna in the VO) and Richard Hook (ESO Reflex : A Graphical Workflow Engine for Data Reduction) talks during the Friday morning tools session**
- **http://taverna.sourceforge.net/**

Why workflows ?

- Capture and preservation of scientific methodology (formalization of the scientific analysis)
  - Tools (different algorithms) to use, data flow, execution details, …
- Management of computation at a large-scale and to mask the complexity
  - Iterations of tasks involving an access to clusters, grids, large DBs,
- A workflow system can provide a collaborative environment for the analysis/design/execution/validation of new use cases
- ...

Workflows in the VO

- **An increasing number of services are developed/deployed in the frame of the Virtual Observatory (registries, data services, Web Services, computing and Grid services, …) : complex use and coordination of the services are possible through workflows**

Workflow use cases in astronomy...

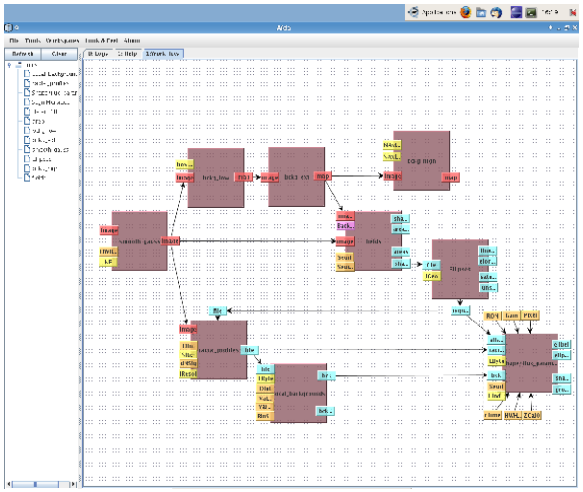
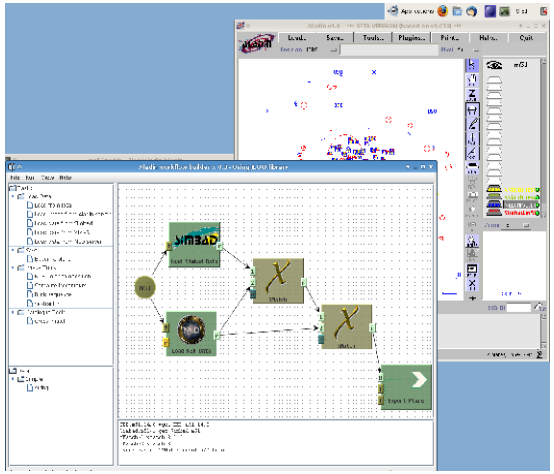
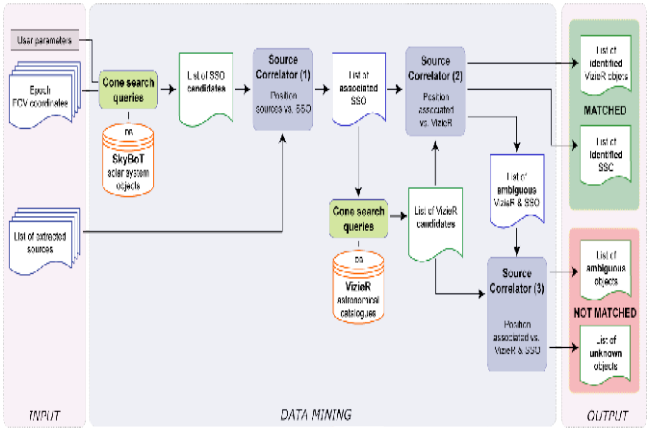


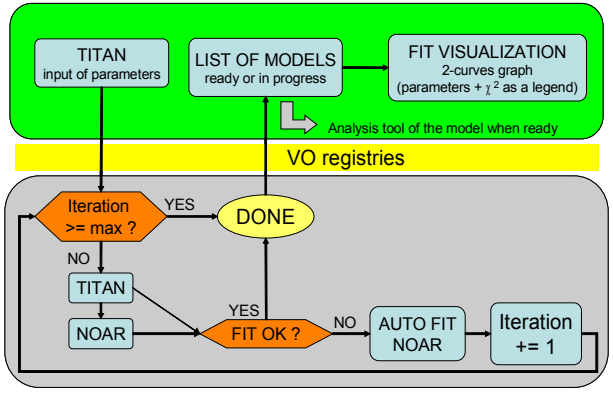
Image processing, E. Slezak.



Aladin scripting,C.Pestel, T. Boch.



Data Mining, J. Berthier et al.



TITAN/NOAR, L. Chevallier.

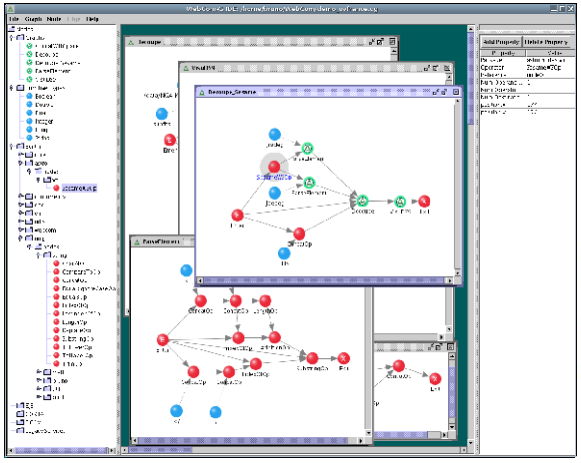
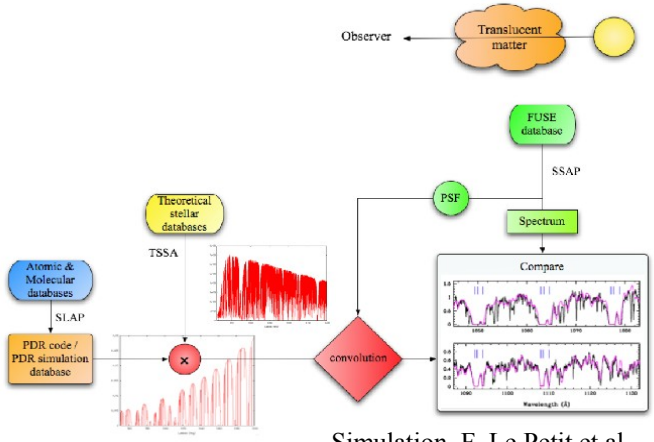


Image extraction from a catalogue, B. Voisin.



Simulation, F. Le Petit et al.

Workflow systems and (some) VO standards

Workflows and VO standards

- **Registry**
  - Adaptive workflows with a choose of tools depending on parameters like the availability (see VOSI), ...
- **VOSpace**
  - Storage of intermediate (deleted after each execution or temporary conserved to replay partially the workflow, ...) or final data produced during the workflow execution, ...
- **UWS**
  - Use of asynchronous VO services in a workflow, ...
- **...**

Common problems in workflows

- **Applications called in workflows are often developed by different persons, with different languages, on different systems, ...**
  - **No unified error management, job failure, etc.**
- **...**
- **A workflow can involve computing resources like clusters, grids and access to databases**
  - **For a 6 steps workflow if the step 3 requires a few hours of computing and the step 4 crashes due to a bad entry value, the workflow will probably end...**
    - How to reduce this investment in CPU and user time ?
- **...**

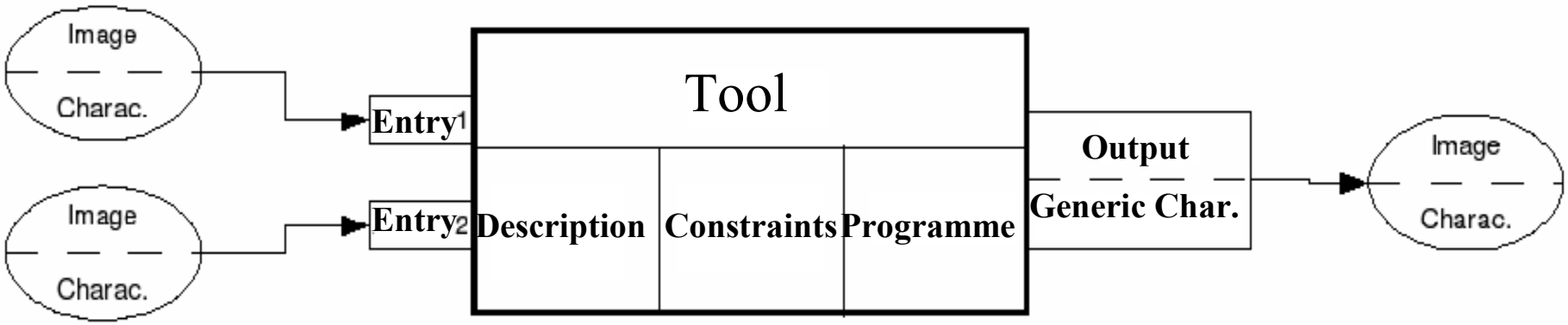
IVOA Characterization

- **From the last reference document**
  - *This document defines the high level metadata necessary to describe the physical parameter space of observed or simulated astronomical data sets, such as 2D-images, data cubes, X-ray event lists, IFU data, etc...The Characterisation data model is an abstraction which can be used to derive a structured description of any relevant data and thus to facilitate its discovery and scientific interpretation. The model aims at facilitating the manipulation of heterogeneous data in any VO framework or portal.*

Characterization of the entries ?

- **Goal : validation of a workflow before its execution in the case of FITS images**
  - **Try to do it for tools with FITS files as entries**
- **Why ?**
  - **Validation is done on the client side before the submission to the engine**
  - **Minimize the use of the external resources if validation fails**
  - **Optimization of the user time**
  - **...**
- **It requires**
  - **A characterization file for the entries**
  - **A good knowledge of the tools to define the constraints**

At the tool level



- **Before the execution**
  - Constraints on entries are defined for each tool
  - A validation step checks the entries
- **During the execution**
  - After the step i, a characterization file is generated for the outputs and checked with the step i+1 constraints before its execution

Workflow test bed

Astronomical Image processIng Distribution Architecture

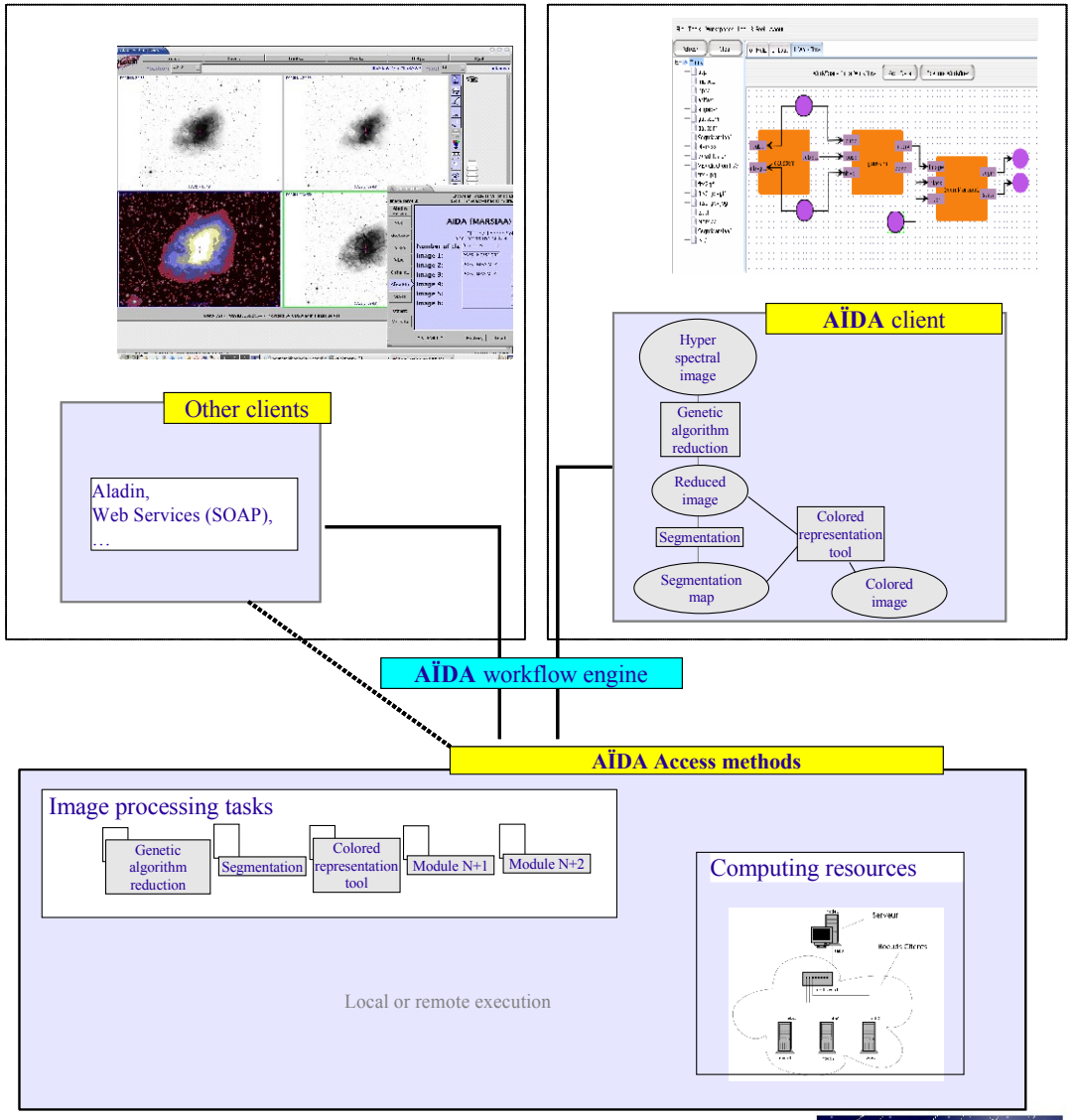
Contributors

O. Benjelloun, characterization integration
J. Beugnot*, packaging
F. Bonnarel, architecture
J.-J. Claudon*, core development
B. Gassmann, characterization & Camea
M. Louys, architecture
G. Mantelet*, characterization integration
C. Pestel, JLOW - design capabilities, new developments
A. Schaaff, architecture

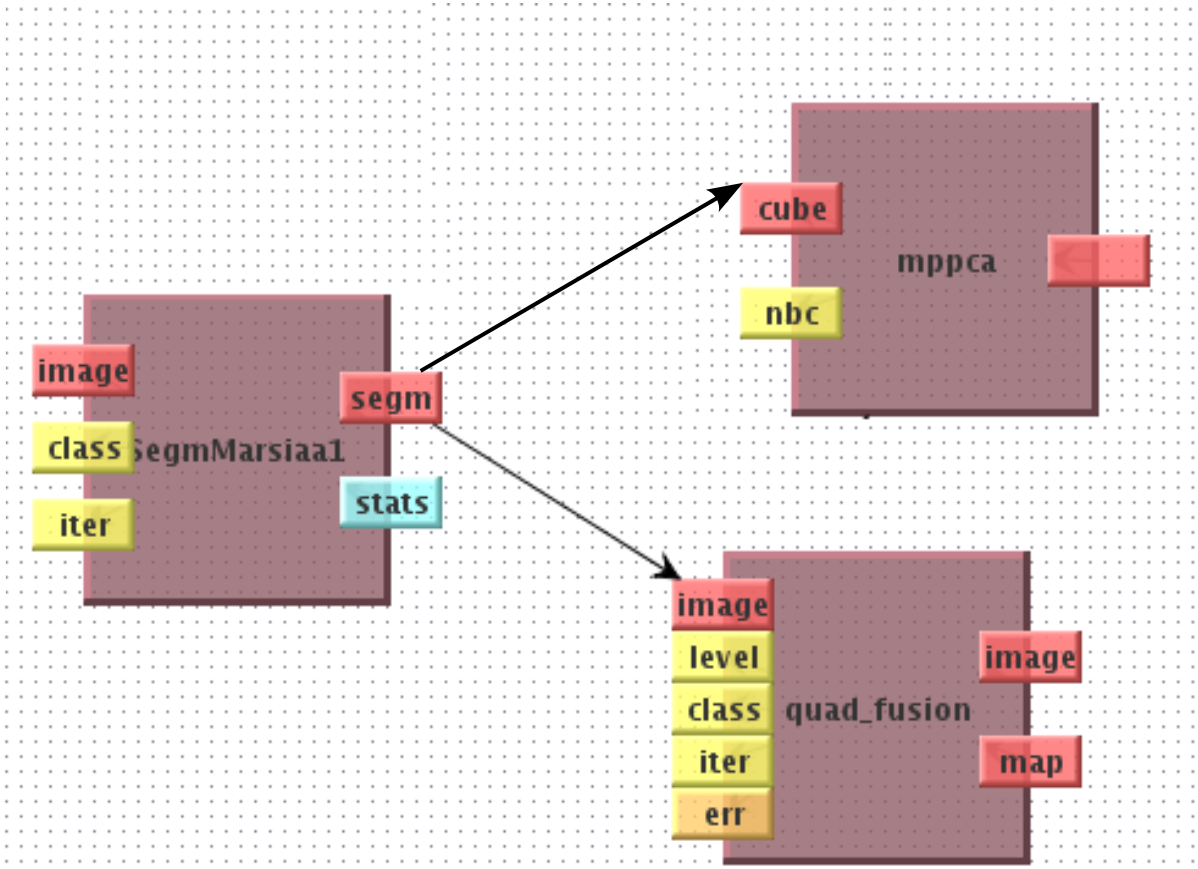
CDS & LSIIT

(have left)*

Work done in the frame of the French « **Massive Data in Astronomy** » project (2003-2006), **OV France** and **VOTECH**

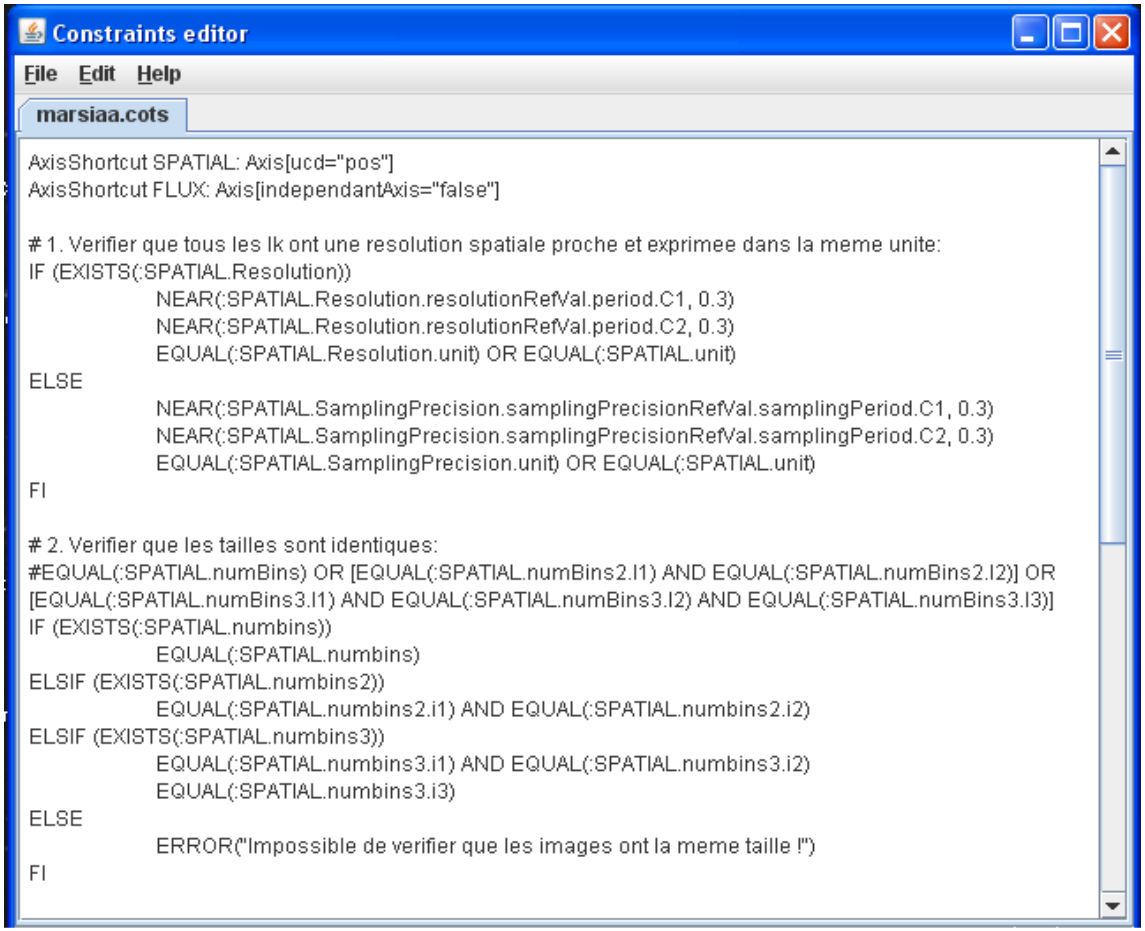


First step : a use case



Second step : write the constraints for each tool

- **We have added a simple constraints editor to AÏDA**



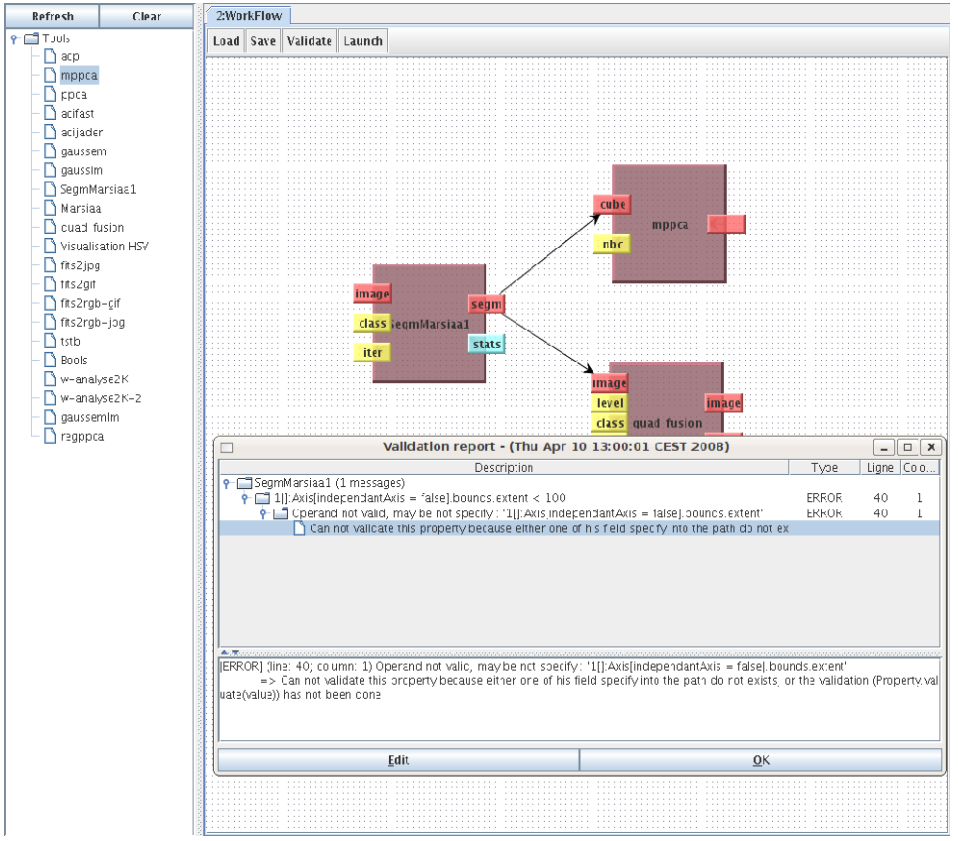
Definition of the constraints

- We have defined the grammar to generate the constraints parser
  - Very close to our needs (and to Characterization)
  - It should be replaced by a more standardized one

```
 AxisShortcut SPATIAL: Axis[ucd="pos"]
AxisShortcut FLUX: Axis[independantAxis="false"]

# 1. Verify that all the Ik have a close spatial resolution and are expressed in the same unit
IF (EXISTS(:SPATIAL.Resolution))
   NEAR(:SPATIAL.Resolution.resolutionRefVal.period.C1, 0.3)
   NEAR(:SPATIAL.Resolution.resolutionRefVal.period.C2, 0.3)
   EQUAL(:SPATIAL.Resolution.unit) OR EQUAL(:SPATIAL.unit)
ELSE
   NEAR(:SPATIAL.SamplingPrecision.samplingPrecisionRefVal.samplingPeriod.C1, 0.3)
   NEAR(:SPATIAL.SamplingPrecision.samplingPrecisionRefVal.samplingPeriod.C2, 0.3)
   EQUAL(:SPATIAL.SamplingPrecision.unit) OR EQUAL(:SPATIAL.unit)
FI

# 2. Verify if the sizes are identical
IF (EXISTS(:SPATIAL))
   EQUAL(:SPATIAL.numbins)
ELSIF (EXISTS(:SPATIAL.numbins2))
   EQUAL(:SPATIAL.numbins2.i1) AND EQUAL(:SPATIAL.numbins2.i2)
ELSIF (EXISTS(:SPATIAL.numbins3))
   EQUAL(:SPATIAL.numbins3.i1) AND EQUAL(:SPATIAL.numbins3.i2)
   EQUAL(:SPATIAL.numbins3.i3)
ELSE
   ERROR("Impossible de vérifier que les images ont la même taille !")
FI

# 3. Vérifier que toutes les images sont superposables
EQUAL(:SPATIAL.Coverage.location.unit) OR EQUAL(:SPATIAL.Coverage.unit) OR EQUAL(:SPATIAL.unit)
EQUAL(:SPATIAL.Coverage.location.coord_system_id)

# 4. Observable : (min-max)>=100 else WARNING
EQUAL(1[]:FLUX.coverage.bounds.unit) OR EQUAL(:SPATIAL.Coverage.unit) OR EQUAL(:SPATIAL.unit)
IF (1[]:FLUX.bounds.limitHi - 1[]:FLUX.bounds.limitLo >= 100)
   WARNING("(Observables: min-max <100) Il faut faire une normalisation en niveau de gris !")
FI

# 5. ...
EQUAL(:FLUX.ucd)
1[]:FLUX.bounds.extent < 100
.....


 FI
```

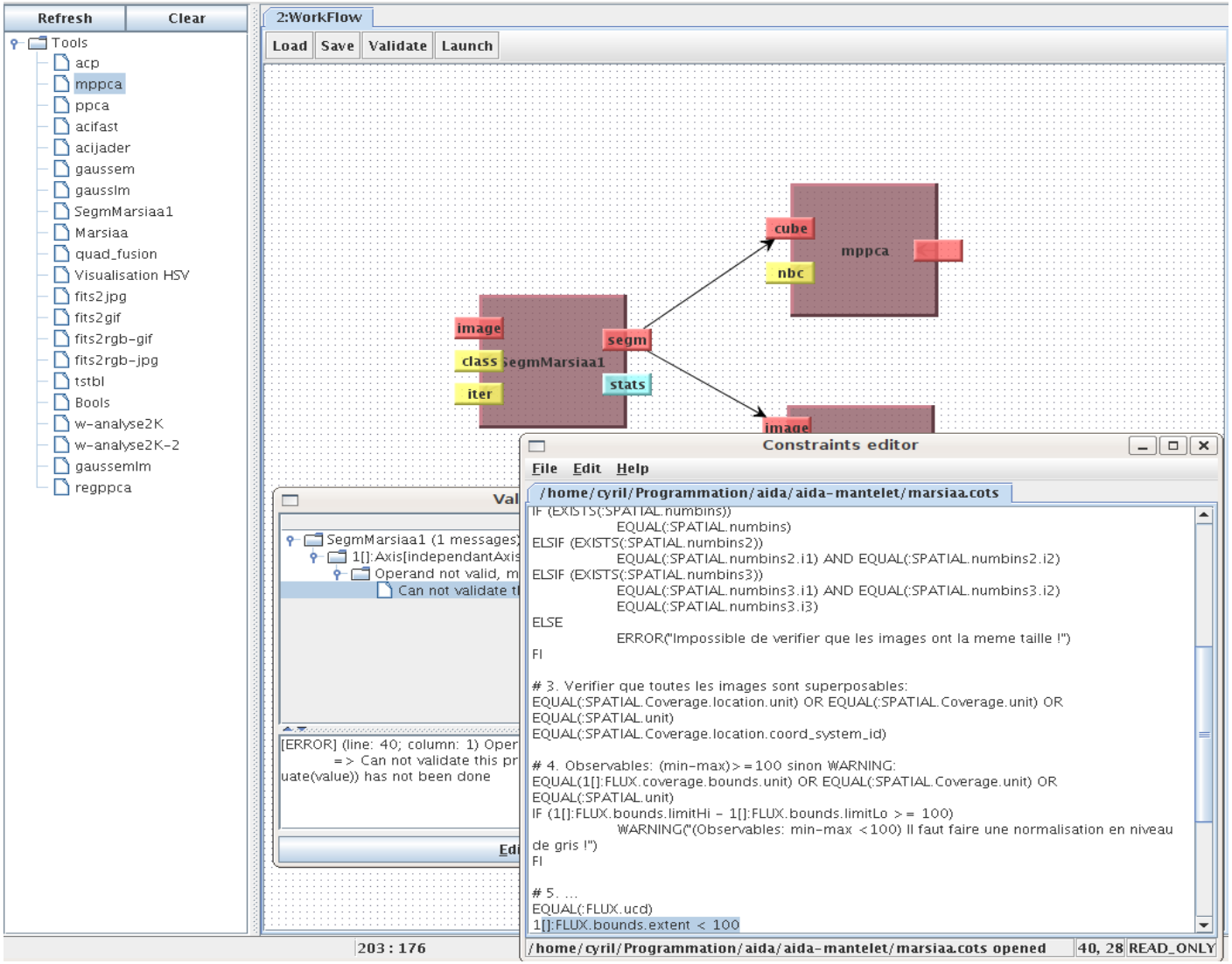
Third step : validation report generation

- It reports, for each tool of the workflow, all the errors and warnings detected during the analysis of all the Characterization files

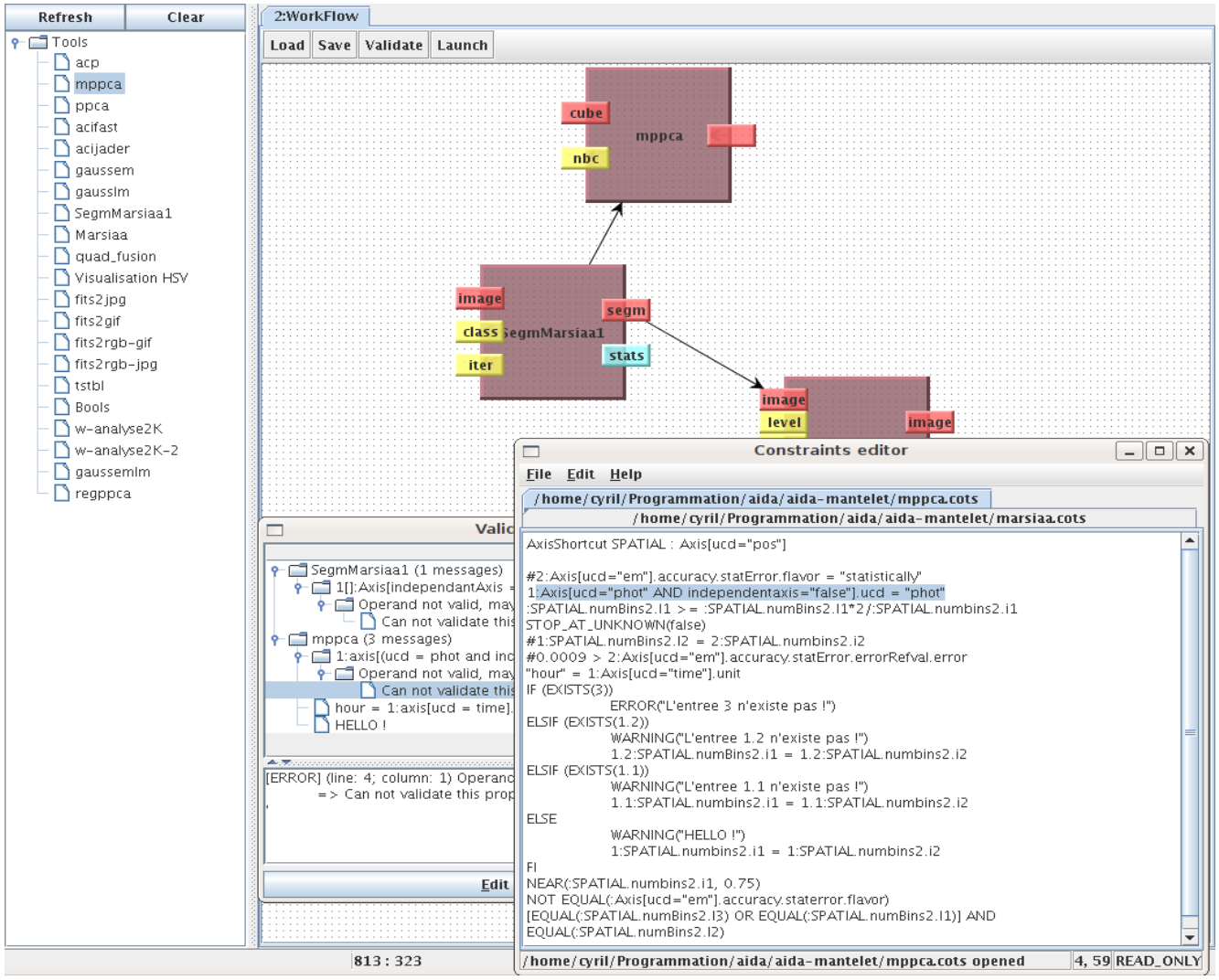


- Last step : execute ? modify the entries with errors ?

AÏDA client with validation capabilities



Other example



Summary of this study

- **Done**
  - **Definition of workflow use cases with Characterized image entries**
  - **Definition of a constraint language and integration in AÏDA**
  - **Definition of constraint files for the use cases tools**
  - **...**
- **Ongoing work**
  - **Increase the validation scope**
    - During the execution : Characterization file generation for the FITS outputs
    - Before the execution : study how to define a virtual Characterization file for an output before the execution...
  - **Replace the constraint language with a more standardized one**

Abstract

- After a quick introduction to workflow systems, the presentation will focus on the use of Characterization, an IVOA standard, in a workflow test bed architecture. The execution of a workflow may require substantial computing resources and this can take a significant amount of time. Our goal is to introduce a validation step in the workflow process before the "real" execution. This work is done in the frame of the VOTECH project.