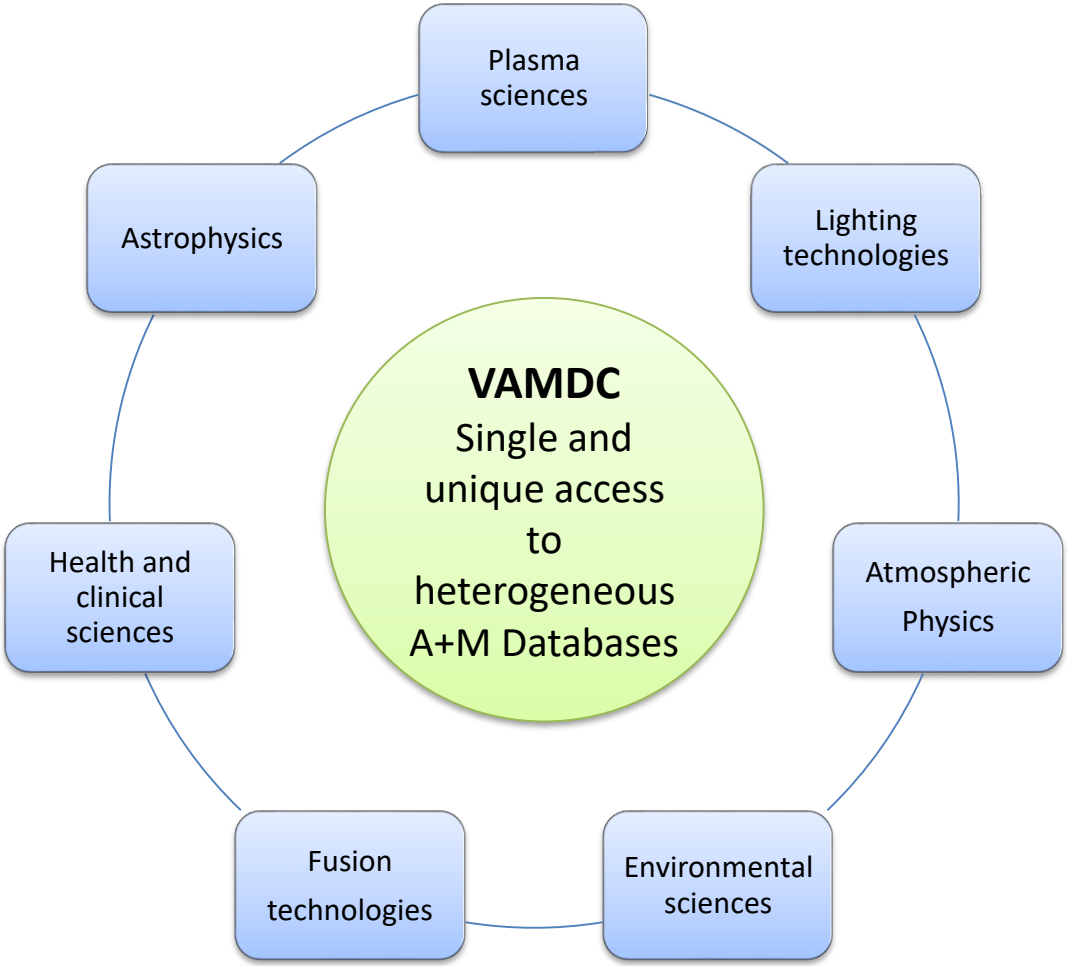
From RDA Data Citation Recommendations to new paradigms for citing data from VAMDC

C.M. Zwölf and VAMDC consortium

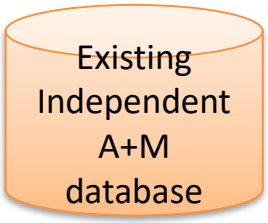
Trieste Interop – October 2016

The Virtual Atomic and Molecular Data Centre



- Federates 29 heterogeneous databases http://portal.vamdc.org/
- The "V" of VAMDC stands for Virtual in the sense that the e-infrastructure does not contain data. The infrastructure is a wrapping for exposing in a unified way a set of heterogeneous databases.
- The consortium is politically organized around a Memorandum of understanding (15 international members have signed the MoU, 1 November 2014)
- High quality scientific data come from different Physical/Chemical Communities
- Provides data producers with a large dissemination platform
- Remove bottleneck between data-producers and wide body of users

The VAMDC infrastructure technical architecture



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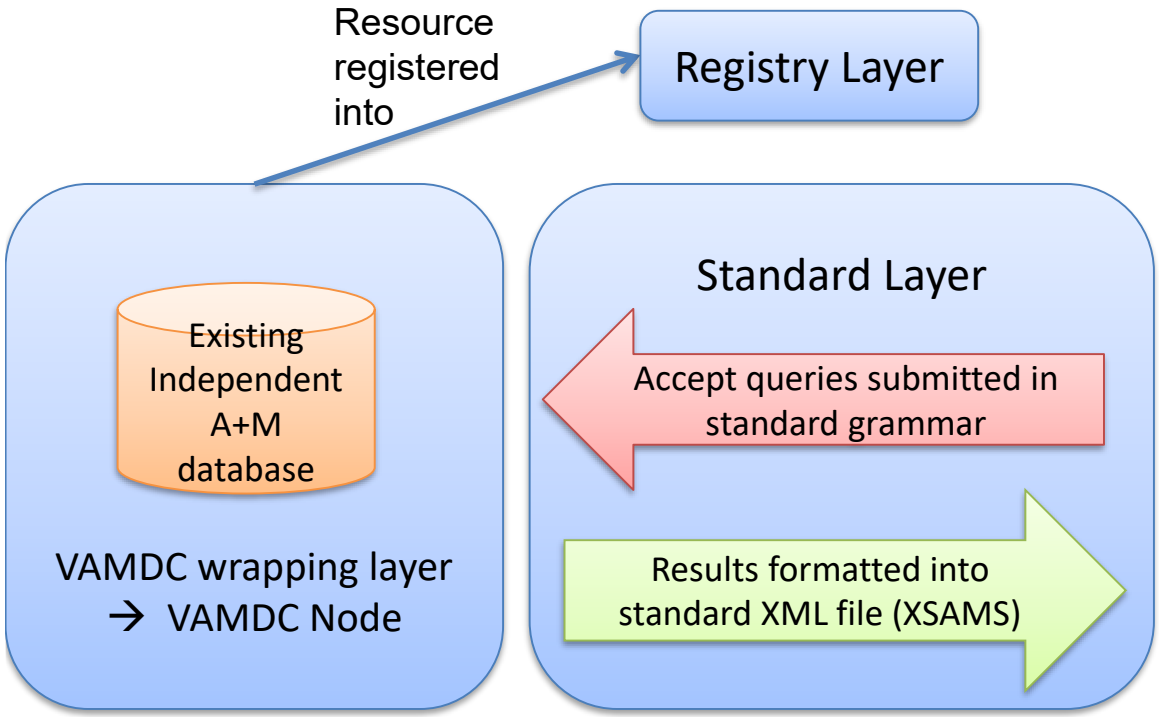

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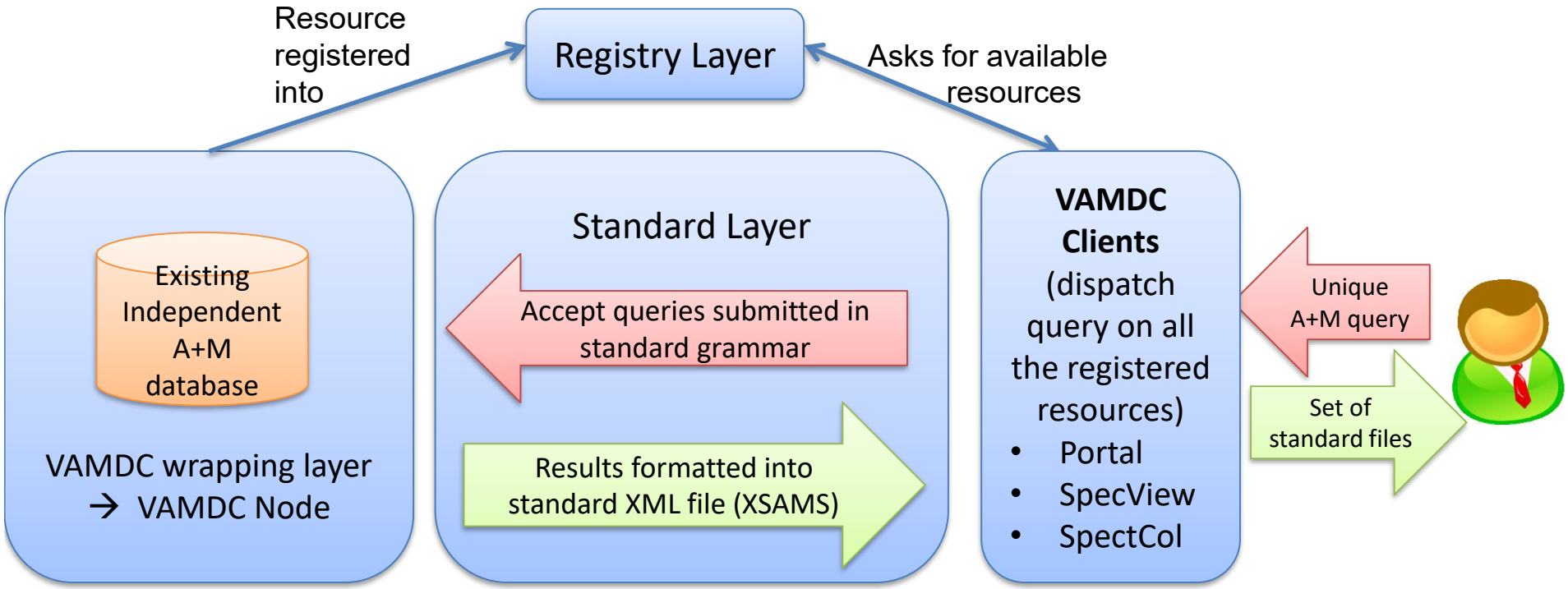

Importance of citation in building new knowledge

Citation is a key element in the production of new knowledge

Gives credits to the author of the intellectual product cited

VAMDC consortium

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The nowadays adopted citation model works well for papers.
It cannot be easily transposed to citation of digital data…

VAMDC consortium

Issues in data citation: case of the Atomic and Molecular data

The evolution of digital data:

- Is very rapid
- Is not systematically reported

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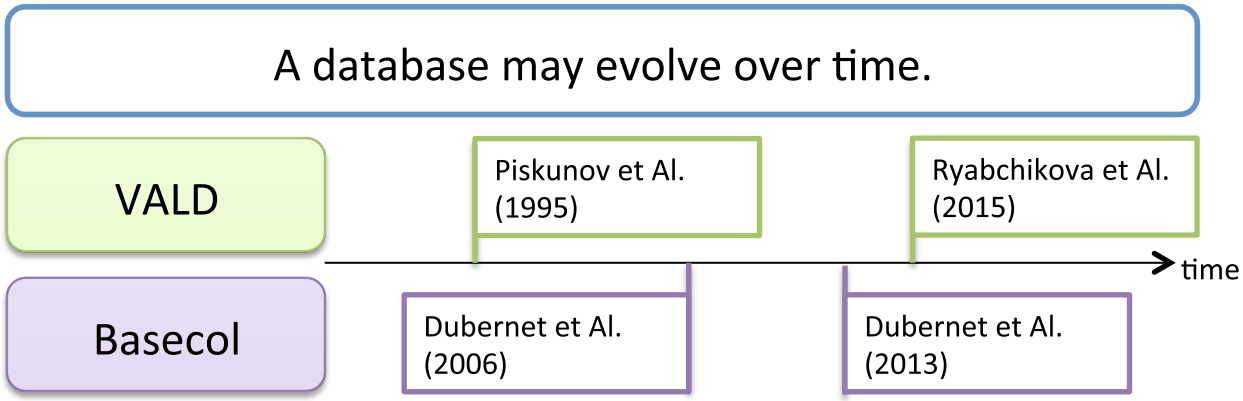

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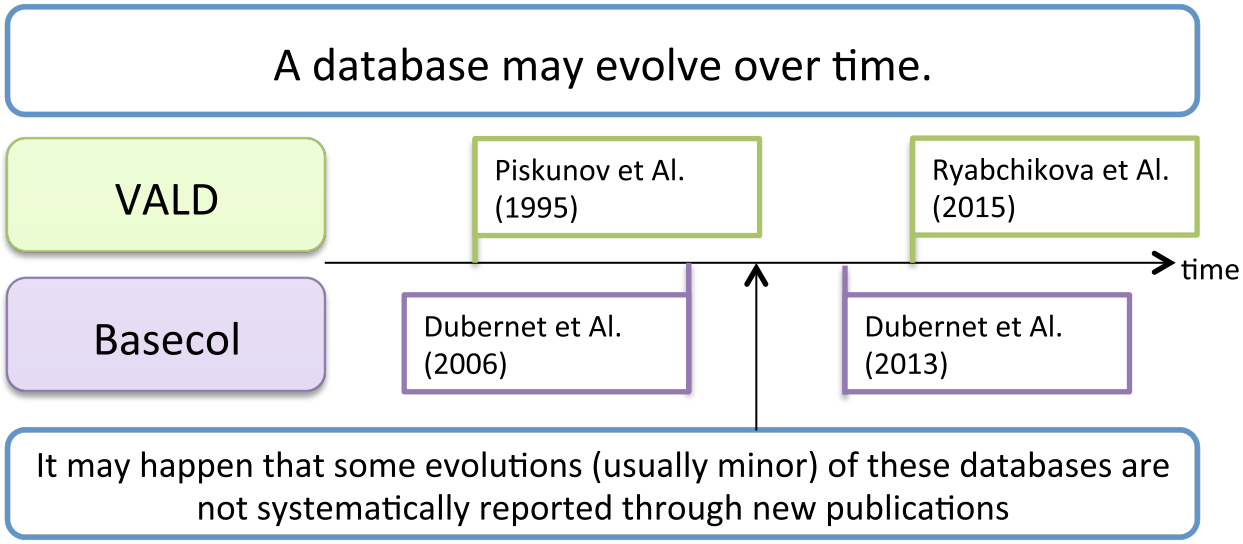

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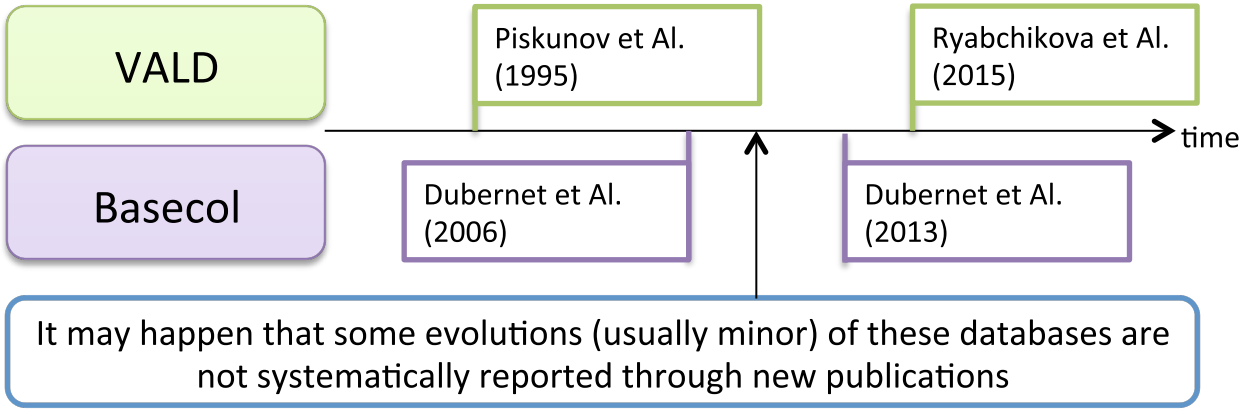

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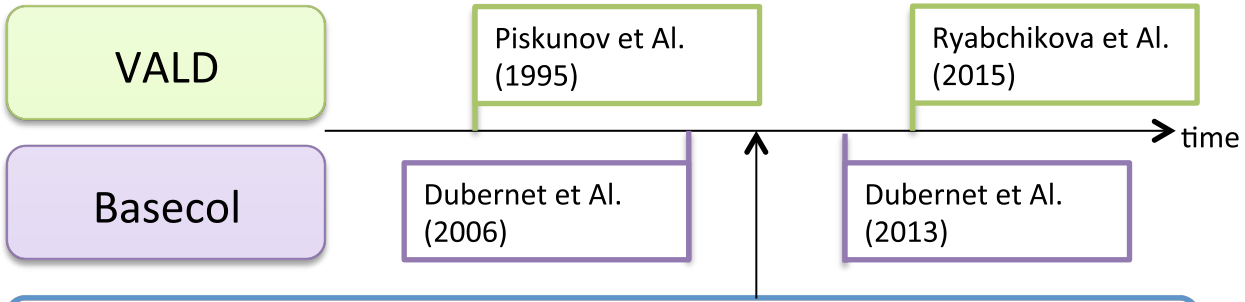

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The volume of digital data is wide and constantly growing.

A given surveys may use thousands of spectroscopic data coming from many experimental/theoretical authors.

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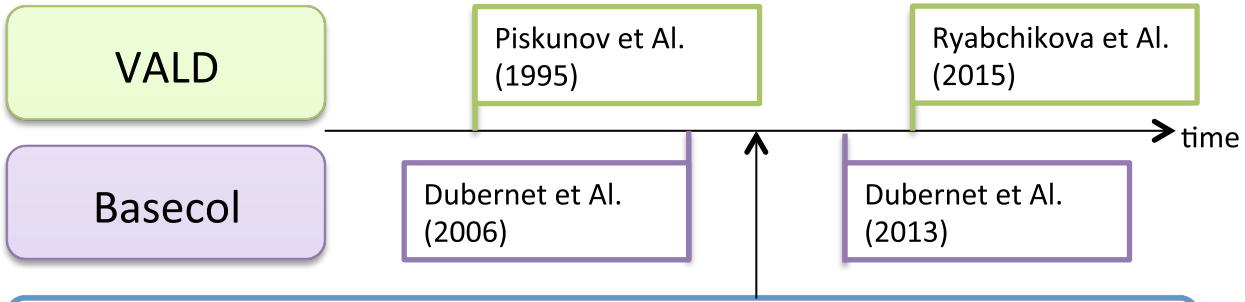

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It is impossible to effectively cite the origin of thousand of data with the required fine grained granularity.

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The survey by *[Ginard et al. (2012)]* covers frequencies from 83302Mhz to 262404Mhz detecting emission from about 36 species:

- They used catalogues from two public databases *[Picket et al. (1998)]* and *[Müller et al (2005)]* and a private communication from J. Cernicharo.
- There is no knowledge of the exact dataset used → **Their analysis is not reproducible**.
- There is no citation of the authors who produced the spectroscopic data used in their analysis.
- The collisional data are properly cited.
  - Dozen of papers for collisional data vs. hundreds of papers for spectroscopic data.

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Track the versioning of data

Having a mechanisms to speed up the citation process

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- Address these issues at the VAMDC federated level (not database by database)
- Discuss these issues at the data-community level: we joined (spring 2014) the **RDA Data Citation Working Group**.

VAMDC has become one of the RDA use-cases.

VAMDC consortium

The Research Data Alliance and the Data Citation WG

Data Citation WG

Group details

Status: Recognised & Endorsed
Chair(s): Andreas Rauber, Ari Asmi, Dieter van Uytvanck
Case Statement: Download

The RDA Working Group on Data Citation (WG-DC) aims to bring together agroup of experts to discuss the issues, requirements, advantages and shortcomings of existing approaches for efficiently citing subsets of data. The WG-DC focuses on a narrow field where we can contribute significantly and provide prototypes and reference implementations.

Goals of this WG are to create identification mechanisms that:

- allows us to identify and cite arbitrary views of data, from a single record to an entire data set in a precise, machine-actionable manner
- allows us to cite and retrieve that data as it existed at a certain point in time, whether the database is static or highly dynamic
- is stable across different technologies and technological changes

Solution: The WG recommends solving this challenge by:

- ensuring that data is stored in a versioned and timestamped manner.
- identifying data sets by storing and assigning persistent identifiers (PIDs) to timestamped queries that can be re-executed against the timestamped data store.

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- The RDA recommendations comes from standalone databases or warehouse.
- VAMDC is a distributed infrastructure, with no central management system.

Let us implement the recommendation!!

The problem is more **anthropological** than technical…

Tagging and versioning data

What does it really mean *data citation?*

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Ok, but What is the data granularity for tagging?

Naturally it is the dataset (A+M data have no meaning outside this given context)

But each data provider defines differently what a dataset is.

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Everyone knows what it is!

Yes, but everyone has its own definition

RDA →cite databases record or output files.
(an extracted data file may have an H-factor)

VAMDC →cite all the papers used for compiling the content of a given output file.

Let us implement the recommendation!!

Implementation will be an overlay to the standard / output layer, thus independent from any specific data-node

Tagging versions of data

Two layers mechanisms

1 → Fine grained granularity:
Evolution of XSAMS output standard for tracking data modifications

2 → Coarse grained granularity:
At each data modification to a given data node, the version of the Data-Node changes

With the **second mechanism** we know that something changed : in other words, we know that the result of an identical query may be different from one version to the other. The detail of which data changed is accessible using the **first mechanisms**.

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Query Store

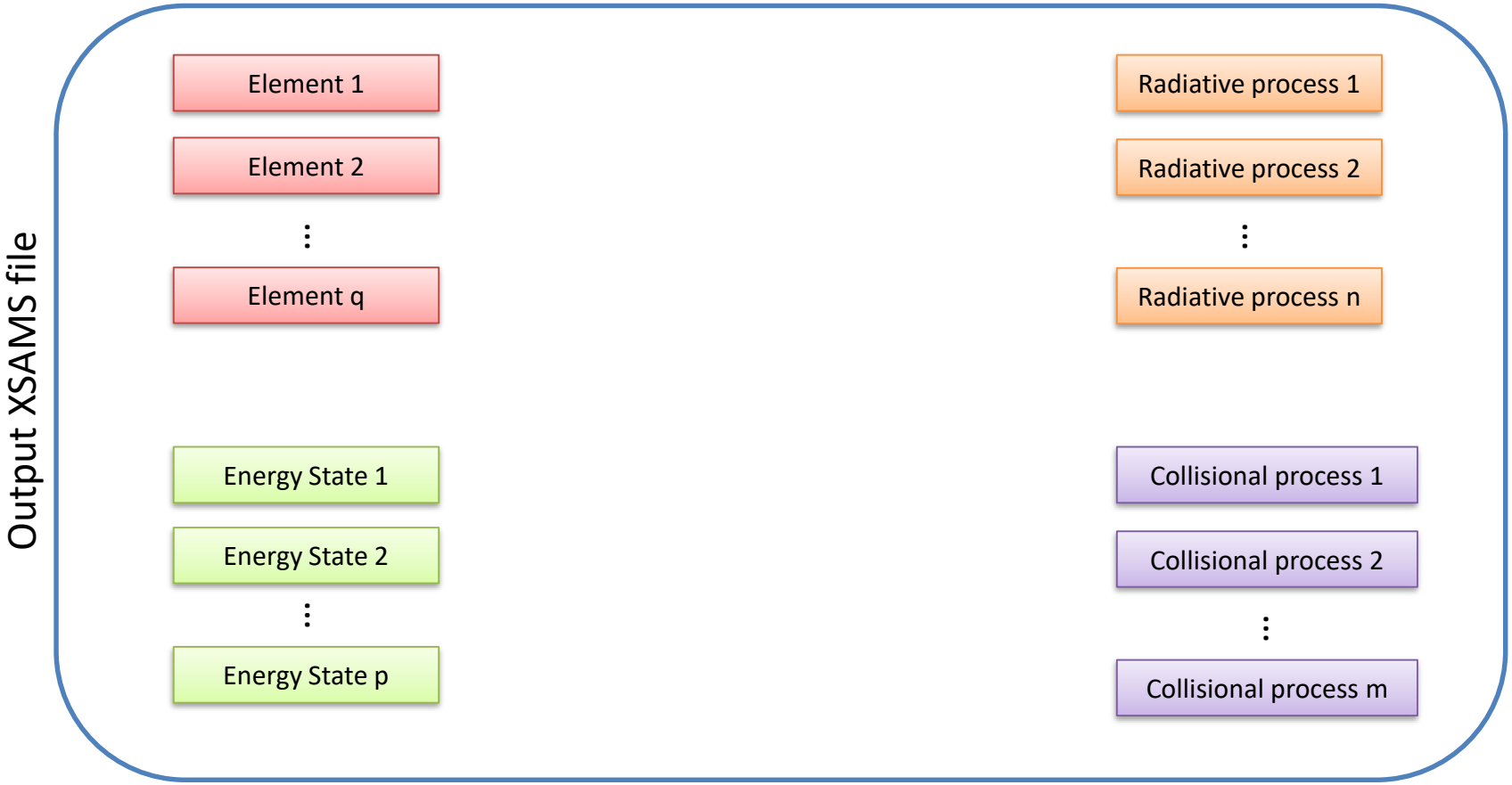
Is built over the versioning of Data

Is plugged over the existing VAMDC data-extraction mechanisms.

Due to the distributed VAMDC architecture, the Query Store architecture is similar to a log-service.

Data-Versioning: overview of the fine grained mechanisms

We adopted a change of paradigm (weak structuration):



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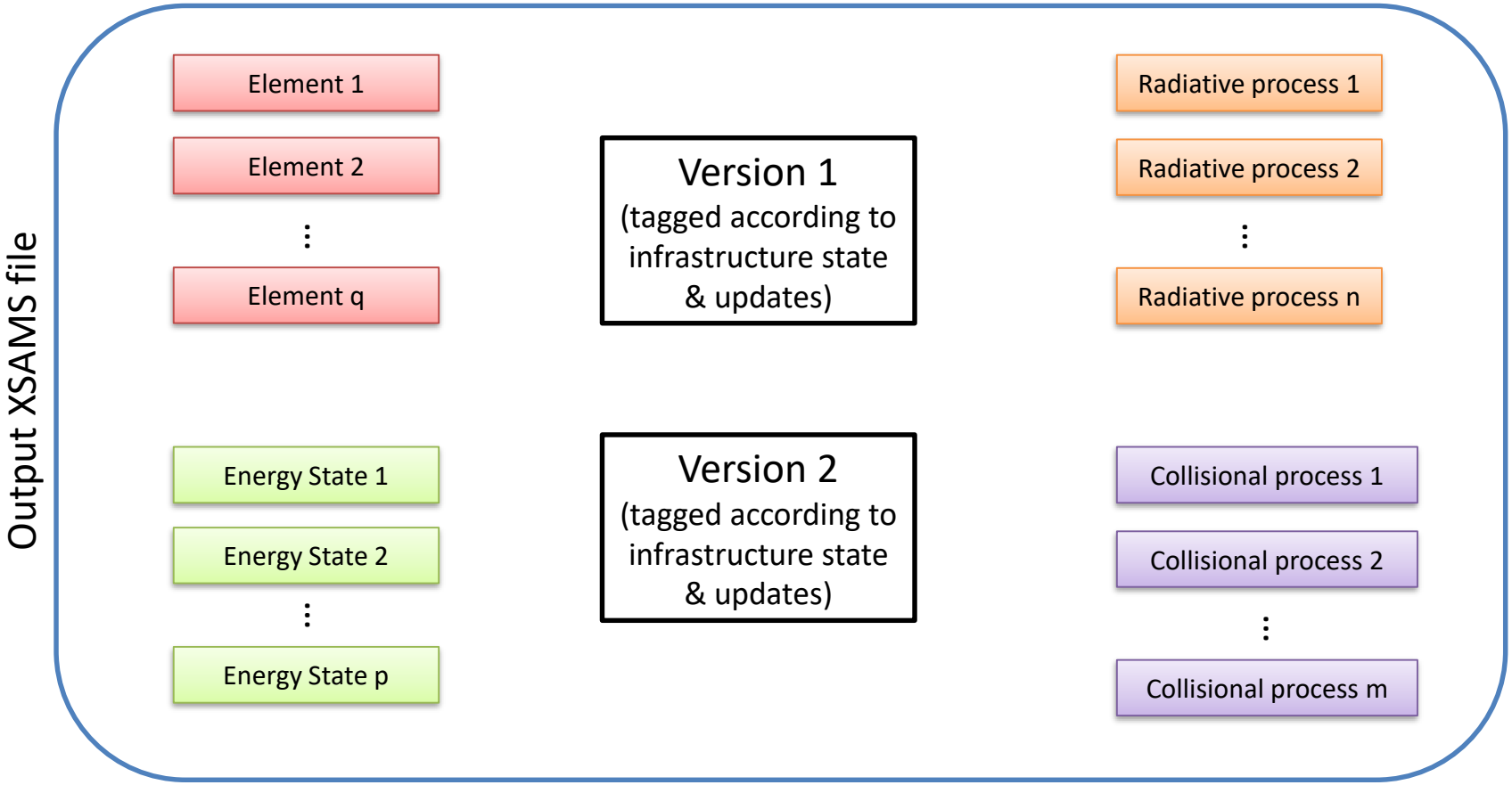

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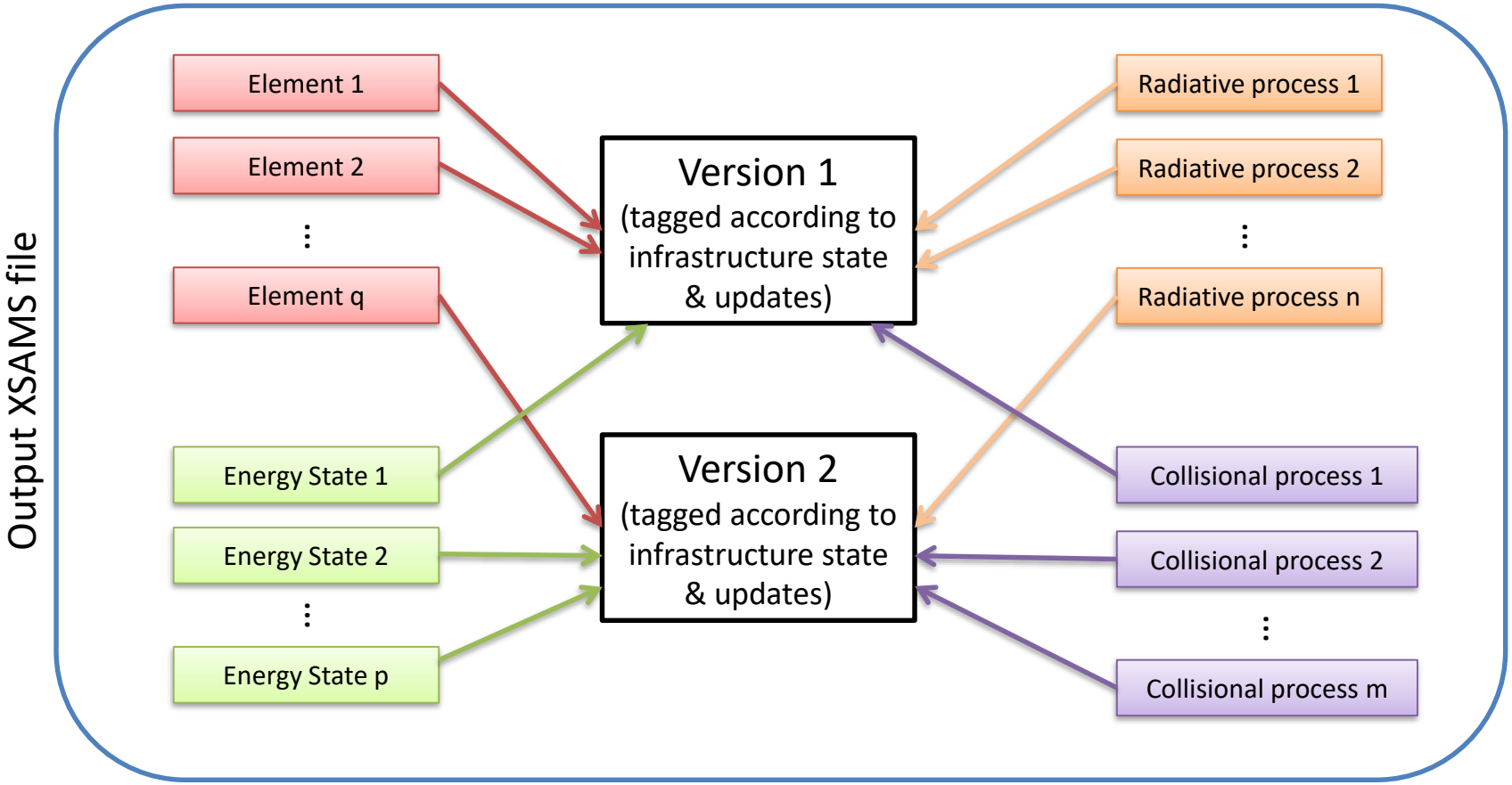

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This approach has several advantages:

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Technical details described in
New model for datasets citation and extraction reproducibility in VAMDC,
C.M. Zwölf, N. Moreau, M.-L. Dubernet,
In *press J. Mol. Spectrosc. (2016)*, http://dx.doi.org/10.1016/j.jms.2016.04.009

Arxiv version: https://arxiv.org/abs/1606.00405

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The difficulty we have to cope with:

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Collaboration with Elsevier for embedding the VAMDC query store into the pages displaying the digital version of papers.
Designing technical solution for

- Paper / data linking at the paper submission (for authors)
- Paper / data linking at the paper display (for readers)

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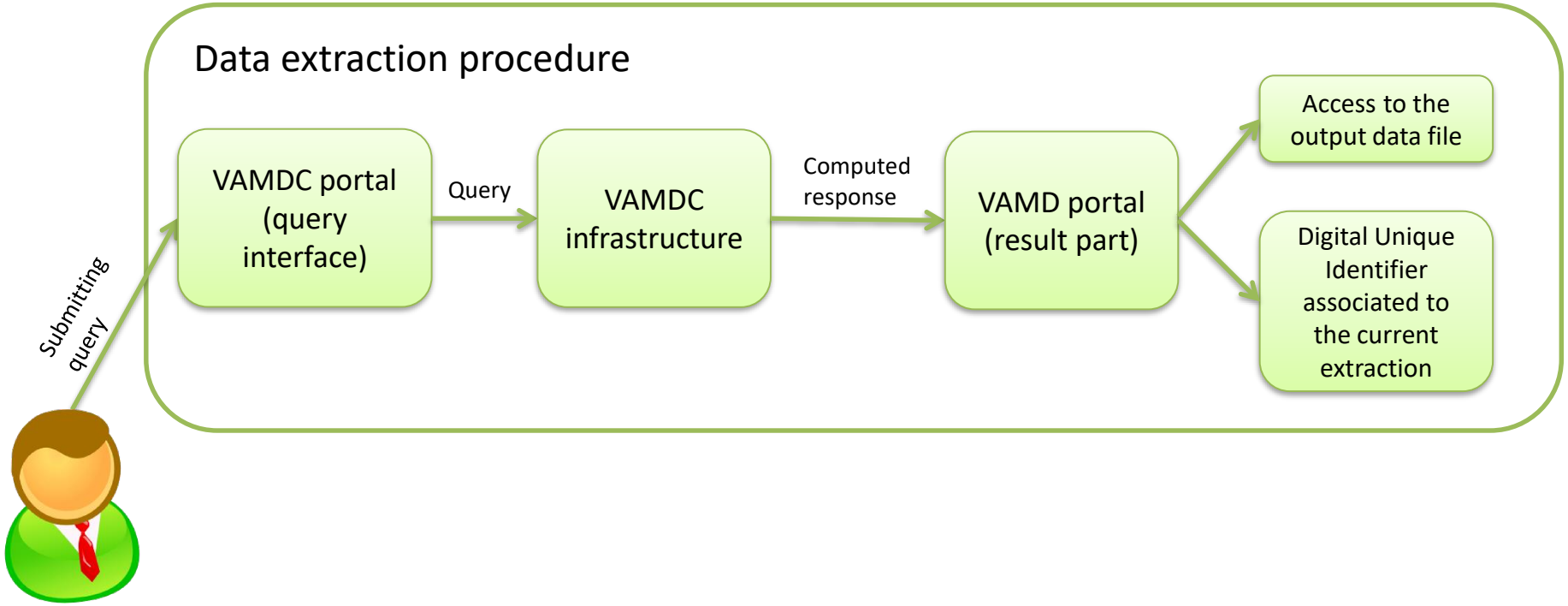
Sketching the functioning – From the final-user point of view:



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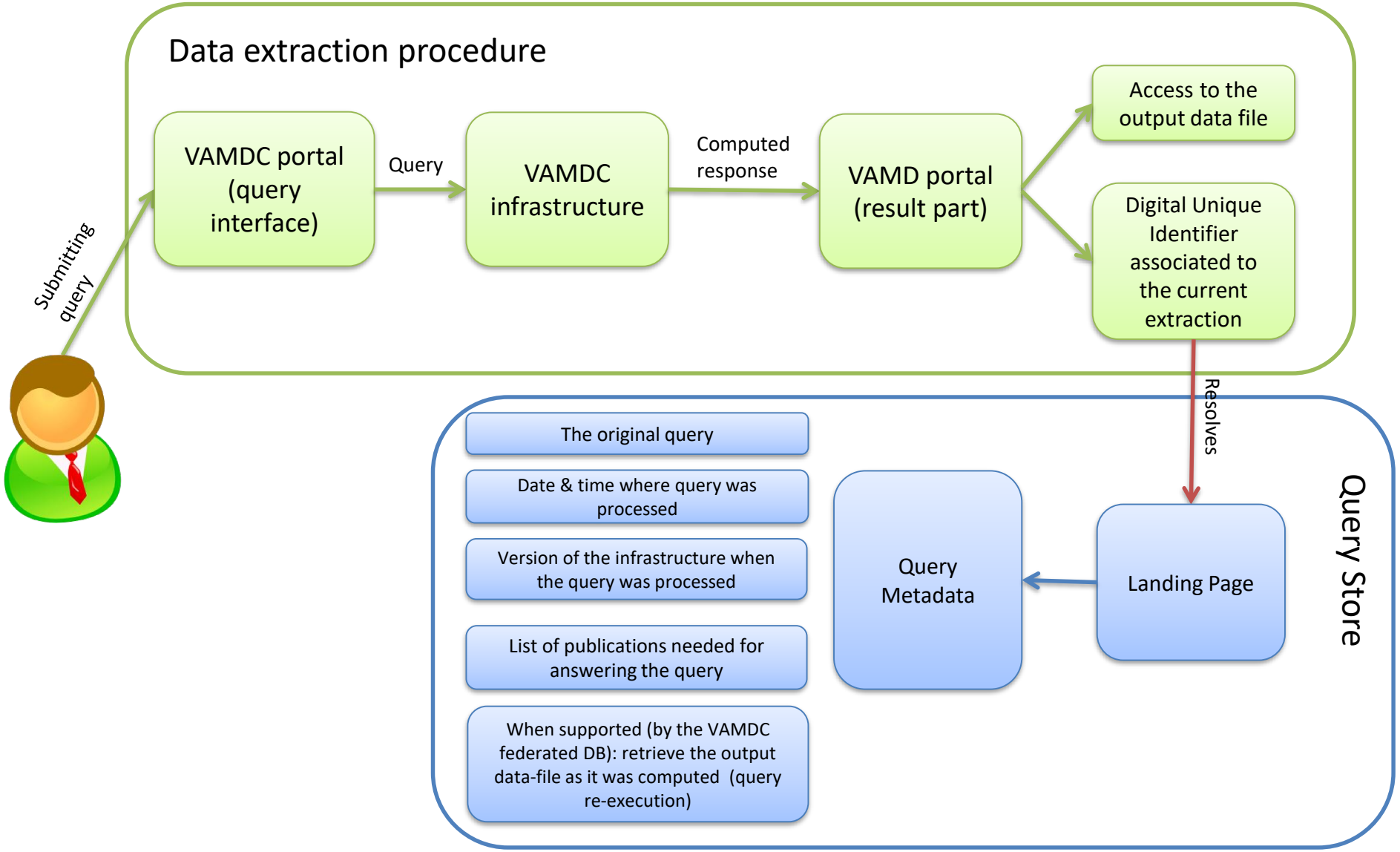

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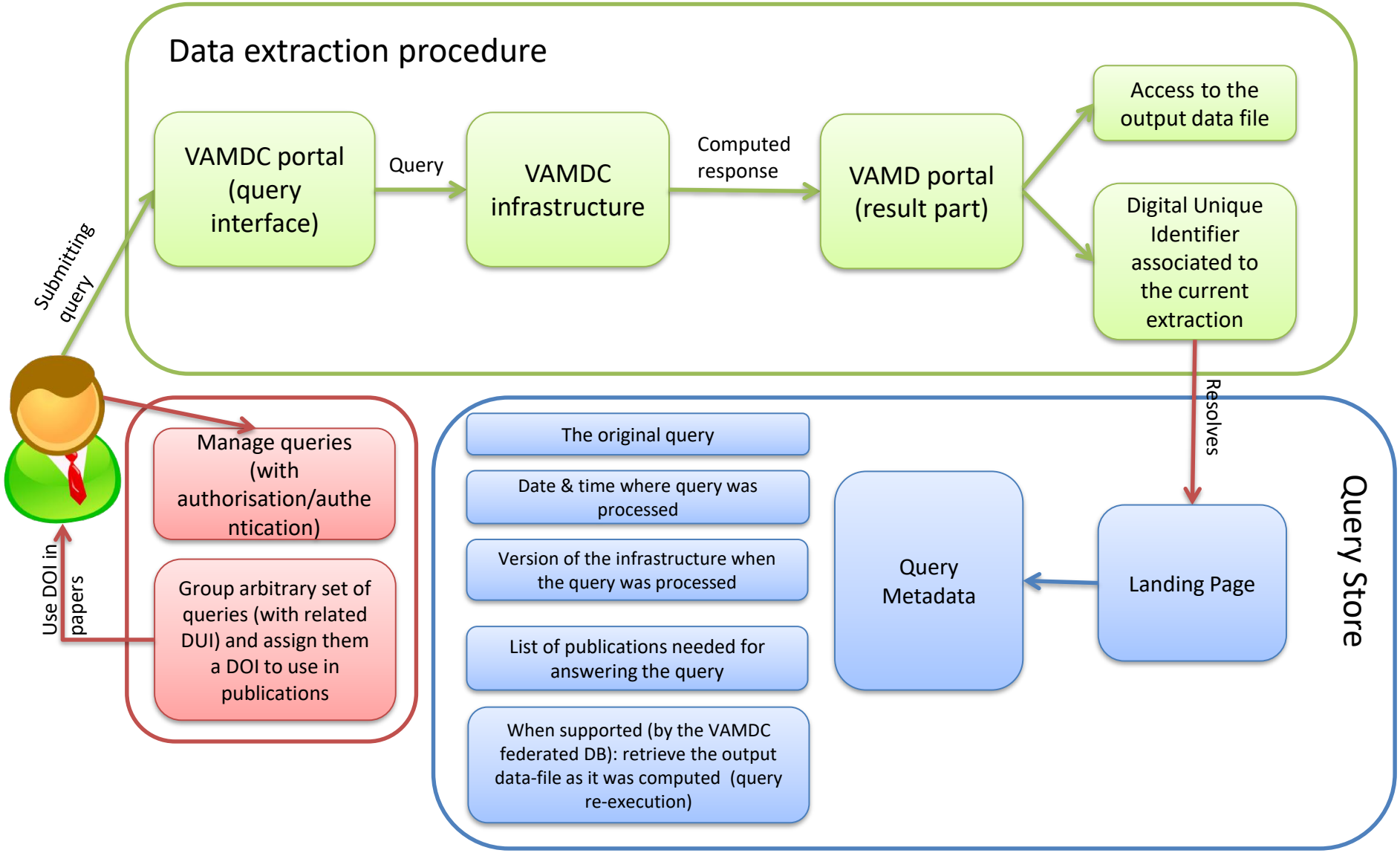

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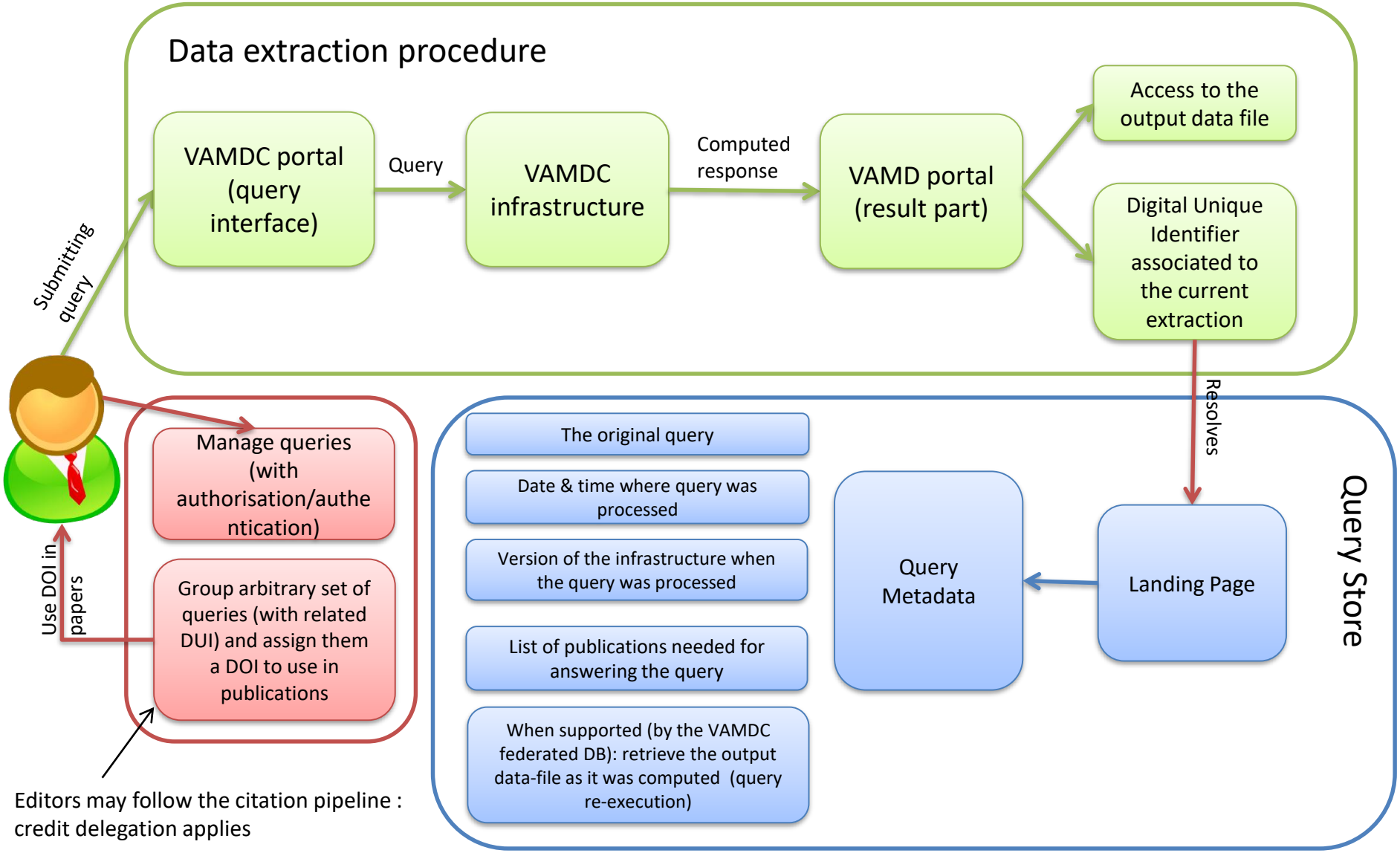

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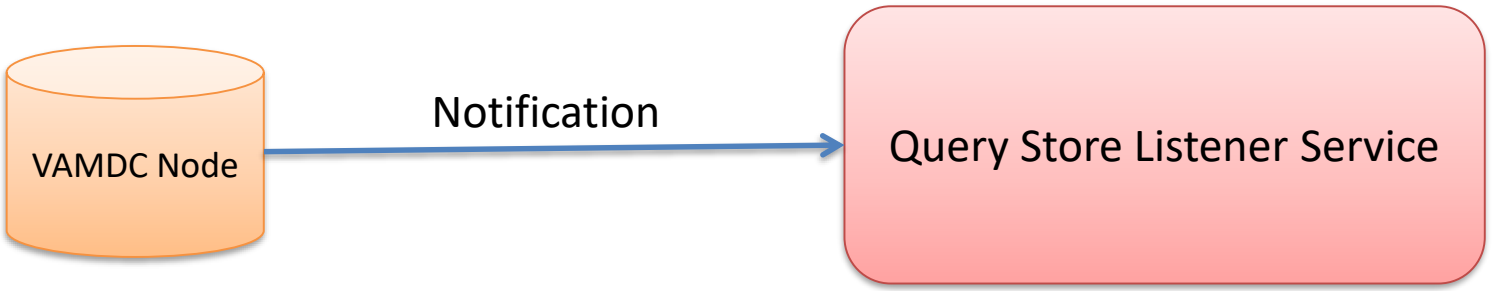

1 → When a node receives a user query, it notifies to the Listener Service the following information:

- The identity of the user (optional)
- The used client software
- The identifier of the node receiving the query
- The version (with related timestamp) of the node receiving the query
- The version of the output standard used by the node for replying the results
- The query submitted by the user
- The link to the result data.

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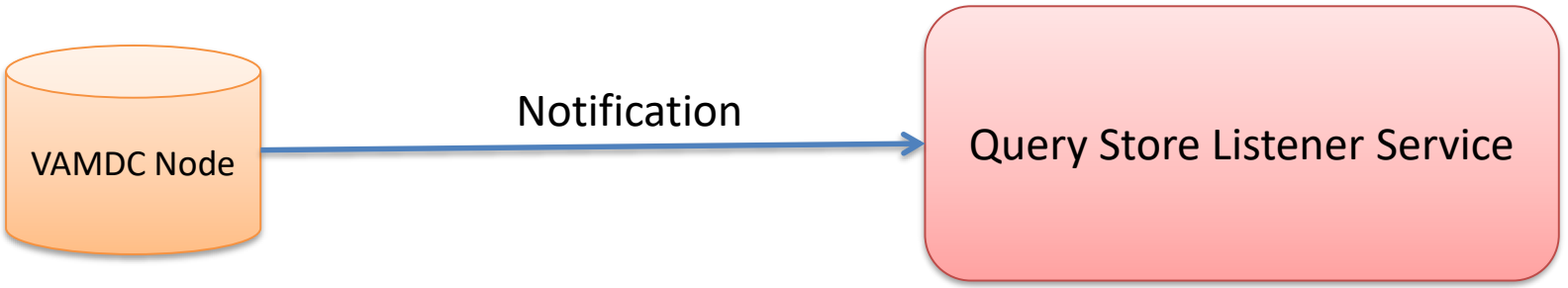

2 → For each received notification, the listener check if it exists an already existing query:

- Having the same Query
- Having the same node version
- Submitted to the same node and having the same node version

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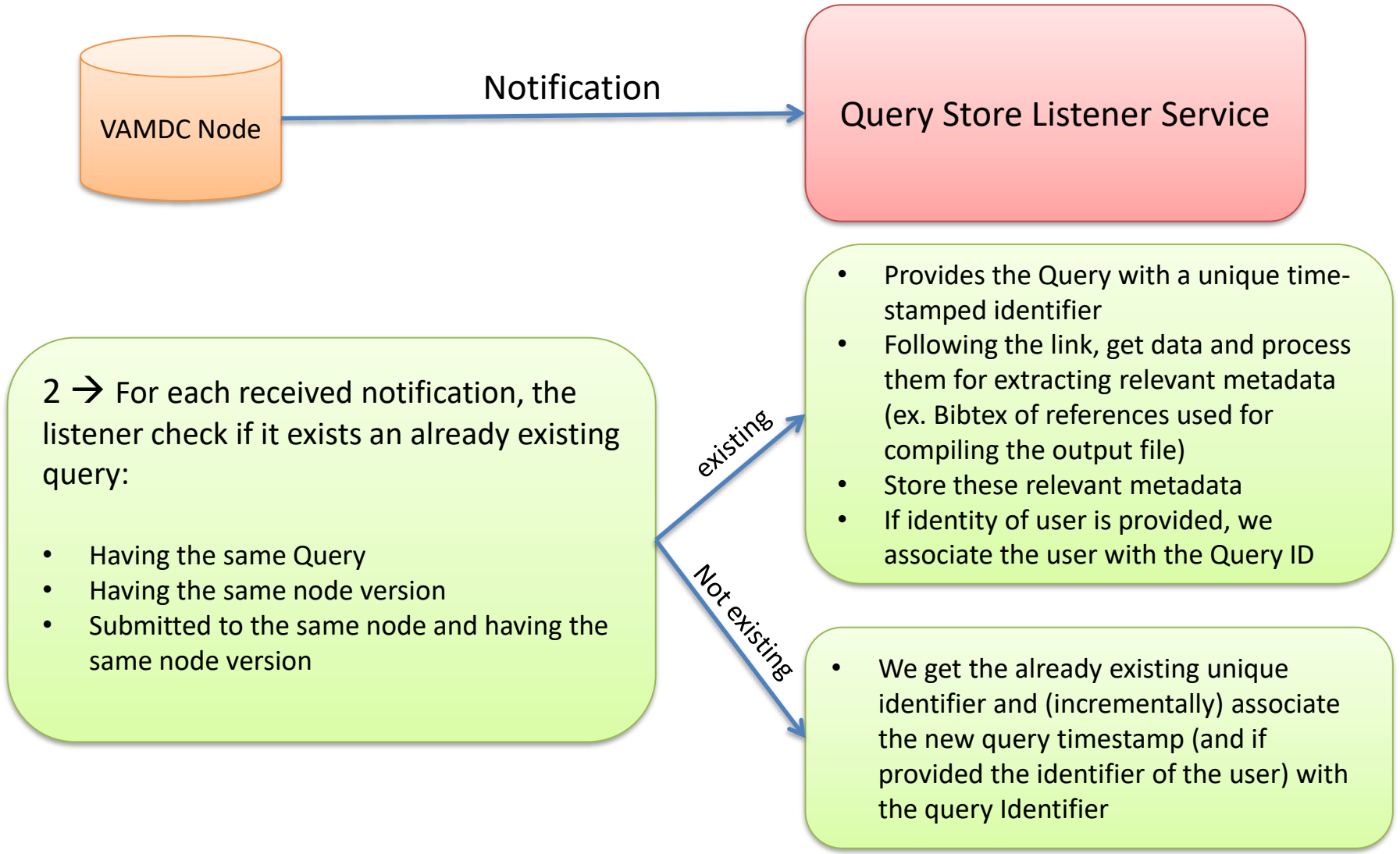

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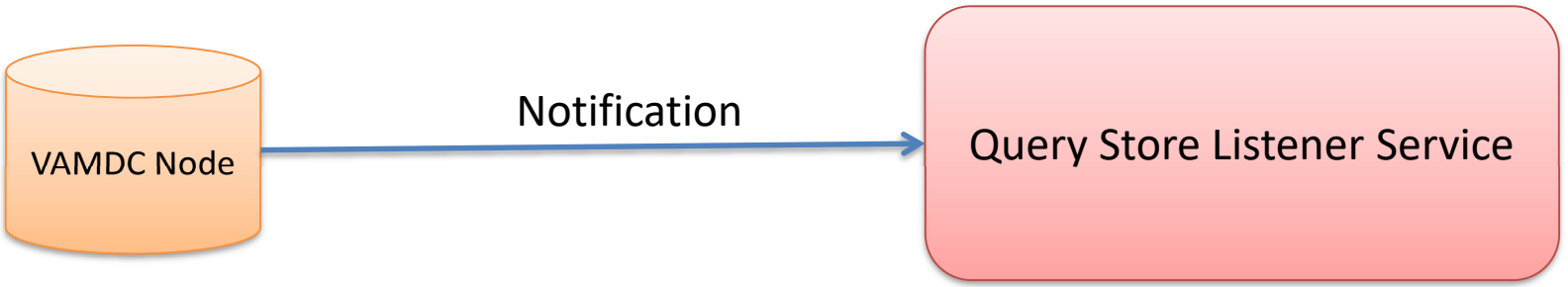

Remark on query uniqueness:

- The query language supported by the VAMDC infrastructure is VSS2 (VAMDC SQL Subset 2, http://vamdc.eu/documents/standards/queryLanguage/vss2.html).
- We are working on a specific VSS2 parser (based on Antlr) which should identify, from queries expressed in different ways, the ones that are semantically identical
- We are designing this analyzer as an independent module, hoping to extend it to all SQL.

Final remarks:

- Our aims:
  - Provide the VAMDC infrastructure with an operational query store
  - Share our experience with other data-providers
    - Provide data-providers with a set of *libraries/tools/methods* for an easy implementation of a query store.
    - We will try to build a generic query store (i.e. using generic software blocks)