VAMDC Interoperability

http://www.vamdc.eu (.org)

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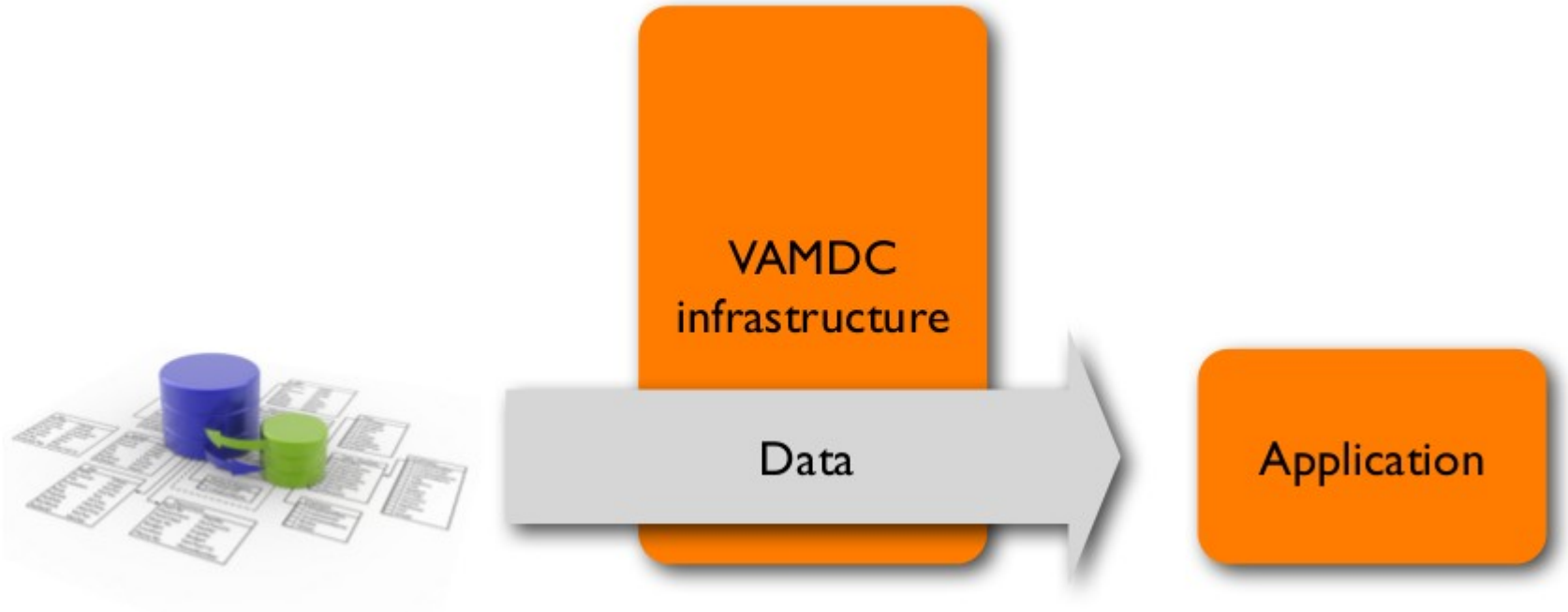
VAMDC
Virtual Atomic and Molecular Data Centre

I. Infrastructure
II. XSAMS format
III. XSAMS Processors

SEVENTH FRAMEWORK PROGRAMME
e-infrastructure

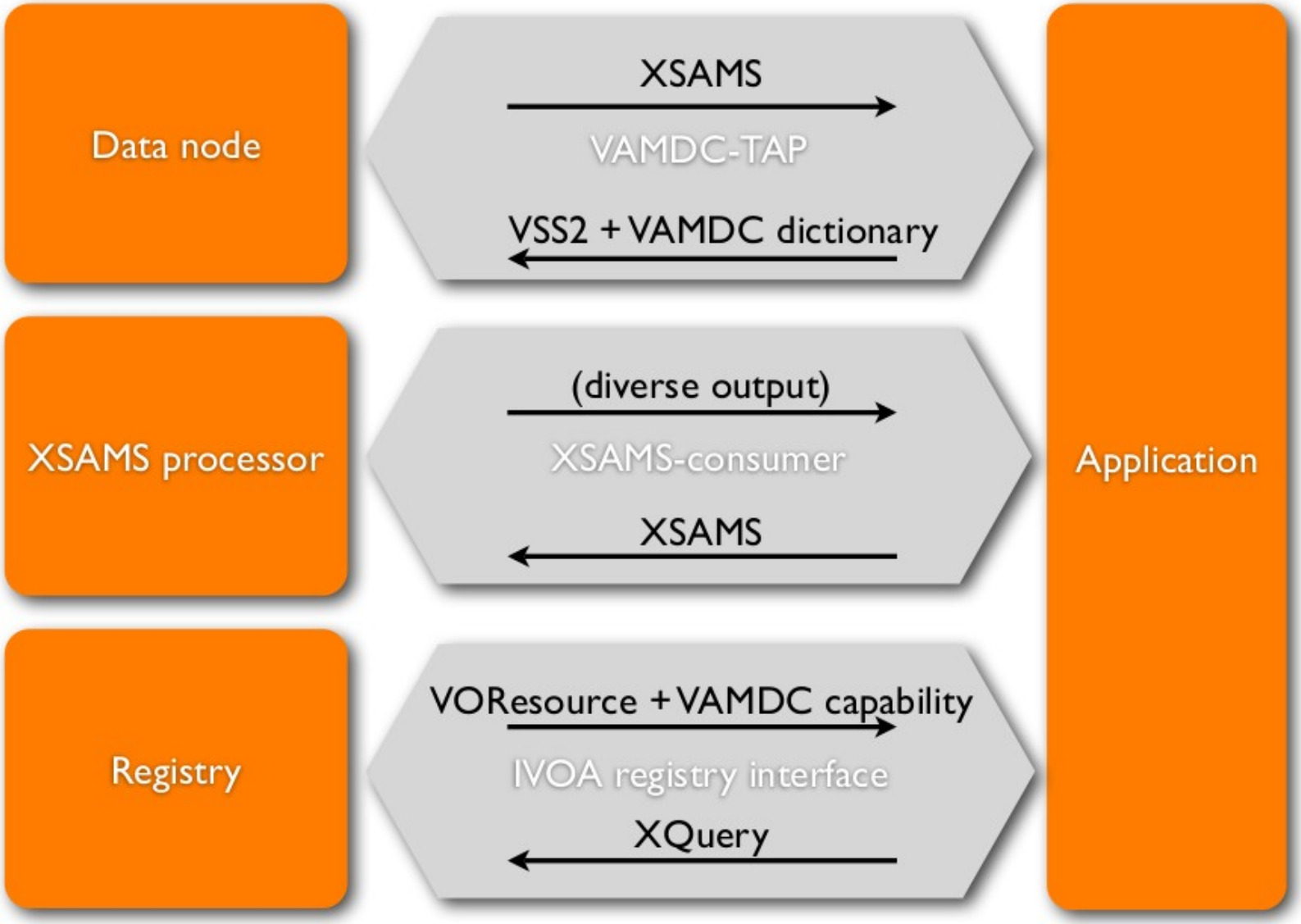
Infrastructure role



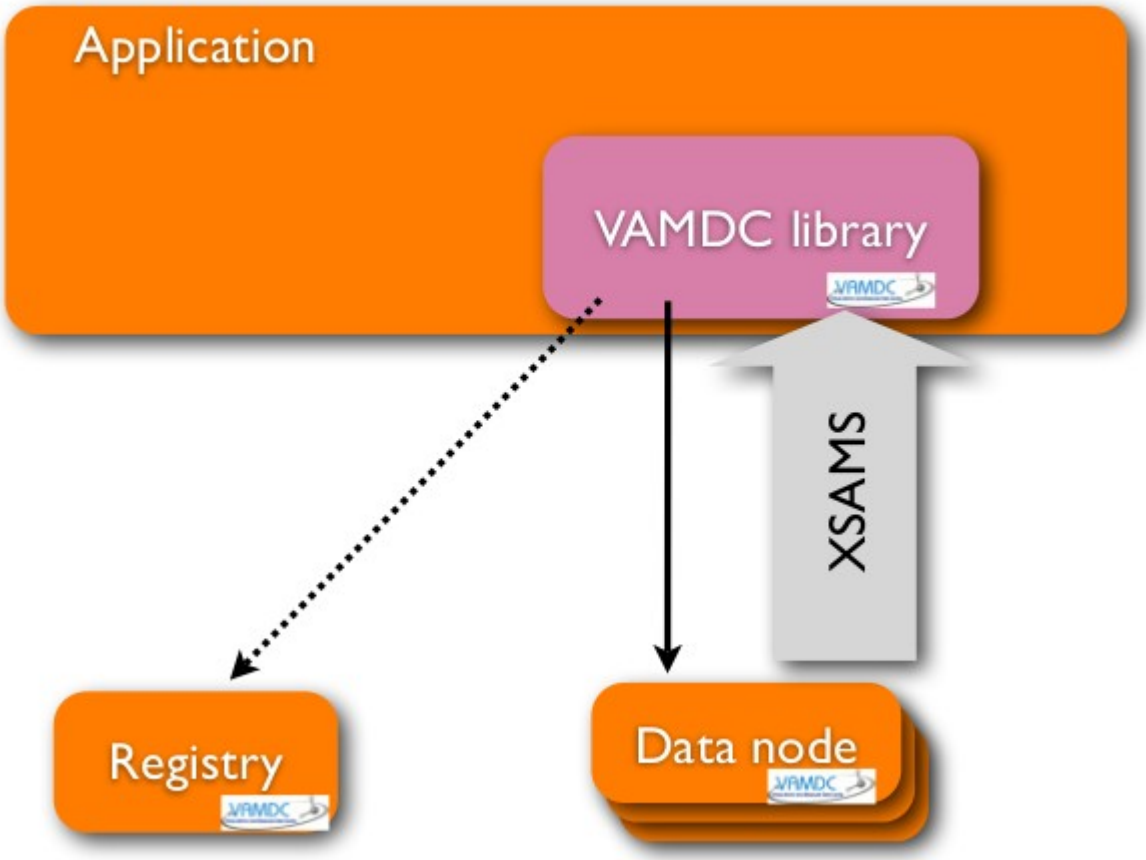
The VAMDC infrastructure is an intermediary layer between DBs and applications

The infrastructure imposes a number of standards on the data flow.

The core standards



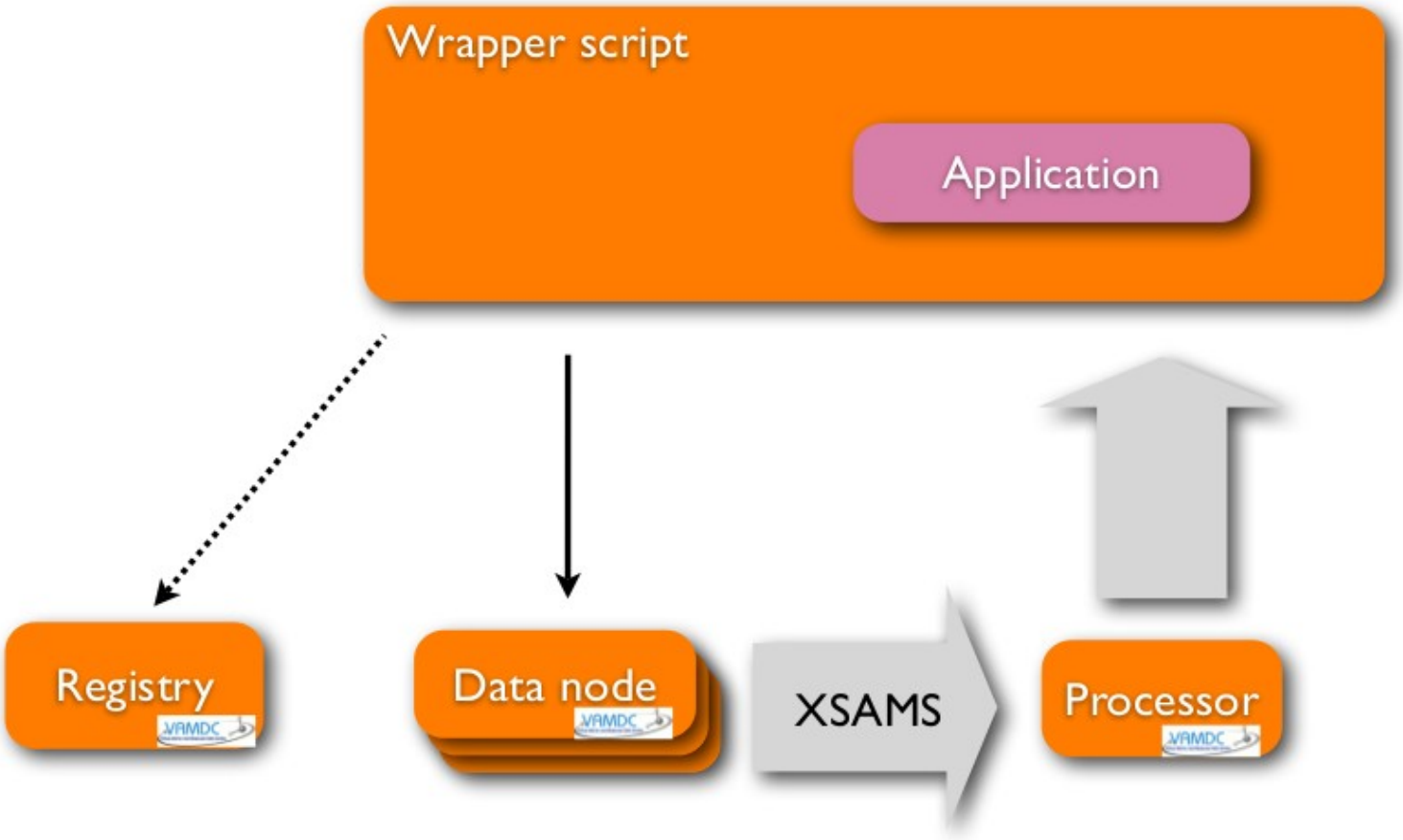
Adapted application



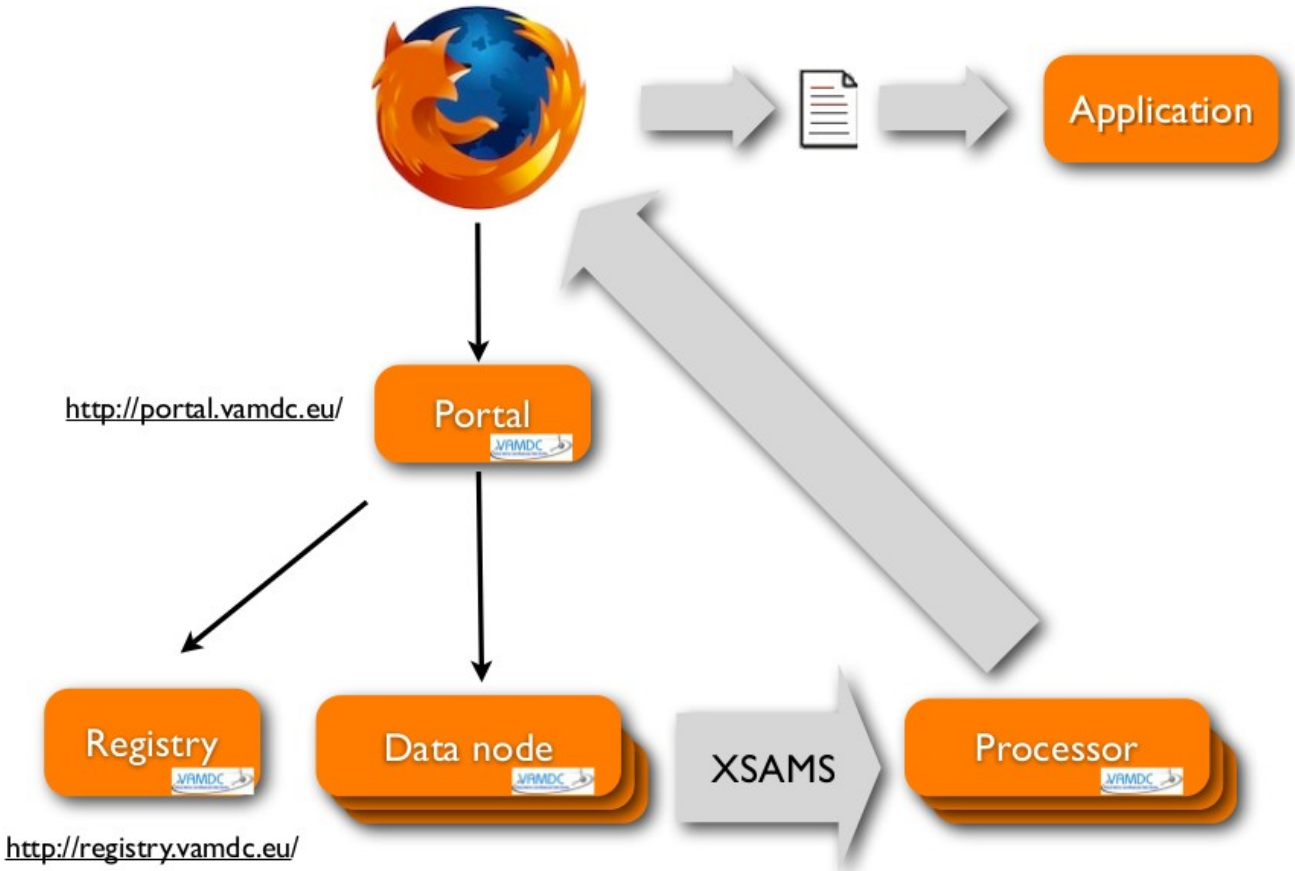
Available Java libraries :

- XSAMS file parsing
- Querying registry
- Query Builder GUI

Wrapped application



Portal, nodes & processors



VAMDC provides a web portal as a proxy for a connected application.
The user drives the portal with a web browser and forms the queries interactively, typically routing the results to a processor for transformation into a desired format.

= “infrastructure”

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XSAMS goals

- XSAMS stands for XML Schema for Atomic, Molecular and Solids

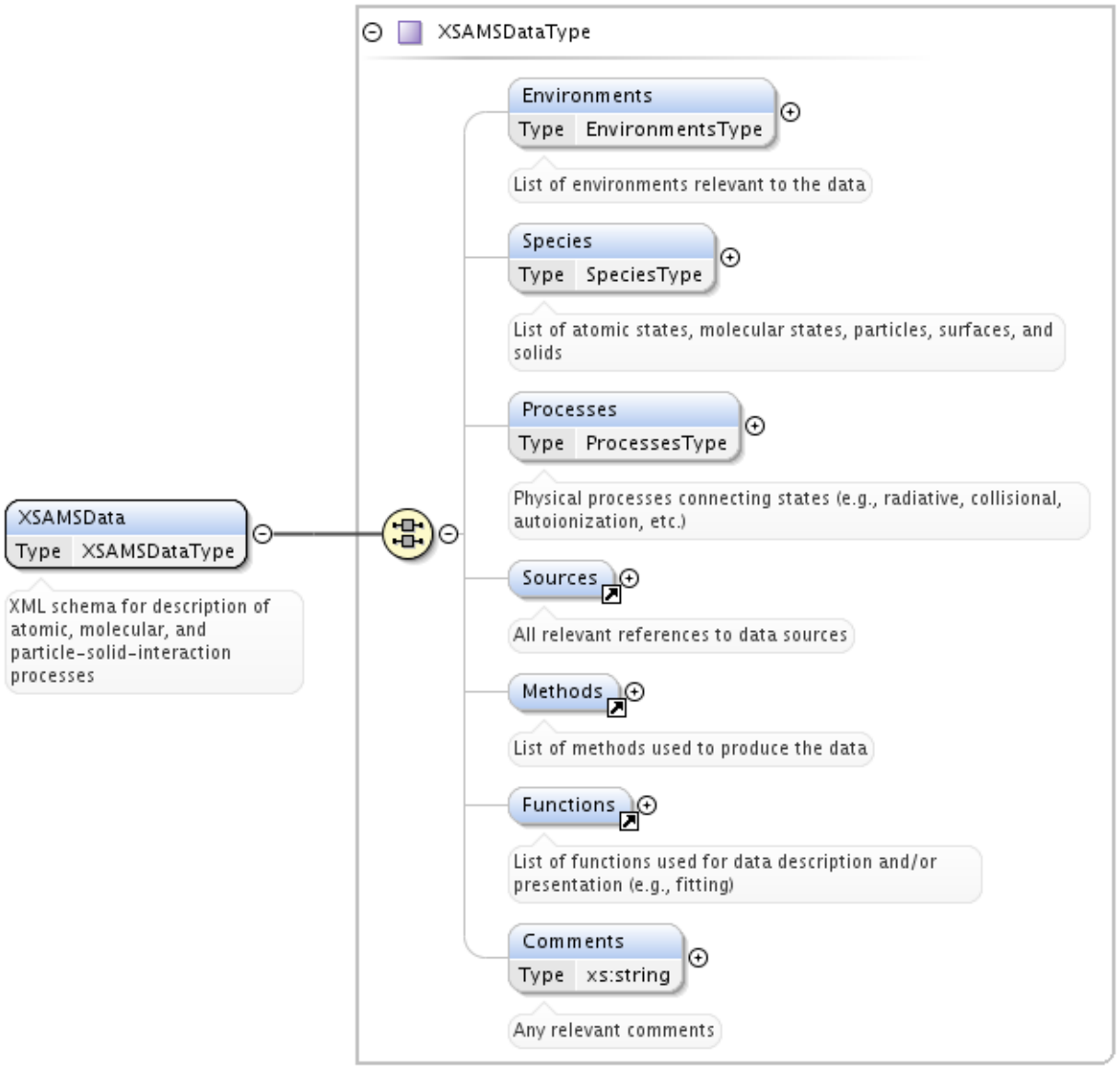
- A common format was necessary because VAMDC includes databases providers from very different fields (atomic, molecular and solid spectroscopy)

- Standard for exchange of atomic, molecular and particle-surface-interaction (AMPSI) data

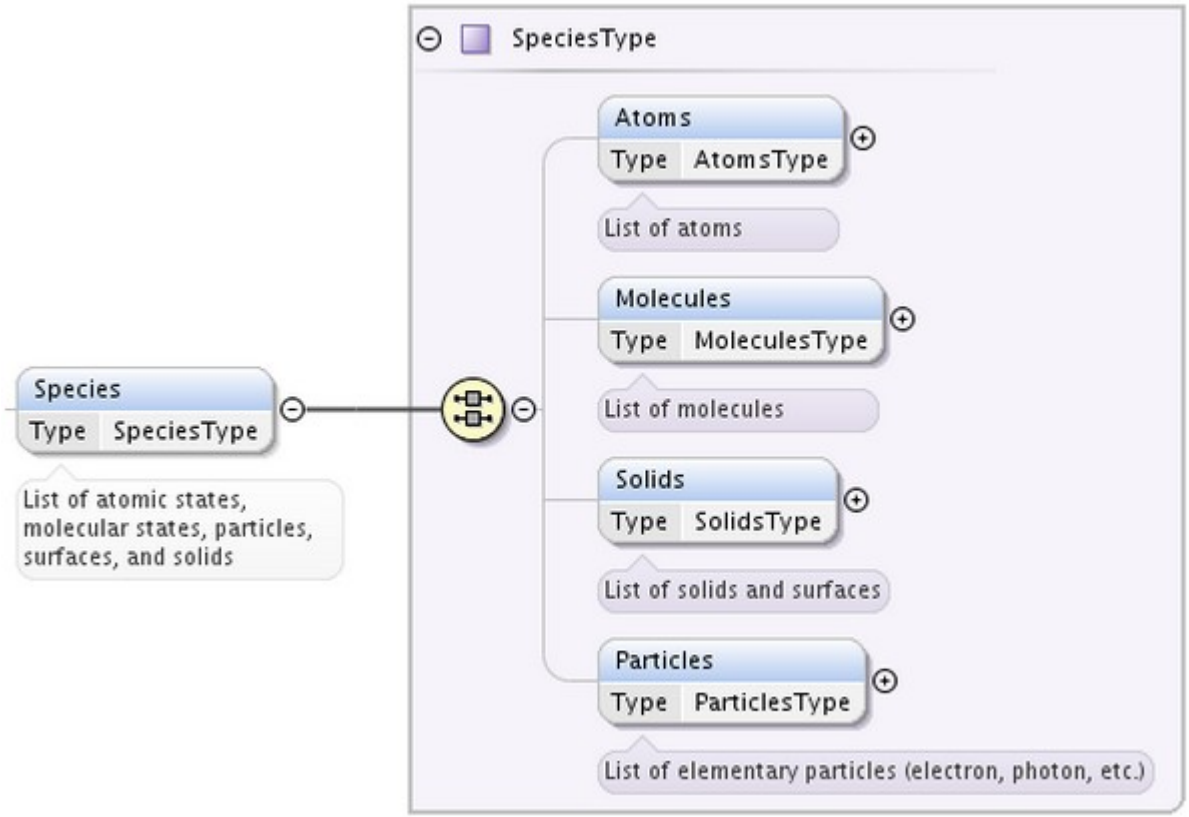
- Informations concerning sources and generation of the data must be provided

- Correctness or applicability of the data is left to the producer responsibility

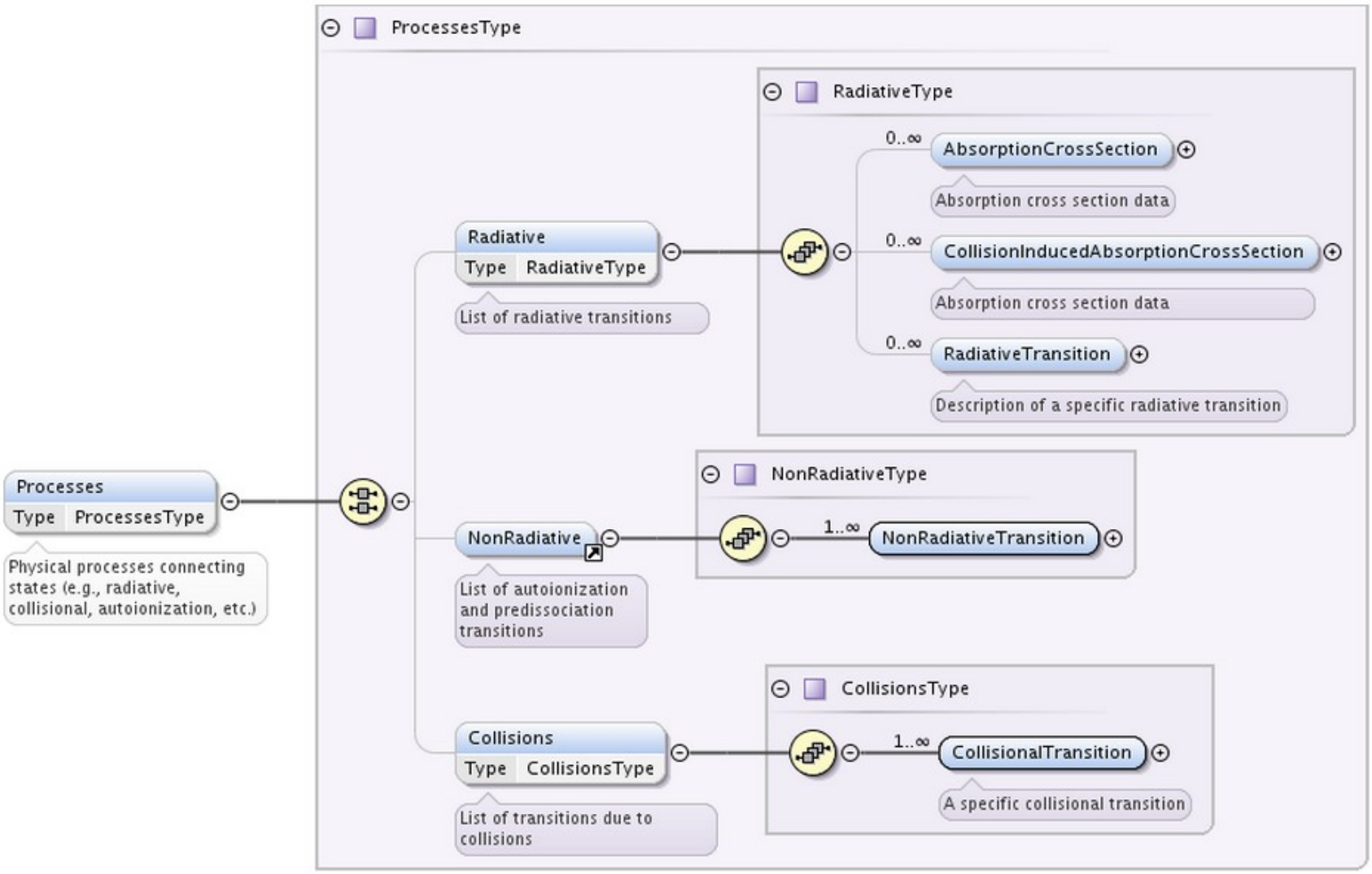
XSAMS structure : root element



XSAMS structure : species element



XSAMS structure : processes element



Data presentation II

```
<RadiativeTransition id="Pchianti-R277588">
    <EnergyWavelength>
        <Wavelength methodRef="Mchianti-EXP">
            <Value units="A">5005.51</Value>
        </Wavelength>
        <Wavelength methodRef="Mchianti-THEO">
            <Value units="A">5037.84</Value>
        </Wavelength>
    </EnergyWavelength>
    <UpperStateRef>Schianti-4014026</UpperStateRef>
    <LowerStateRef>Schianti-2014026</LowerStateRef>
    <SpeciesRef>Xchianti-14026</SpeciesRef>
    <Probability>
        <TransitionProbabilityA>
            <Value units="1/s">0.008762</Value>
        </TransitionProbabilityA>
    </Probability>
</RadiativeTransition>
```

Experimental wavelength

Theoritical wavelength

Reference to lower and upper states

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XSAMS Processors

- They are web services applying transformations to one or more input files giving one output file as a result

- Aims at:
  - Simplifying XSAMS format usage through a transformation into other formats
  - Combining/Comparing files (for example level identification between databases)

- Existing processors use XSL stylesheets to transform XSAMS files (not a requirement)

- They are accessible from the VAMDC portal

- They are standardized :
http://www.vamdc.org/documents/xsams-processor_v12.07.pdf

XSAMS Processors

- As they are registered in the VAMDC registry, they must provide VOSI capabilities functionnality

- Capability element from VOResource schema has been extended, adding versionOfSoftware, versionOfStandards, numberOfInputs and cacheLifeTime (http://www.vamdc.org/xml/XSAMS-consumer/v1.0/)

- They provide a simple web interface to upload XSAMS files and can be called directly from scripts

- Parameters :
    - GET/POST : url (one or more, leading to the XSAMS file)
    - POST : upload (one or more, contains the document itself)

- The job receives an ID that is used to identify it, the newly created document then stays available on the server with this id

Current Processors

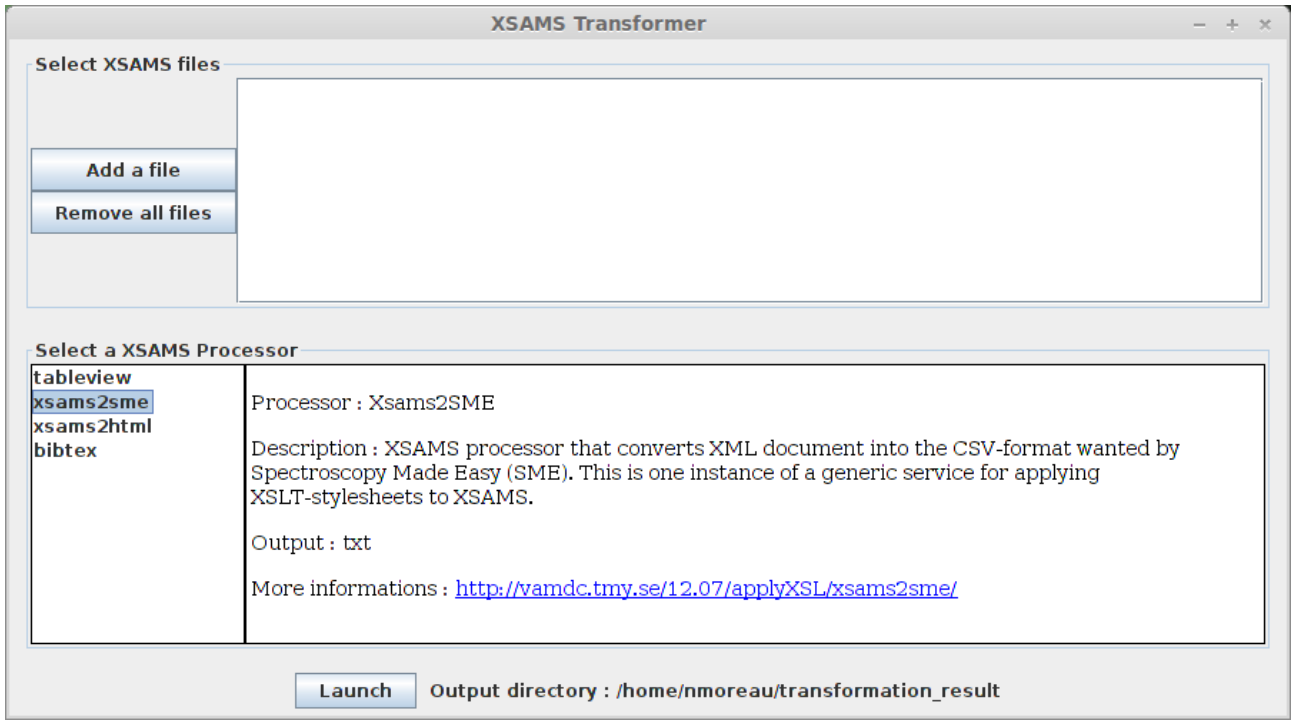
- Bibtex : extract references informations from a XSAMS document and returns them as an Bibtex file

- XSAMS to SME : converts XSAMS file to SME compatible file (Spectroscopy Made Easy (SME) is IDL software and a compiled external library that fits an observed high-resolution stellar spectrum with a synthetic spectrum to determine stellar parameters)

- Table view : presents XSAMS document as an HTML table

- Atomic XSAMS to HTML : presents atomic XSAMS data as an HTML table with sort functions and SAMP functionnalities (selected content is converted into votable and sent to Topcat for example)

Standalone Processor application



- Java application executing processors locally
- Does not require a network connection
- Provide both a GUI and a CLI so that it can be used in scripts
- Execute the XSL stylesheets on one or more input files

Future developments

- We provide a processor web service skeleton to help new implementation, only XSL file must be implemented

- New processors that we will implement :
  - Molecular spectroscopy
  - Collisional data
  - Asking to user to identify other needs