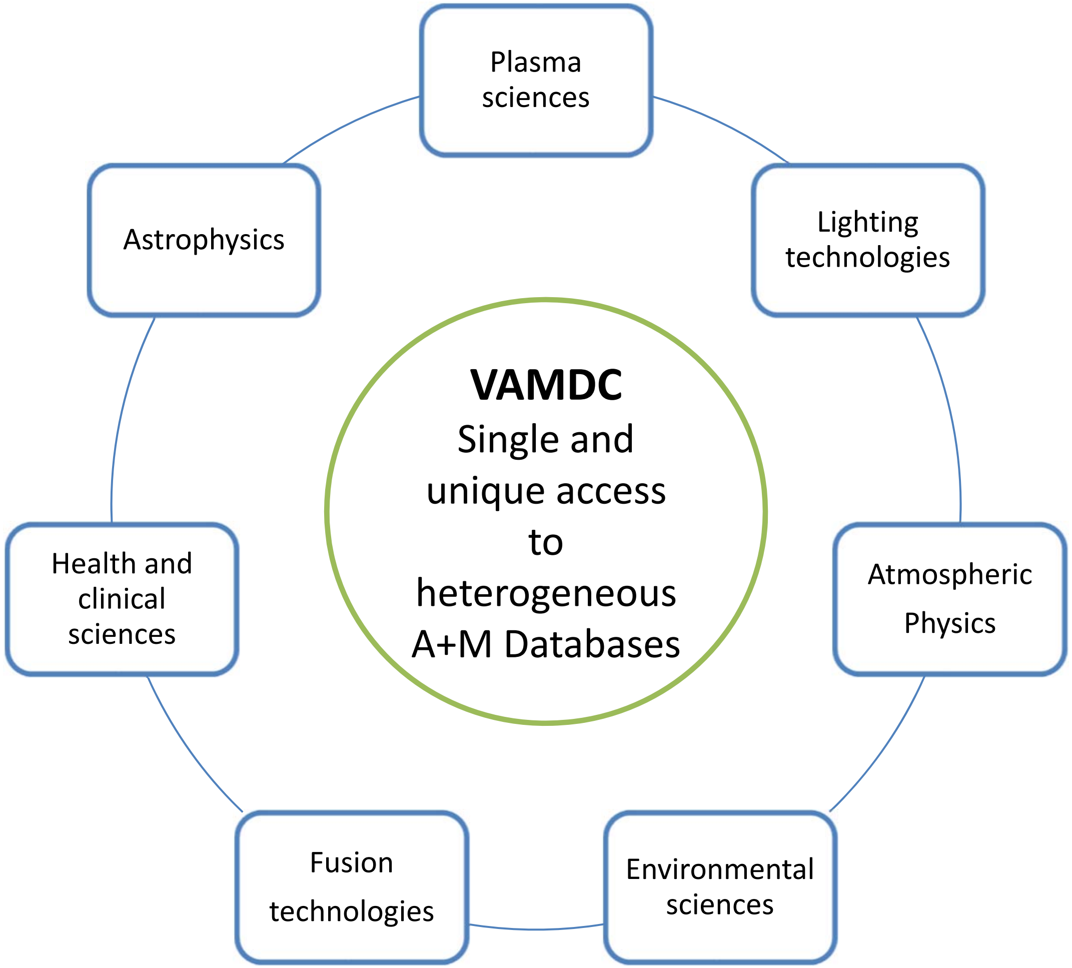
Implementing the RDA data citation recommendations in the distributed Infrastructure of the Virtual Atomic and Molecular Data Centre

C.M. Zwölf, N. Moreau and VAMDC consortium

VAMDC consortium

PADC
Paris Astronomical Data Centre

The Virtual Atomic and Molecular Data Centre



- Federates ~30 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.

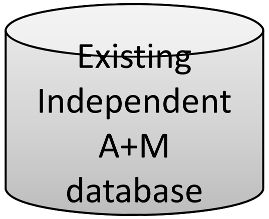
- The consortium is politically organized around a Memorandum of understanding (15 international members have signed the MoU, 1 November 2014)

- 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



Existing Independent A+M database

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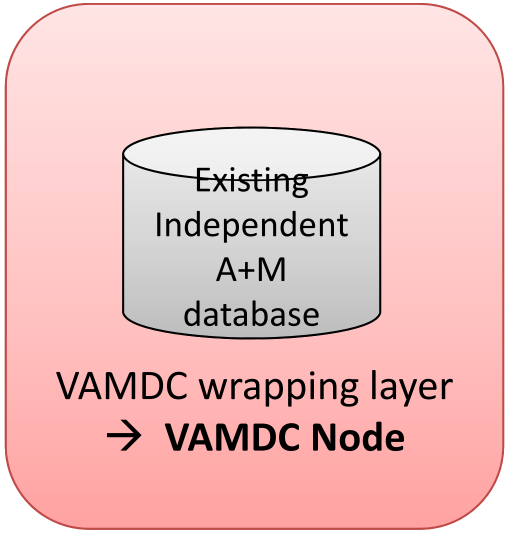
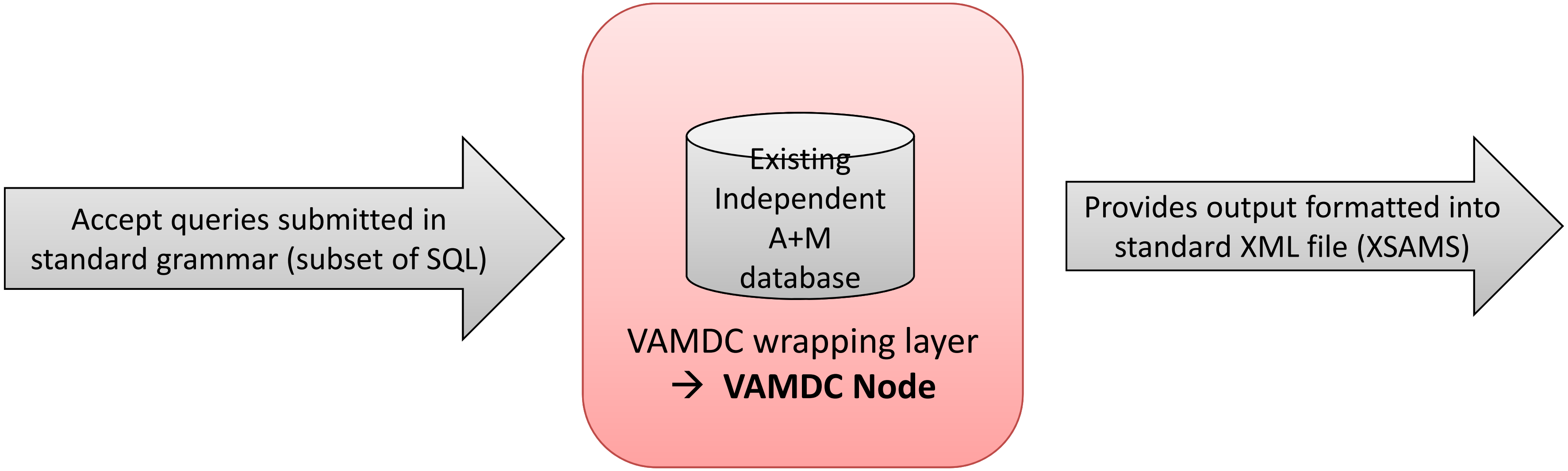


Existing Independent A+M database

VAMDC wrapping layer

→ **VAMDC Node**

The VAMDC infrastructure technical architecture



Accept queries submitted in standard grammar (subset of SQL)

Existing Independent A+M database

VAMDC wrapping layer

→ **VAMDC Node**

Provides output formatted into standard XML file (XSAMS)

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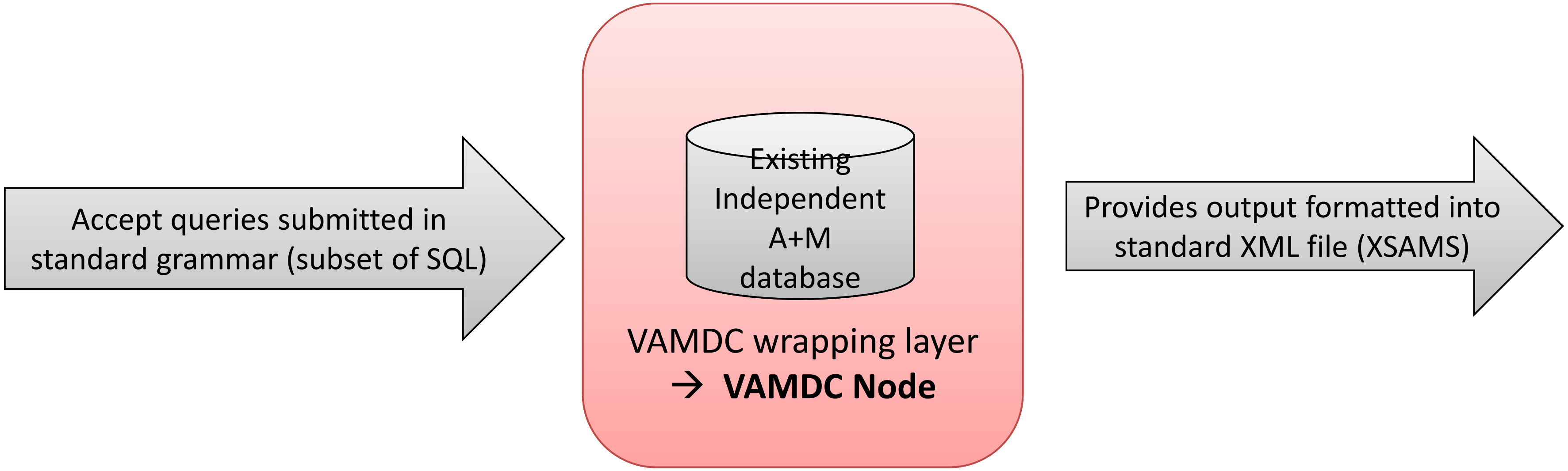

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Existing Independent A+M database

VAMDC wrapping layer
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Provides output formatted into standard XML file (XSAMS)

For further details, cf.
http://standards.vamdc.eu

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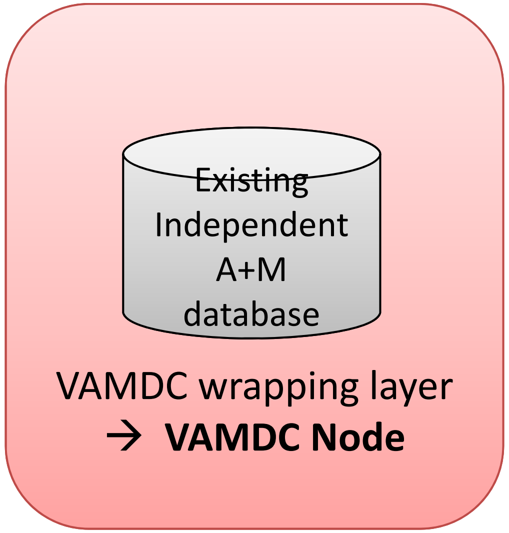
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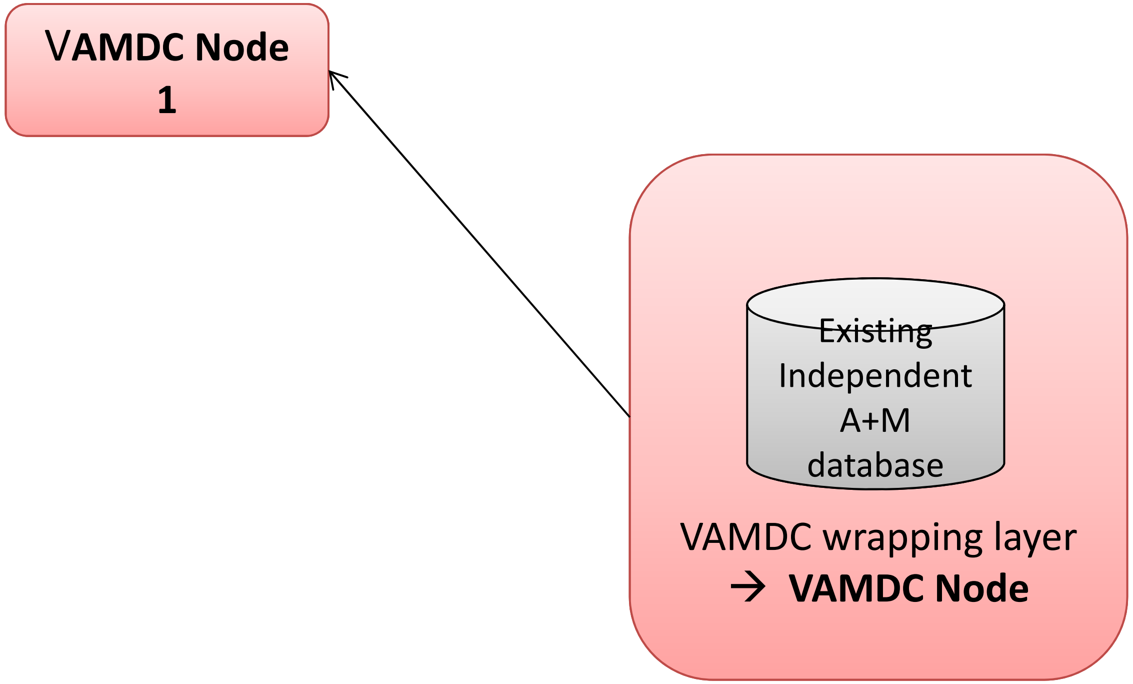

VAMDC Node 1

Existing Independent A+M database

VAMDC wrapping layer → **VAMDC Node**

The VAMDC infrastructure technical architecture

VAMDC Node 1

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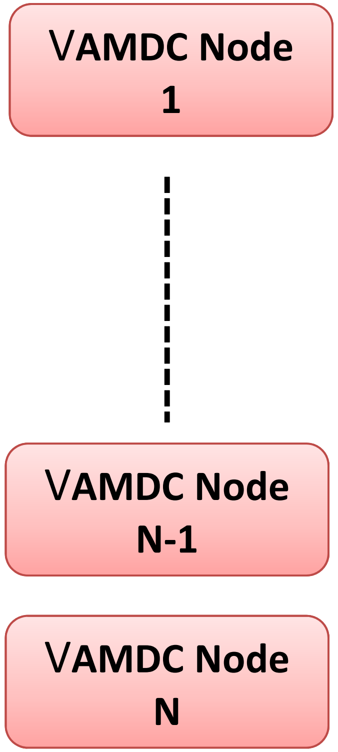
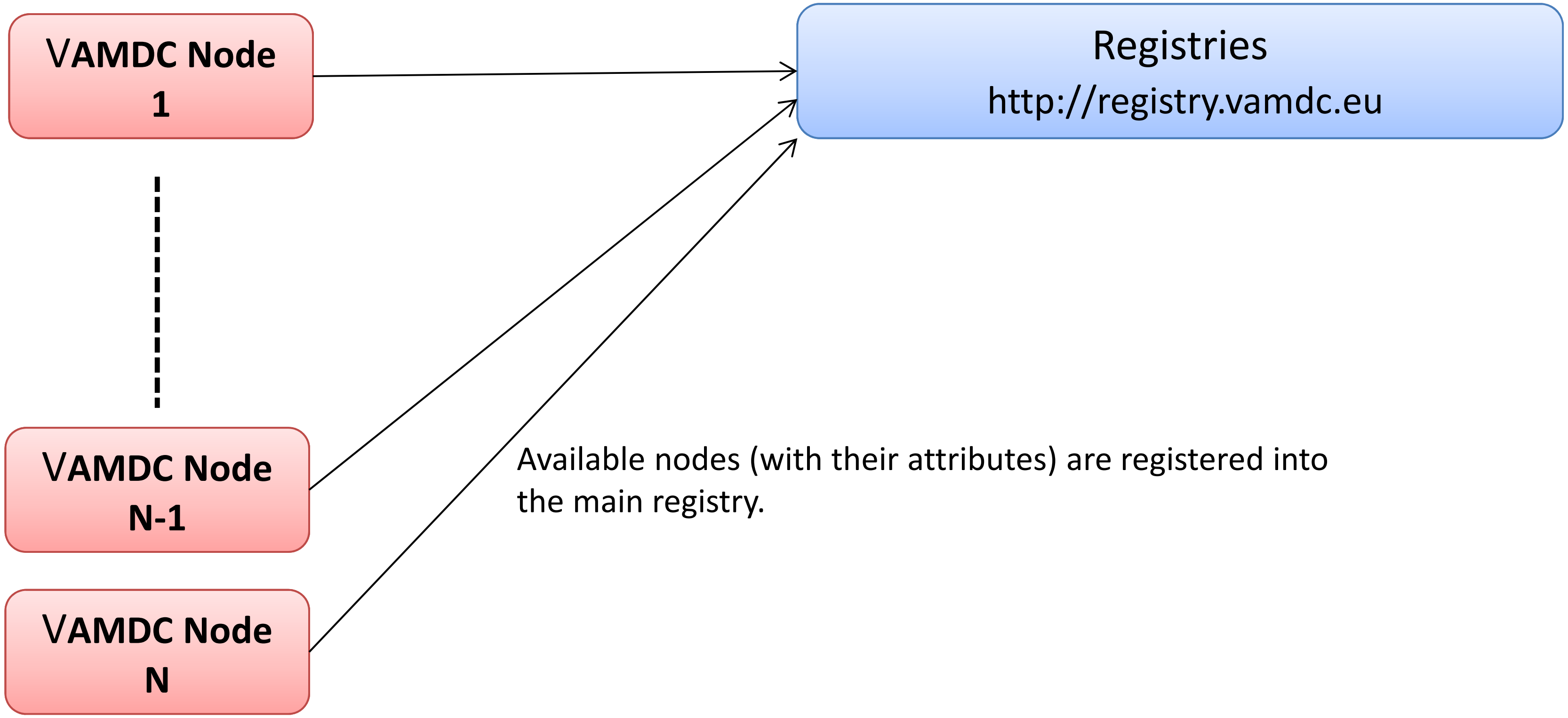


VAMDC Node 1

VAMDC Node N-1

VAMDC Node N

The VAMDC infrastructure technical architecture



Available nodes (with their attributes) are registered into the main registry.

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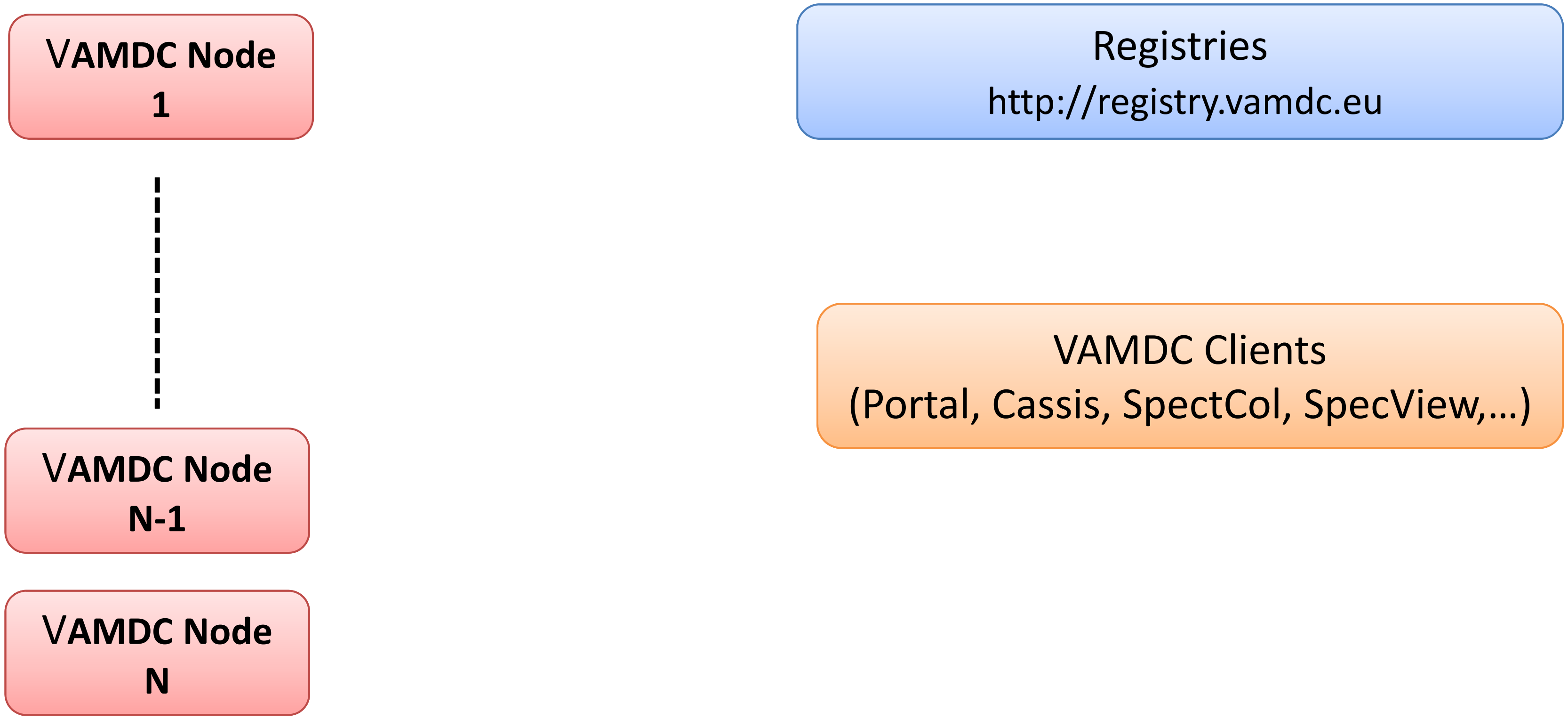

VAMDC Node 1

VAMDC Node N-1

VAMDC Node N

Registries
http://registry.vamdc.eu

VAMDC Clients
(Portal, Cassis, SpectCol, SpecView,…)

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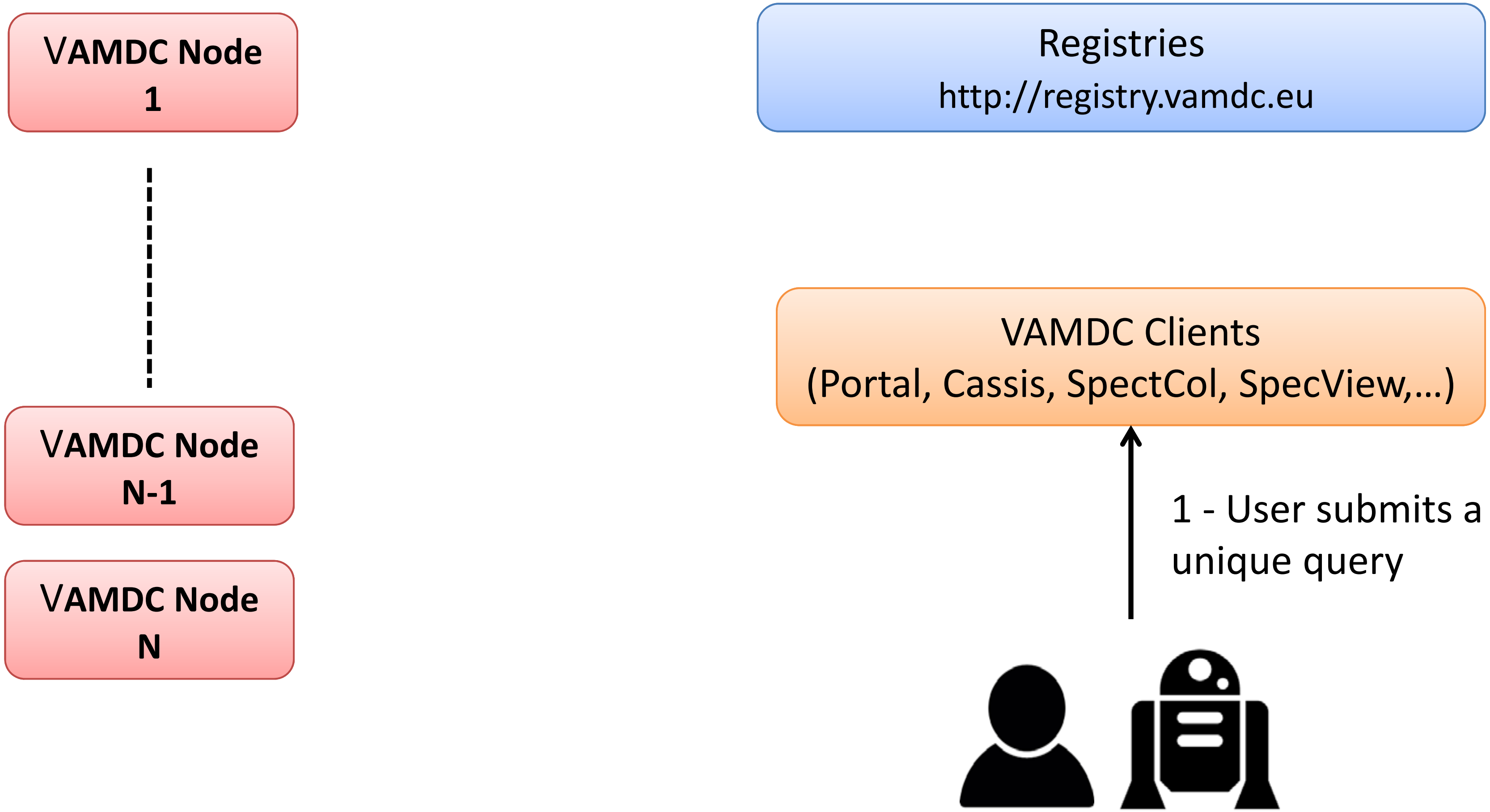

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1 - User submits a unique query

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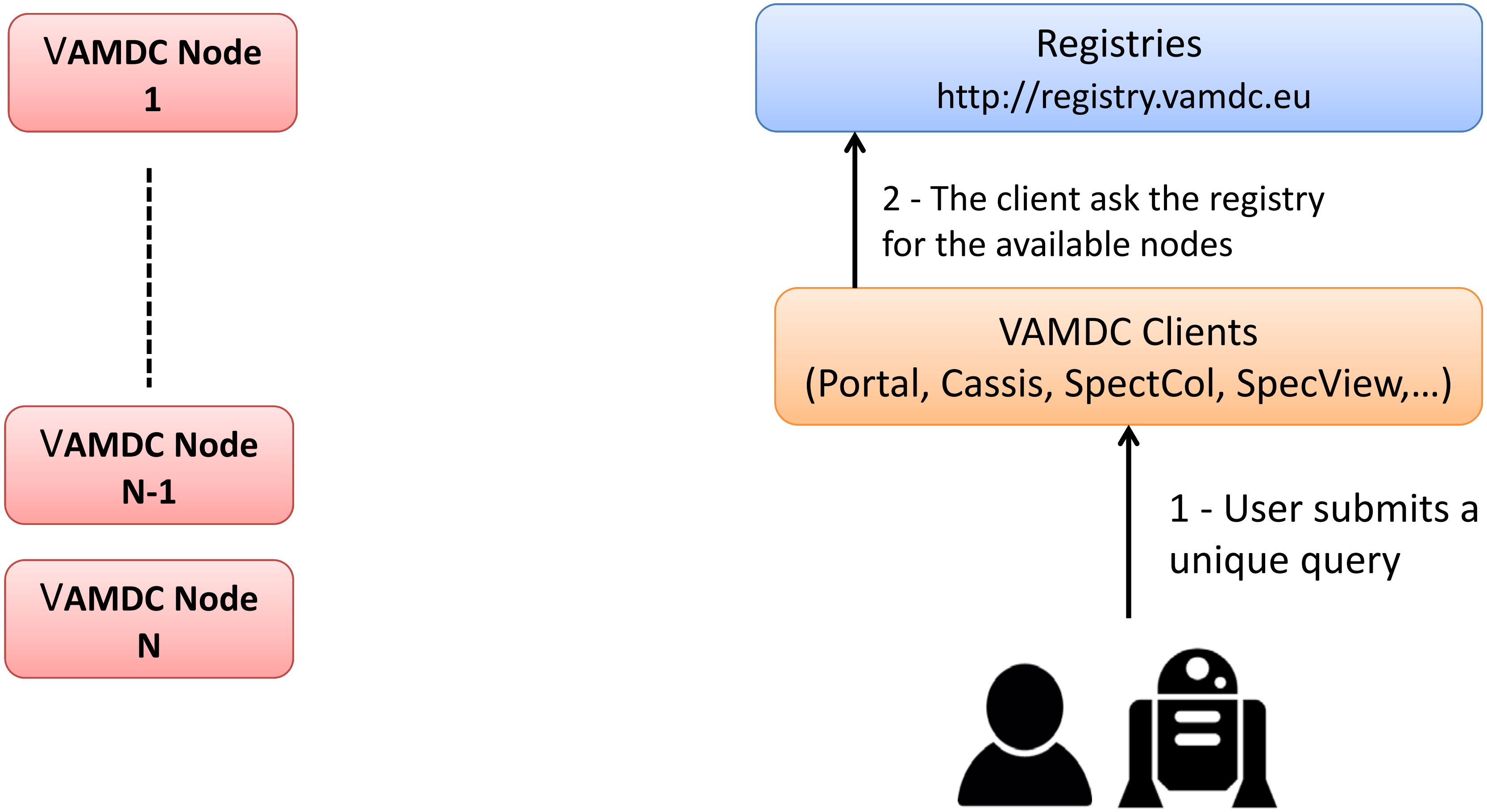

VAMDC Node 1

VAMDC Node N-1

VAMDC Node N

Registries
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2 - The client ask the registry for the available nodes

VAMDC Clients
(Portal, Cassis, SpectCol, SpecView,…)

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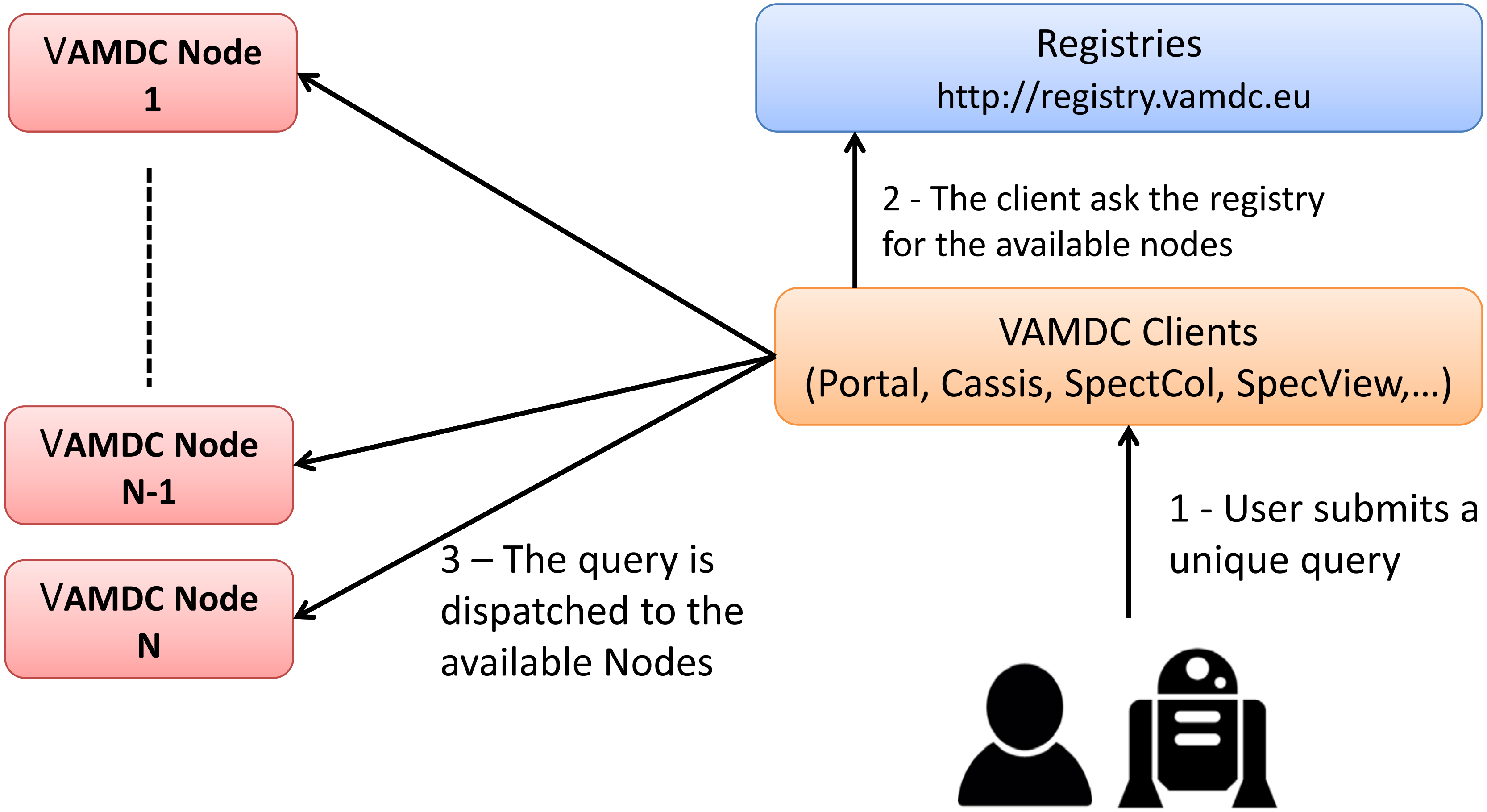
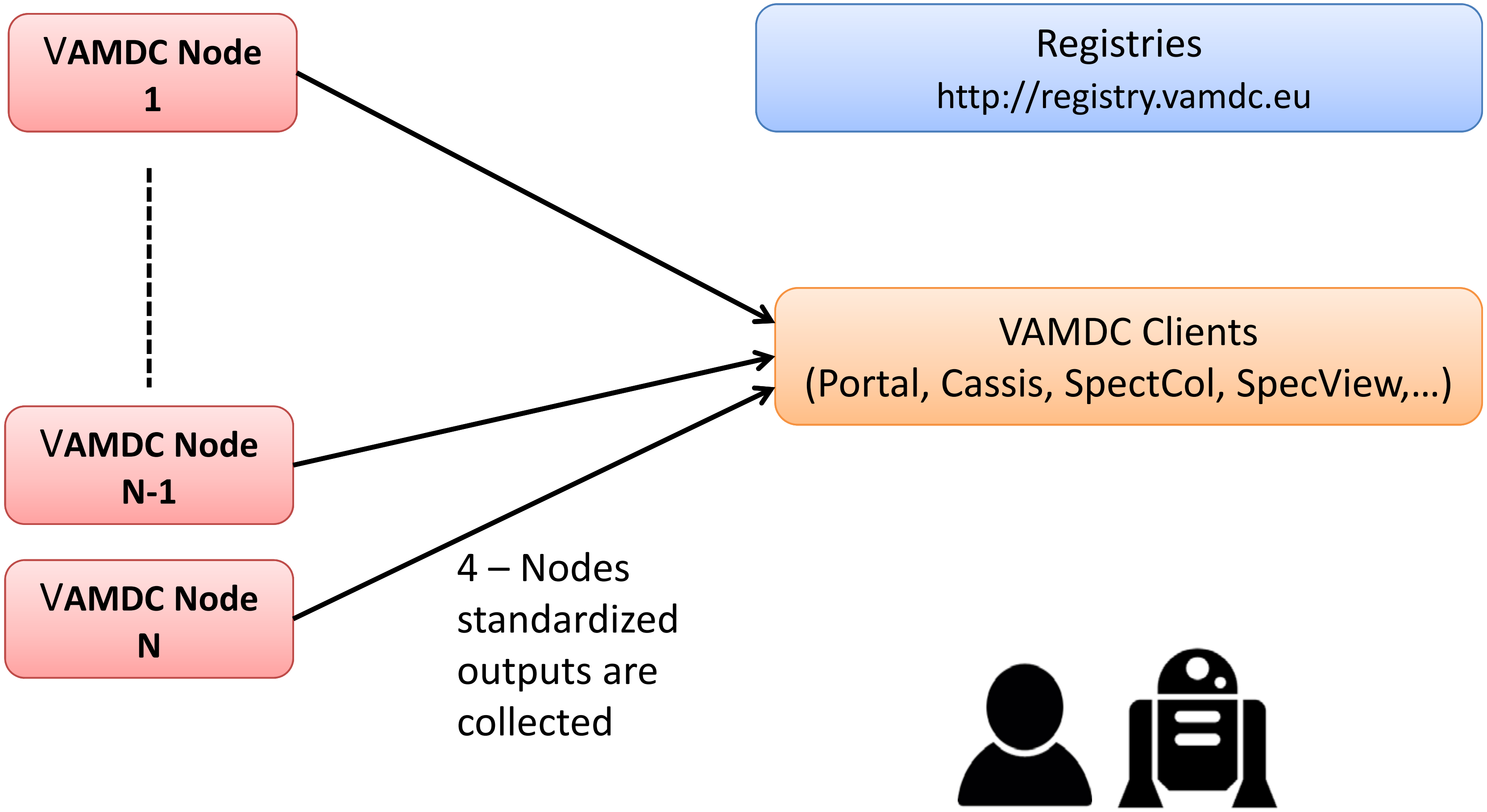


1 - User submits a unique query

2 - The client ask the registry for the available nodes

3 – The query is dispatched to the available Nodes

The VAMDC infrastructure technical architecture



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4 – Nodes standardized outputs are collected

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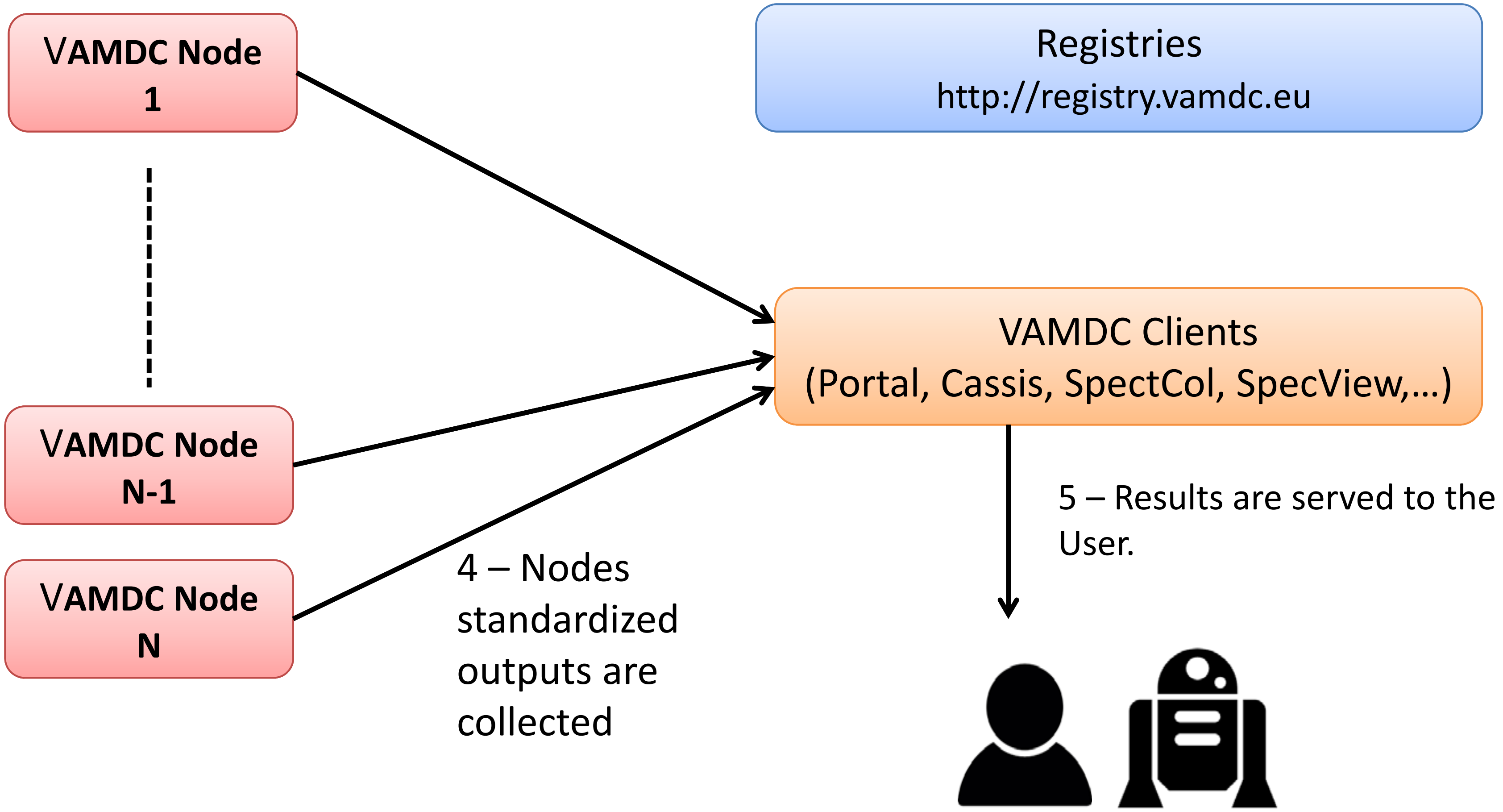

VAMDC Node 1

VAMDC Node N-1

VAMDC Node N

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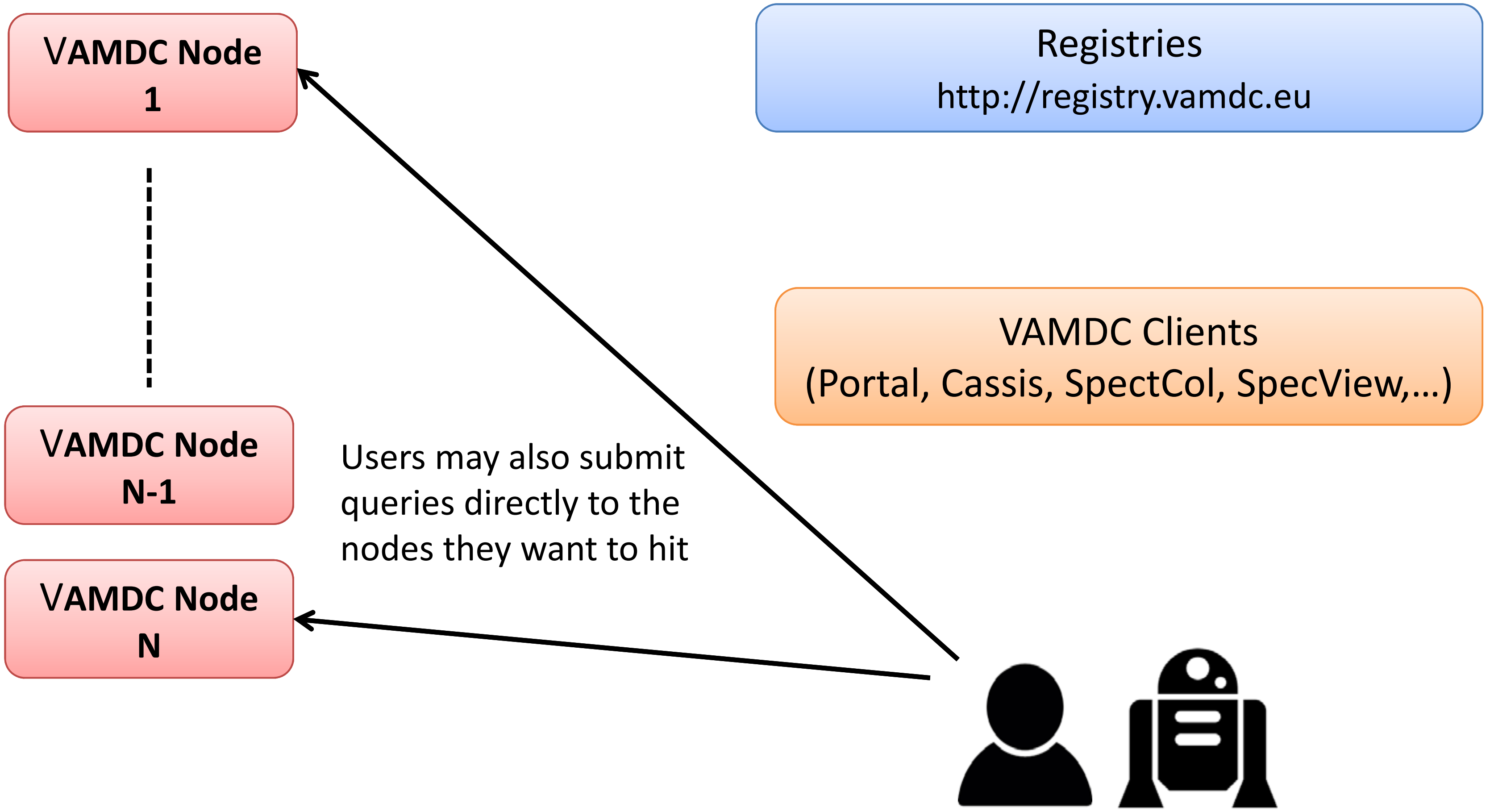
(Portal, Cassis, SpectCol, SpecView,...)

4 – Nodes standardized outputs are collected

5 – Results are served to the User.

The VAMDC infrastructure technical architecture



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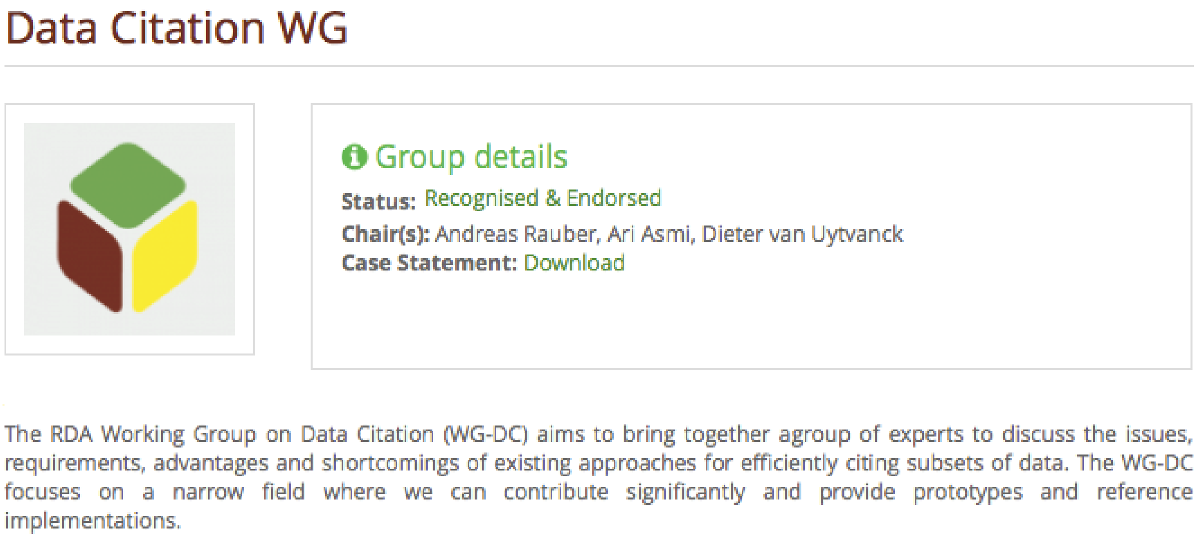
Users may also submit queries directly to the nodes they want to hit

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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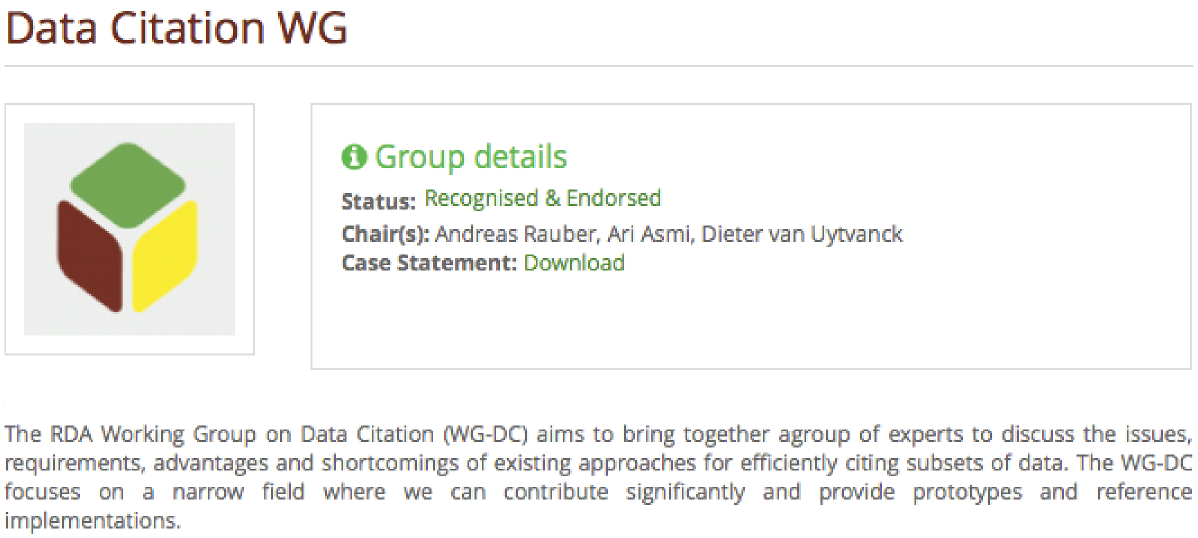

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- The RDA recommendations comes from standalone databases or warehouse.
- VAMDC is a distributed infrastructure, with no central management system.

Highlighting the main issues

How to build a Query Store in our distributed infrastructure?

- The solution belongs to a space with lot of constraints
  - Any choice will impact each of the ~30 databases federated by VAMDC.
  - Any technological change of the infrastructure must be validated by the majority of the members

The solution must cause least effects on the existing infrastructure and have minimal implementing cost for the database owners.

- This constraint suggest to fit the solution into the standard wrapping layer transforming an autonomous Database into a VAMDC node.

Highlighting the main issues

But the problem not only technical, it is **anthropological** too…

Tagging and versioning data

What does it really mean *data citation?*

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Tagging and versioning data

We see technically how to do that

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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What does it really mean *data citation?*

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.

Sketching the solution strategy

Implementation is 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**.

Query Store

Is built over the versioning of Data (the coarse-grained mechanism)

Is plugged over the existing VAMDC data-extraction mechanisms.

Due to the distributed VAMDC architecture, the Query Store may be seen as a smart log-service.

* http://dx.doi.org/10.1016/j.jms.2016.04.009
arxiv version at https://arxiv.org/abs/1606.00405

Let us focus on the query store:

The difficulties we have to cope with:

- Handle a query store in a distributed environment (RDA did not design it for these configurations).
- Integrate the query store with the existing VAMDC infrastructure.

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The implementation of the query store is the goal of a joint collaboration between VAMDC and RDA-Europe 3.

- Development started during spring 2016.
- Final product released during 2017.

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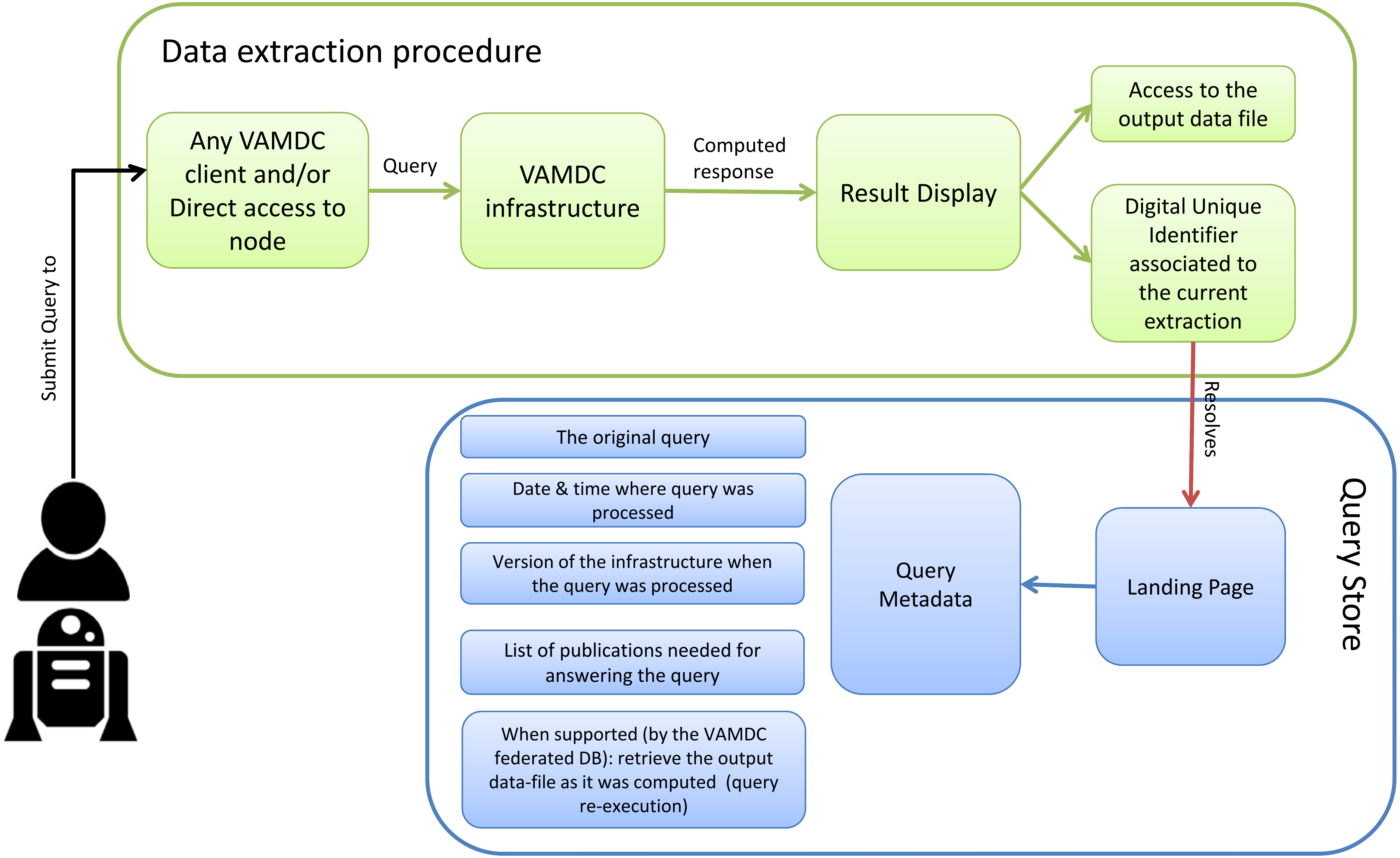
Collaboration with Elsevier for embedding the VAMDC query store into the pages displaying the digital version of papers.

Designing technical solution for

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

A functional overview of the Query Store

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



Data extraction procedure

Any VAMDC client and/or Direct access to node

Query

VAMDC infrastructure

Computed response

Result Display

Access to the output data file

Digital Unique Identifier associated to the current extraction

Submit Query to

Resolves

Query Store

The original query

Date & time where query was processed

Version of the infrastructure when the query was processed

List of publications needed for answering the query

When supported (by the VAMDC federated DB): retrieve the output data-file as it was computed (query re-execution)

Query Metadata

Landing Page

Strengths of the Query Store:

- The QS usage is transparent for users (complexity is hidden).
- Live monitoring of all the queries and users of the VAMDC e-infrastructure
    - Data providers may measure their impact and have detailed statistics of usage.
- It will be easy for authors to cite data coming from VAMDC. Credit to producers will be automatic.

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Minimal impact for federated database owners for dealing with the Query Store

Database owners just need to install the latest version of the VAMDC wrapping software

Data providers has to fill a “version” field (~ a simple string), which is just the version label.

- When the database is modified and/or data node software changes, the version label should evolve.

Remarks before the live demo:

- We provided the VAMDC infrastructure with a working Query Store
- The concept adopted and the implemented code are quite generic and both can be adapted to other use-cases:
  - If it worked in our complex distributed case, it may work in many contexts
  - The cost for adapting an existing service/database to a VAMDC-type Query Store is minimal
    - All the complexity is handled and masked in our generic software.

Live demo link: https://youtu.be/kDDWFpi22cU