Inside a VAMDC data node—putting standards into practical software

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Abstract
Access to molecular and atomic data is critical for many forms of remote sensing analysis across different fields. Many atomic and molecular databases are however highly specialised for their intended application, complicating querying and combination data between sources. The Virtual Atomic and Molecular Data Centre, VAMDC, is an electronic infrastructure that allows each database to register as a ‘node’. Through services such as VAMDC’s portal website, users can then access and query all nodes in a homogenised way. Today all major Atomic and Molecular databases are attached to VAMDC. This article describes the software tools we developed to help data providers create and manage a VAMDC node. It gives an overview of the VAMDC infrastructure and of the various standards it uses. The article then discusses the development choices made and how the standards are implemented in practice. It concludes with a full example of implementing a VAMDC node using a real-life case as well as future plans for the node software.

Keywords: databases, atomic and molecular physics, stellar atmospheres, data analysis, science infrastructure

((Some figures may appear in colour only in the online journal)

1. Introduction

The problem of analysing remote sensing data is encountered in a wide variety of scientific and technological fields, ranging from astronomy and climate research to computer tomography and movie production. Its solution requires detailed knowledge about absorption, scattering/reflection and emissivity of matter. This in turn builds on insight to the electronic and nuclear structure of atomic and molecular species, its dependence on the environment, as well as radiative and collisional processes leading to transitions between energy levels. Ray tracing, spectral analysis and other types of remote sensing tools are well-established in research and industry. By contrast, the collection of relevant atomic and molecular data has remained challenging. This is due to the heterogenous nature of individual data collections: atomic and molecular (A&M) databases are often created to serve very specific applications (e.g. modelling of stellar atmospheres) or as repositories storing the output from experimental or theoretical work by atomic physicists. Thus a particular data collection is often specialised not only in terms of content but also in terms of units, format and query language.

The Virtual Atomic and Molecular Data Centre (VAMDC, http://vamdc.eu) is an electronic infrastructure that solves these problems by providing standardised ways to both formulate queries and to retrieve data. All the data collections that are part of VAMDC, henceforth called data nodes, provide their internally heterogenous data in a commonly agreed-to, machine-readable form. VAMDC was originally created with support from an EU FP7 grant and is now maintained and further developed by a large international consortium. It offers atomic- or molecular data providers the possibility to quickly bring their results to their users. At the same time it provides the attributes of published work through including the valid references for proper citations. All major A&M databases are either integrated in VAMDC or support standards and protocols developed within this project.

To make uniform access to data possible, VAMDC maintains an infrastructure of web services. The VAMDC registry lists data nodes and other services together with their respective capabilities. This allows users and programs to find
resources and only select those containing the sort of data they need. Most visible from the perspective of the data-user community is the VAMDC portal\(^1\). The portal is a web interface that helps with formulating queries and collecting data from the connected data nodes. The portal also acts as an intermediary to services that process the machine-readable results; these services can perform calculations and export to various file formats or human-readable presentations. For a full overview, see Dubernet et al (2016).

In this paper we focus on VAMDC’s data provider infrastructure, consisting of the aforementioned data nodes. A node is hosted and maintained either by the data producer or by a group interested in collecting data from several sources. Each node may offer a wide variety of scientific data depending on its history and purpose. Regardless of its internal layout and content, a node can join VAMDC by implementing the interface defined by the VAMDC standards. This interface must:

- Understand queries formulated using the VAMDC query language.
- Produce data output in the standardised data format (XSAMS) used by VAMDC for data exchange.
- Implement the VAMDC application programming interface (API) to receive queries, to send back the results and to report additional information to clients and to the registry.

The node software is the software package supplied by VAMDC. It aims to help individual data nodes set up and operate. In the following we will first go into some detail on the VAMDC standards. We then describe the node software implementation and the intricacies that arise from balancing versatility, simplicity of use and performance at the same time. Finally we take an existing data node as an example to illustrate the node software in action and the process of using the -bundled publishing tools to import and update node data content.

2. The VAMDC standards for data nodes

The VAMDC standards are publicly available online at [http://standards.vamdc.eu/](http://standards.vamdc.eu/) and we refer the reader to that resource for all details omitted here. The purpose of this section is to summarise the parts of the standards that are particularly relevant to the node software and to highlight a few aspects that directly affect the implementation, as described in the subsequent sections.

2.1. The data format: XSAMS

Data returned by a node must conform to the XML Schema for atoms, molecules and solids (XSAMS). XSAMS originated at the International Atomic Energy Agency (IAEA) and is now maintained and further developed by VAMDC in collaboration with NIST. XSAMS defines a strict layout for where and how data is represented in the XML document. This includes for example how to describe atomic and molecular structure, processes like collisions or radiative transitions, as well as supplemental information such as environmental properties. In addition, associated references are included and cross-referenced within the XML structure. The top levels of the XSAMS structure are shown in a simplified form in figure 2.

XSAMS documents are validated against the schema. This ensures that the document is self-contained with consistent referencing (no dangling cross-references) and that no essential information is missing. The schema makes heavy use of its own types and classes to make sure that properties like data accuracies and evaluations are always represented in the same way.\(^2\)

VAMDC publishes its standards in an online dictionary\(^2\). The returnables section of the standard defines exactly how a node returning XSAMS should name a specific data property as well as what unit and data type should be used. For example, the life time of an atomic state must be identified as AtomStateLifeTime and be a float given in seconds.

2.2. The query language: VSS2

The query language that data nodes understand is called VAMDC SQL-subset 2 (VSS2). It consists of severely restricted SQL-like SELECT statements. VSS2 supports querying with binary operators (\(=\), \(\neq\), \(<\), \(\ge\), \(\le\), \(\sim\), \(\in\)) and IN as well as logical relations with AND or OR. Other standard SQL features, like BETWEEN, are not included in the SQL-subset. Instead of database column names, SELECT statements use keywords from the VAMDC standard dictionary in a similar way as described for XSAMS in section 2.1.

Below is a full example of a query for atomic lines in FeIII:

```sql
SELECT * WHERE RadTransWavelength = 858.4
AND AtomSymbol = 'Fe'
AND AtomIonCharge = 2
```

Note that there is no SQL FROM-clause in the above query. This is because the internal table structure is hidden from users. The query is written as if the data existed in one large in-line table. The keys used in the WHERE-clause in place of column names are called restrictables. Restrictables are derived from the XSAMS itself and thus generally correspond to a certain location in the data hierarchy. While the definition of a restrictable is fixed, it is up to each node to decide how to go about supplying it. For example, a given node may need to do convert units or perform an internal query against more than one database column or table.

It is important to note that, since XSAMS needs to be a self-contained document, one cannot expect to receive only the isolated data type specified in the SELECT-clause. That is, if the radiative transition we seek references a certain state which in turn refers to a certain ion, both the state and the ion must be included in the returned document for it to be valid XSAMS. The VAMDC dictionary however specifies a select

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1. [http://portal.vamdc.eu/](http://portal.vamdc.eu/)
2. [http://dictionary.vamdc.eu/](http://dictionary.vamdc.eu/)
number of requestables. One or several such requestables can replace the " wildcard in the query to request only a certain type of data. For instance, using the ‘species’ requestable in

SELECT species WHERE... will only return the atoms and molecules part of XSAMS. Leaving out the WHERE altogether will return all species that a node has data about.

The exact same query can be sent to any VAMDC data node. It is the node’s task to convert the standard keys into a query relevant to the node’s internal database. Each node also needs to specify and report just which keys are actually relevant for querying its data. This allows clients (like the VAMDC portal) to send a query only to nodes that can answer it, instead of gathering unnecessary empty results.

2.3. The API: VAMDC-TAP

A data node communicates with the world via HTTP, using GET/POST/HEAD requests. The definition of this web-API is known as VAMDC-TAP, where TAP stands for table Access Protocol. This, in turn, is a subset of the International Virtual Observatory Alliance TAP standard (Demleitner et al 2012). VAMDC-TAP is a RESTful API that operates on the basis of a single request and reply. No sessions are stored or maintained. There is no connection between subsequent queries and there is no authentication.

At the specified URI endpoint data nodes accept requests (HTTP GET/POST) containing a VSS2 query as described in section 2.2. If the request is instead made using HTTP HEAD, the node answers with statistics about the given query (in the form of HTTP headers). Such statistics include the number of species and processes that match the query as well as the expected size of the selected dataset. This allows gathering information without actually executing a potentially expensive query and subsequent big data transfer. This mechanism is used by the VAMDC Portal to gather preliminary statistics from all nodes. Nodes can choose to truncate the data if the result would be too large, reporting the truncation as part of the header return.

This is an example of a URI that uses VAMDC-TAP to query a data node:

http://<node-url>/tap/sync?
LANG=VSS2&
REQUEST=doQuery&
FORMAT=XSAMS&
QUERY=(VSS2-query)

The URI specifies the language, return format and the type of request. The QUERY parameter holds an SQL-like string as specified in section 2.2. This example accesses the tap/sync endpoint to initiate a synchronous query to the node, meaning that the data is returned right away, in the response to the same HTTP request. There is currently no asynchronous alternative to avoid blocking the server in the case of very expensive queries. This is planned for the next iteration of VAMDC-TAP and node software releases.

The VAMDC-TAP definition includes the additional administrative URI endpoints /tap/availability and /tap/capabilities. The former allows the node to report planned node maintenance or downtimes. The node’s capabilities, a short XML document, include information like the URL addresses to various services, the version of the node software used as well as sample queries for testing the node in question. The capabilities document also specifies which returnables (see section 2.1) and restrictables (see section 2.2) this node supports. This API can be accessed by tools like the VAMDC portal as well as by custom use-case-specific applications. It is also intentionally easy to script.

VAMDC offers processor services. A processor takes an URI with a query as input, like in the example above. It then fetches the data and processes it before presenting the result to the user. A complication arises in the form of the same-origin policy that web-browsers implement for security reasons. This means that browsers do not make cross-site requests unless the website or service explicitly announces that it is fine with accepting them. Since VAMDC is inherently distributed and the various parts of the infrastructure are meant to interact with each other at the user’s behest, data nodes thus need to announce their willingness to take cross-site requests. This is done by answering HTTP SERVICE requests with the appropriate HTTP headers according to the cross-origin resource sharing (CORS) standard.

3. Node software implementation

From the description of the VAMDC Standards above, it should be clear that there are obvious advantages with data nodes sharing a common software. The nodes need not only answer to the same API—incoming queries are also node-independent, as is the data output format that needs to be assembled for the reply. However, depending on the type of data they hold, nodes can be quite different internally. This concerns mainly the table layout of the underlying database and is reflected in the list of restrictables and returnables they support.

There are currently two implementations of the VAMDC standards for data nodes. One is built on the Python programming language while the other is using Java. All but two of the currently ~30 registered data nodes use the Python node software which is the subject of this paper. The Python node software can be obtained from its online git repository. It is released under the GPL version 3 open-source license.

Python is an open-source high-level language with a mature ecosystem of utility libraries. It is widely used within e.g. the astronomical science community and tends to be fast to learn for users with any previous programming experience. This has in our experience lowered the barrier of entry for data providers wanting to start up their own node.

3 https://w3.org/TR/cors
4 https://github.com/VAMDC/NodeSoftware
3.1. Django and data model abstraction

The Python implementation of a VAMDC Node relies on the Django web framework\textsuperscript{5}. Django is widely used as the underpinnings of professional large-scale websites, is actively developed and has an active community. It features a powerful and flexible object-relational mapping (ORM) which allows us to define a database schema and formulate queries to it using Python rather than SQL. This abstraction allows Django to support a wide range of different relational database engines. In effect, data providers already storing their data in an SQL database will likely find that Django can make use of it.

The database engine is not formally part of the node software, but MySQL with its MyISAM storage engine is used at many nodes. This also is the setup that has been recommended to new nodes that do not already have their data in a relational database. The recommendation still holds even though MySQL now uses InnoDB as default storage engine, because in our use-case with de-facto read-only access to the database, MyISAM has performance advantages once it has been set up.

Django’s abstraction layer between the database and the node software API implementation allows us to write code that is agnostic about a single node’s intricacies. This allows a large portion of the code to be reused by all data nodes. When a node has special needs that makes the common implementation insufficient, we add hooks where node-specific code can be plugged in.

The node software only uses a sub-set of Django’s capabilities. Still, it allows us to keep the code volume of the node software small: The core functionality is only some 1000 lines, plus another 2000 for the XML-generator. This has made maintenance and upgrades over the last seven years relatively easy, even when seen over many major Django versions. Similarly, the effort of porting the node software from Python 2.x to Python 3.x was measured in hours rather than days; both are now supported with the same code-base to ensure a smooth upgrade path for nodes.

The choice of Django has turned out to have a beneficial impact on several data nodes, beyond their involvement with VAMDC Django’s relative ease of developing new custom interfaces for data collections has allowed nodes to significantly improve their own web presence, often heavily tailored to their pre-existing user communities. Examples of this are seen with for example CDMS\textsuperscript{6} (Müller \textit{et al} 2005) and HITRAN\textsuperscript{7} (Rothman \textit{et al} 2013).

3.2. Publishing tools

Some atomic and molecular data are produced through \textit{ab initio} calculations of atomic and molecular energy structure, transition probabilities and collisional cross-sections etc. Other data come from experimental measurements of wavelengths, line strengths and lifetimes. Both approaches have advantages and problems. Occasionally, data producers merge the two e.g. by combining experimental lifetimes with theoretical branching ratios. In all cases, the new data comes in form of tables, often in peculiar units and with complex assessment of the quality.

A stand-alone part of the node software, dubbed the \textit{publishing tools}, parses such data and populates a new relational database for use by the VAMDC node. Figure 1 shows the top-level structure of the XSAMS output language the node is expected to return. For query efficiency the node should ideally try to organise its schema in a similar way. For example, the atom, molecule and transition data should aim to be separate database tables.

In the simplest case, the node data provider already has an SQL database with a useful schema. Django’s native \texttt{inspectdb} mechanism can use the existing database for creating the Django data model. These auto-generated Python classes usually only need small modifications before the node software can access the database properly. In particular, the

5 https://djangoproject.com
6 http://cdms.berkeley.edu
7 https://cfa.harvard.edu/hitran

\textbf{Figure 1.} Graphical overview of the VAMDC infrastructure.
foreign key relations between tables have to be transferred to the Django model.

However, in many cases the original data is either stored using some non-SQL solution or using a schema less optimised for VAMDC queries. This is where the publishing tools come into play: they can perform various operations on the data before inserting it into the node SQL database. The goal is to do as much work as possible at database creation, when execution time does not matter, instead of repeating work every time an incoming query is processed. Possible operations include, but are not limited to, proper parsing of near-arbitrary table formats, interpretation of header information, tagging of missing data, unit conversions and pre-creation of derived quantities that are useful in the XSAMS output.

The first step for doing this data import is to define the new (empty) database schema. The new schema is formulated using Django’s model classes. Each such class represents a table in the new database, including the relationships between them. Every instance of these classes is one record in the table. This model is then used to create the actual tables in the database, again granting nodes the flexibility to choose any of the database engines that Django supports.

The mapping of data from the old data store to the new database can be the most work-intensive part of setting up a VAMDC data node, depending on the original form of the data. This is done by writing a mapping file that contains a Python dictionary in a form understood by the conversion tool. It must be created uniquely for each node. The components of this dictionary describe how to read and parse the records of each input file into one or more output files. Multiple inputs can for example be combined into a single output or vice versa.

It is often not possible for the parser to work in parallel with all input files; for example, inter-table relations may not be possible to construct until all relevant files have been read. This requires multiple passes, something which is supported by the mapping mechanism. Since the mapping file can contain Python code, this process can be further customised with helper functions to account for any peculiarities in the input data. The publishing tool includes a set of functions for processing and handling common data formats.

Running the mapping file through the execution script produces a series of text files that exactly match the database schema—one file per database table with matching columns. These files can be efficiently read using the database’s own import functions. The syntax of this import is the only part of the node creation that depends on the particular choice of SQL database. For example, a user of MySQL would open the database client and execute:

```
mysql> LOAD DATA INFILE filename INTO TABLE table;
```

Once the mapping file exists, it is easy to re-run and tweak the process, or to add new data to the node at a later time. The publishing tools are not part of the day-to-day operations of the VAMDC node.

With the data loaded in the new database, one can set up additional database indices or perform other optimisations. This bit highly depends on the individual node’s database schema, size and engine.

Updates to the database schema often coincide with an update of the data itself, meaning that it can be convenient to simply use the publishing tools to recreate the entire database from an updated mapping file and input data files. If this is not desired or possible, Django comes with a very flexible system for database migrations, using small Python files that describe the changes to the database over time. These are executed in sequence by Django and, if written correctly, can even be used to revert changes and roll back to a previous version of the database in case of errors.

### 3.3. Receiving and executing queries

One of the two main tasks of the node software is to receive queries of the form described in section 2.2 above, and execute them on the node’s database.

In order to do this, the node software needs to be told which VAMDC restrictables correspond to what column in which table of the database. We implement this in the most straight-forward way, a Python dictionary where the key is the restrictable and the value is the name of the Django model and the relevant data field, concatenated by an underscore. This is the Django-internal way of referring to model fields and we
refer readers to the excellent Django documentation for more information. An example of this restrictables dictionary is shown in section 4. The point is that this dictionary connects the (node-independent) restrictable keywords to the (node-specific) names of the right table and column in the database.

An incoming VSS2 query is validated as a first step. We use the third-party package pyparsing\(^8\) to formulate an SQL-dialect strictly limited to the supported SQL subset. Rejecting any SQL statements except SELECT right away also offers protection from a large set of potential malicious queries.

The parsed and validated query is then handed to what we call a node’s *query function*. This is the only piece of Python logic that is custom to each node. The query function’s goal is to turn the input query into QuerySets. A queryset are Django’s internal objects representing the result of an SQL query. A queryset is *lazily evaluated*, meaning that the query is only executed on the database once the result values are accessed. This allows the query function to quickly set up the result and pass it on to the XSAMS generator which is described in section 3.4 below. Only then, as we describe below, will the database deliver data that get wrapped in XML and streamed directly to the user that initiated the query.

Nodes have, by design, near-total freedom on how to write the query function. Covering all of the complexity and subtleties of A&M data collections would not be possible. Thus the only constraint the system impose is that a node’s custom query function returns the appropriate QuerySets. Documentation and examples are provided to help data providers with this step and most nodes use the method described in the following.

The node software offers a utility to convert a (parsed and validated) query into a Django *Q-object*. Most nodes use this first thing in their query function. A Q-object is Django’s way of representing a *database-agnostic* query. It is suitable for direct interaction with Django’s ORM.

The next step is to apply the Q-object to the data model. This is where nodes differ largely. For example a node that contains atomic transition line lists is likely to first restrict on the transition model. It would then use the ORM to figure out the corresponding species and states along with the references that need to be attached. Other nodes might restrict the species first or use a totally different strategy.

As mentioned above, the query function returns QuerySets that can be used to populate the output XML document. Each QuerySet needs to correspond to a top-level organizational group of XSAMS, like atoms, molecules, transitions, collisions, sources and so on. The return value of the query function is therefore a Python dictionary where the keys identify the part of XSAMS to be used, and the values are the (yet to be evaluated) QuerySets. The names of the keys to be used are listed in the node software documentation.

The total overhead for receiving a query, parsing it and setting up the result, i.e. running a node’s query function, is typically below 0.5 s which is negligible compared to the total response time, especially for large queries. This means that nodes typically are responsive and start returning data soon after the query is initiated.

### 3.4. Generating XSAMS

The second main task of the node software is to take the data that comes from the database and put it into an XSAMS document (see section 2.1). In the previous section we described how nodes return QuerySets from their query function. These are passed directly into the node software’s XSAMS *generator*.

This generator is named such not only because it assembles the XSAMS data output, but also because it is a proper Python *generator* in the sense that it uses *yield* statements. Generators in Python are structures that can be looped over without being fully in memory when the loop starts. Expressions get evaluated only for the current loop element. This nicely matches the input QuerySets; only what is currently needed for the next piece of output gets fetched from the database and put into XML. Especially for large data set this is not only much more memory efficient, it also means less of a delay before the first piece of data is ready to return.

The main task of the XSAMS generator is to go through the different parts of XSAMS in turn, passing each loop through the QuerySet it received. Each iteration of the QuerySet produces an instance of the Django data model (a row in the database) and the generator accesses its fields’ values to build up the corresponding piece of XSAMS. We do not use an XML library or a document object model for assembling the XML. For maximum control we instead use plain Python string concatenations, placeholders and `'\s'.join()` on lists of strings.

In order to know which attribute of the current model instance needs to be mapped to which element or attribute of XSAMS, the generator needs the returnables dictionary. This is analogous to the restrictables dictionary from the previous section, but in the opposite direction. Again the dictionary keys are the (node-independent) keywords; these are hard-coded in the XSAMS generator to the proper XML-location. Since the list of returnable keys is derived from XSAMS, there is a one-to-one correspondence.

The values of the dictionary tell the generator how to access the (current iteration) model instance to retrieve the wanted information. We use an internal function called `GetValue()` for this, allowing nodes to fill the returnables dictionary values in several ways. Firstly, they can contain a static string, useful when a value is the same for all data and not even stored in the database (like units). Secondly, it can be the name of a model field in which case its value gets retrieved. Thirdly, it can be the name of a model field in a different model, connected by a foreign key relation; as common with Django, table traversal in models is possible by simply concatenating fields and foreign keys with periods.

The fourth possible option for filling the dictionary value is the name of a custom method on the data model. `GetValue()` calls this method and inserts whatever it returns into the current place in XSAMS. This allows for maximal flexibility, but for performance reasons nodes are encouraged not to use this if they can pre-calculate data instead. Note that

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\(^8\) This is the node software’s only additional dependency apart from Django and the Python driver for the database engine in question.
3.5. VAMDC-TAP implementation

The previous sections describe how queries are parsed and how the reply content is assembled. What remains is the implementation of the VAMDC-TAP API. Django offers a straightforward way to connect Python code to URL endpoints. Since the API is simple, a single view function per endpoint is enough. The capabilities and availability (see section 2.3) endpoints are implemented by rendering simple templates with a few configuration variables, using Django’s own template mechanism. For example, the keys from the returnables and restrictables dictionaries go into the capabilities to tell other parts of the VAMDC infrastructure which keys are understood by the data node in question.

The sync endpoint receives and answers queries. All this view needs to do is to call the query validation, the node’s query function and then pass its result to the XSAMS generator. Note that due to the lazy evaluation of both the query and the generator, the main queries have not yet run at this point and no XML is yet held in memory. Only when the XSAMS generator is passed to Django’s StreamingHTTPResponse does the whole machinery start churning and gradually producing the XSAMS document for the client. XSAMS documents can be hundreds of MB in size, this method has proven superior for our needs, compared to early attempts with Djangos templates or XML libraries.

The view-function behind sync also needs to distinguish between GET and HEAD requests, the latter allowing for returning statistics. In addition, incoming OPTION requests are answered according to CORS to allow cross-site requests (see section 2.3). Thanks to Django’s high-level tools for handling requests, the whole API implementation is only about 150 lines of code and therefore easy to understand and maintain.

3.6. Deployment

A data node’s performance depends to a large extent on the underlying database itself. However, the assembly of large XML documents can also become computationally expensive, not the least because the XSAMS generator is generalised for use by all nodes. Instead of spending effort on optimisation, it has proven beneficial for several nodes to replace the standard Python interpreter by PyPy⁹, an alternative interpreter employing just-in-time compilation for large gains in speed. Django and the node software run nicely with PyPy, including the recent PyPy3.

The node software must be run by an application server able to serve data over HTTP. Since data providers generally host their nodes themselves, the setup should be light weight and easy to manage. We recommend to use gunicorn¹⁰, an application server with minimal configuration. It is also written in Python and a common choice for deploying Django apps. Alternatives include Apache mod_wsgi and uWSGI. Nodes frequently choose set-ups that deviate from the recommendation, for example due to integration with other services on the same machine or local expertise with certain tools.

Furthermore, it is good practice to put a proxy between the application and the client. Its most important task is to offer gzip compression to clients (XML is highly compressible). The proxy can also do load balancing and provide HTTPS/TLS. The most common and recommended choice of proxy is Nginx¹¹ but again, data providers often choose whatever webserver they have running already. Caddy¹² is a relatively new webserver that can act as proxy, do compression and automatically handle free certificates for HTTPS, with minimal configuration effort.

4. A data node in practice: VALD

The Vienna Atomic Line Database (VALD, Ryabchikova et al 2011) stores atomic and molecular transition data of astronomical interest¹³. This section describes the process and experiences of using the node software to adapt VALD into a VAMDC data node.

VALD originally uses a custom binary storage method. Since the original VALD database will continue operation alongside its VAMDC counterpart, this data was extracted using VALD’s own tools into a series of text files:

- The species and their properties (charge, composition, ionisation energy, isotopic fractions, InCHI keys designation etc. Each record of this file also contain a unique species number.
- A list of transitions and the corresponding energy levels, sorted by wavelength. This file has two lines per transition containing transition probability, line

⁹ http://pypy.org
¹⁰ http://gunicorn.org
¹¹ http://nginx.org/en
¹² https://caddyserver.com
¹³ http://vald.astro.uu.se
broadenings and the upper and lower level description (energy, Landé factor, coupling model, term designations etc).

- A list of the quantum numbers for each level in the same order as the previous file (J, L, S, parity etc).
- A list of the custom reference-ID strings used in VALD, tied to a number identifier.
- A list of all data collections included in VALD identified by an id string. Often such compilation has an associated critical evaluation paper that contains valuable quality analysis work.
- A BibTeX file linking VALD’s reference-ID strings to actual BibTeX entries.

Note that no less than three different files are involved in tracking references making the import process quite involved.

The next step was to prepare the VAMDC database. As discussed in section 3.2, this is done using Django models, each representing a database table in the database. In the VALD case, the most relevant models are:

- **Species**, containing all species data like mass number, ionisation energy and identifiers. This model also holds a many-to-many relationship to other species if this is a part of a molecule.
- **State** describes all atomic or molecular states and references the species involved, the energy, Landé factor and quantum mechanical properties. Also the literature sources for the main properties are referenced.
- **Transition** contains the wavelength for each transition alongside references to the states and species involved. It also refers to all sources used for the data and which line list the transition data comes from.
- **Linelist** represents the line lists and sources used for every species. It also designates if the data was obtained through empirical observations, calculations etc.
- **Reference** stores the actual bibtex references for all data in the database.

This data model was then used by Django’s **migrate**-mechanism to create the tables in an empty database. With the database schema in place we now used the publishing tools’ mapping system to map the raw data files of VALD to the VAMDC schema. Due to the layout of the raw data files the mapper was set to read several lines simultaneously and collate the lines (or groups of lines) from each file to build an output record. The first pass created the records and the second established the relationships between the tables. For efficiency, a separate run created the many-to-many relationships as extra intermediary data files.

An important re-organisation of data was carried out at this stage. The original data inlines upper- and lower states as part of the transition record. The XSAMS data model instead separates states and transitions and lets the latter refer to the former. We therefore needed to de-duplicate states and create several output files from the same input file. The relation between the states and transitions also had to be preserved by generating unique keys tying them together.

Since VALD is a large database with 250 million lines, this conversion process is computationally quite heavy. Originally the idea was to have the node software mapper create Django database instances directly. This turned out to be both slow and memory consuming (since a full Python object must be created for each record). Creating intermediary text files that match the database schema (see section 3.2) turned out to be considerably faster and is now a part of the standard workflow. Furthermore we found that the import process benefited greatly from the use of the PyPy just-in-time compiling Python interpreter; we saw a speedup of up to a factor five. Consequently we kept using PyPy also for the node’s normal operation and recommend PyPy in the node software manual.

At this point the mapping tool had created a series of large text files, one for each database table. These files were read directly into the MySQL database using MySQL’s own load mechanism. This is fast as long as the database indices are not in place yet. Django can automatically create indices for certain fields but we chose to defer this until after loading the data. Then we also created additional database indices to speed up the most common types of queries.

With the database ready, we proceed with preparing the dictionaries to enable communication with VAMDC. The restrictables dictionary looks like this:

```python
'AtomSymbol': 'species__name',
'AtomMassNumber': 'species_massno',
...,
'Lower.StateEnergy': 'lostate__energy',
'Upper.StateEnergy': 'upstate__energy',
```

This allows the node software to convert incoming VSS2 request into a Django Q-object. On the left-hand side are the standard VAMDC restrictable keys. The right-hand side contains the corresponding model field name in Django format, using double-underscores __ to denote membership. In the example above, a request for AtomSymbol data leads to querying the name field of the species table.

Next is the query function. As described above, it receives the query and starts by converting the SQL into a Django Q-object. Because VALD is primarily a transition line list, our query strategy is to start from the transitions model and pass to it the Q-object, resulting in the (not evaluated) QuerySet for all matching transitions.

Reconstructing the QuerySets for states and references containing only the records needed for the selected transitions turned out to be slow for this particular database. So in order to prematureley evaluate the transitions-QuerySet we opted for a customised generator instead; the VALD node overrides the main function of the XML generator. Our custom version is a variant of the standard one. It uses all the sub-functions creating the XML but has one important optimisation: it starts outputting the transition data right away, before figuring out which species, states and references will be needed to make the data complete. During the loop over transitions, we collect the ID-keys in Python sets. These sets are then used in simple and fast database queries to retrieve the complementary data.
For queries close to the size limit this reduced the response time of the VALD node by up to a factor ten.

A drawback of this approach is that the VALD node no longer knows how much data it will include in a given request and cannot include statistics in the GET HTTP headers. To get the statistics headers from VALD an explicit HEAD request is needed. This was deemed to be an acceptable compromise for the increase in speed.

The VALD returnables dictionary used by the XSAMS generator to populate the XML looks like follows, making use of the full range of options described in section 3.4:

```
... 'AtomStateID': 'AtomState.id',
'AtomSymbol': 'Atom.name',
...
'RadtransSpeciesRef': RadTran.get_wave_r-efs()',
'RadttransWavelengthUnit': 'Å',
'RadttransUpperStateRef': 'Radtran.upstate_id',
'RadttransLowerStateRef': 'Radtran.lostate_id',
...
```

The VAMDC keys (on the left-hand side) tell the XSAMS generator where in XSAMS to place a certain value. The dictionary values are the constants, model fields or methods returning the content to insert. Note that we make use of Django’s features to access inter-table foreign keys through _id and use a custom model method for the non-trivial way that VALD handles references.

After this, the VALD node was operational and could be registered with the VAMDC network. An important aspect of the setup is that it’s easily repeatable and scriptable: when a new line list is added or a correction is done to VALD one can just re-run the process and get a VAMDC version with the latest update.

5. Concluding remarks

We have in some detail described the VAMDC Standards that concern data nodes, and the implementation of these protocols in practice. The software package that has been the topic of this paper strikes an illustrative balance between diverging requirements from different research groups and the goal to provide common tools that make common tasks easy. It is also a case where a successful web framework like Django becomes highly useful in science.

In summary, the node software carries out the tasks of

- Helping data providers importing existing data to a standard relational database schema, starting from almost arbitrary custom storage formats.
- Making it easy to repeat the process when set up once. Such situations occur when the data is updated/expanded or a new type of data is added to a node.
- Translating the VAMDC standard query language (VSS2) to the internal names/fields-units conventions at a given node.
- Converting the data from the node’s database to the VAMDC common output format (XSAMS).
- Providing the API access needed to make a data node operate within the VAMDC infrastructure, including registry information.

Since its inception, the node software has been developed by a small team of VAMDC consortium members who each are in charge of a data node. This means that developers and users overlap significantly and that flexibility and easy modification were always prioritised over user-friendliness. One can argue that ‘end users’ wanting to use VAMDC to retrieve data never need to use or understand the node software; it is used by data providers only. Nevertheless, significant effort has been spent into documentation, both in text and screencast video form, allowing new data nodes to be set up without significant input or help from the node software developers.

Since its initial launch, there have been several node software releases, marked with Git(Hub) tags. These follow the evolution of the VAMDC standards and have also often offered gradual but significant improvements driven by feedback from the data provider community or new requirements by an individual data node. These custom changes are merged into the main version control branch which is today considered a rolling beta release. The VAMDC standards themselves are stable and currently only evolve in a backwards-compatible manner. This means that unless a data node wants to make use of the latest features, it needs not upgrade in order to stay interoperable with the surrounding infrastructure. This fits well with the reality of data nodes; they are often run with very little manpower for oversight, maintenance and upgrades. To our knowledge this has not yet presented any problems, neither in terms of interoperability nor in security. Nevertheless we are currently preparing a release based on the latest long-term-support version of Django (1.11, April 2017). After release we will encourage all data nodes to upgrade the node software and the underlying stack to the latest version.

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Appendix: XSAMS example

This is an annotated example of an XSAMS document (see section 2.1) returned from a request of Ca lines between 5000.0 and 5000.1 Å. The return data is from the VALD database node. The output was shortened in places for brevity.

```xml
<XSAMDData xmlns="http://vamdc.org/xml/xsams/1.0" xmlns:xml="http://xml-cml.org/schema" xmlns:xsi="http://w3.org/2001/XMLSchema-instance">
```
This return concerns a radiative transition, which is identified using an ID internally consistent within this XSAMS document. Other parts of the document can then reference this as needed.

(EnergyWavelength)
   (Wavelength)
      (Comments) Vacuum wavelength from state energies (RIT2)
      (SourceRef) Bvald-K07
      (Value units = 'Å')5000.04125034
   (/Wavelength)
(/EnergyWavelength)

The wavelength and its units is given. It could reference a Method to show it is a calculated result but in VALD’s case this is instead noted as a comment and the reference to the source is given (later in this document).

(UpperStateRef ) Bvald-26696
(LowerStateRef ) Bvald-46769
(SpeciesRef ) Xvald-191

(Probability)
   (Log10WeightedOscillatorStrenght)
      (SourceRef) Bvald-K07
      (Value units = 'unitless')-3.607
   (/Log10WeightedOscillatorStrenght)
(/Probability)

Similarly, the transition will reference other parts of the XML document (the AtomicState) for the information about the upper/lower states involved in this transition. The transition probability is given with values, units and reference.

(Processes)
   (Species)
      (Atoms)
         (Atom)
            (ChemicalElement)
               (NuclearCharge)20
               (ElementSymbol)Ca
            (/ChemicalElement)
            (Isotope)
               (IsotopeParameters)
                  (MassNumber)40
               (/IsotopeParameters)
            (Ion speciesID='Xvald-191')
   (/Processes)

This describes the species (Isotope) that RadiativeTransition referenced above.

(IonCharge ) 0
(AtomicState stateID='Bvald-26696')
(Description) 3p6.3d.7f 3P'
(AtomicNumericalData)
   (StateEnergy)
      (SourceRef) Bvald-K07
      (Value units='1/cm')60690.2700
   (/StateEnergy)
   (LandeFactor)
      (SourceRef) Bvald-K07
      (Value units='unitless')1.41
   (/LandeFactor)
   (AtomicNumericalData)
      (AtomicQuantumNumbers)
      (Parity)odd
      (TotalAngularMomentum)1.0
   (/TotalAngularMomentum)
   (AtomicComposition)
      (Component)
         (Configuration)
            (AtomicCore)
               (Term) 3p6.3d.7f 3P'
            (/AtomicCore)
         (/Configuration)
         (Term)
            (LS)
               (L)1
               (S)1.0
            (/LS)
         (/Term)
   (/AtomicComposition)
(/AtomicState)

The entirety of the Ion State 3p64d.7f 3P' is described, along with its quantummechanical data. The measurements of its energy and lande factor both come with references to which sources they are coming from. Note that more States would follow after this one.

(InChI) InChI=1S/Ca (/InChI)
The node software will always return a ‘self-reference’ as part of the XSAMS document. This details which query produced this result and is intended primarily for the end user to be able to reproduce their query. It could also potentially be used for bug reporting.

<Source sourceID=’Bvald-2017-02-20-14-58-15’>
Comments
This Source is a self-reference. It represents the database and the query that produced the xml document. The sourceID contains a timestamp. The full URL is given in the tag UniformResourceIdentifier but you need to unescape ampersands and angle brackets to re-use it.
Query was: select * where (RadTransWavelength >= 5000.0 AND RadTransWavelength < 5000.1) AND ((AtomSymbol = 'Ca'))
</Comments>
</Source>

The source reference contains all necessary components for properly crediting the data, including an optional BibTeX field. Note that parts of this entry has been cropped.

</Source>
</Method>

This is an example of the node providing more information than necessary—this method is not referenced from anywhere in the XSAMS document but is still included (other methods have been cut out to shorten the listing).

</Method>

<Methods>
  (Function functionID=’Fvald-stark’)
    (Name) Stark Broadening (/Name)
    (Expression computerLanguage =’Fortran’)
      gammawaal ’ (T / 10000.0) ’” (1.0/6.0) ” N
    (Expression)
    (Y name = ‘gammaL’ units = ‘1/cm3/s’ )
    (Arguments)
      (Argument name = ‘T’ units = ‘K’)
      (Description) The absolute temperature, in K
    (Description)
    (Argument)
      (Argument name = ‘N’ units = ‘1/cm3’)
      (Description) Number density of neutral perturbers (/Description)
    (Description)
    (Argument)
      (Arguments)
        (Parameters)
          (Parameter name = ‘gammawaal’ units = ‘1/cm3/s’)
          (Description) Lorentzian FWHM of the line
        (Description)
        (Parameters)
        (Description) This function gives the temperature dependence of
          Stark broadening. (/Description)
      (Function)
</Function>

</Methods>
</Description>
</Source>
</Authors>
</Source>
</Authors>
</Source>

(UniformResourceIdentifier )http://kurucz.harvard.edu/atoms/1400/gfemq1400.pos (!...–)

(BibTeX )@misc{K07, Author = {{Kurucz}, R.L.}, Title = {{Robert L. Kurucz on-line database of observed and predicted atomic transitions}}, year = 2007, Bdsk-Url-1 = {http://kurucz.harvard.edu/atoms/1400/gfemq1400.pos, ...}}

(Source) http://vald.isinasan.ru/vald-node/lap/sync?LANG=VSS2&REQUEST=doQuery&FORMAT=XSAMS&QUERY=select+’+where+’%28Rad-TransWavelength+%3E%3D+5000.0+AND+RadTransWavelength+%3C+3D+5000.1%29+AND+%28%28AtomSymbol+%3D%2B27Ca%27%29%29+

(UniformResourceIdentifier)
The function block can offer functional code in computer language or other representation. Multiple other functions would follow this one.

```xml
<Environments>
  <Environment envID='Evald-stark'>
    <Comments>A given gamma can be scaled with gamma = gamma_given * (T / T_ref)¹/⁶ * number density of free electrons.</Comments>
    <Temperature>
      <Value units='K'>1.0E4</Value>
    </Temperature>
    <TotalNumberDensity>
      <Comments>The broadening parameters are given in Hz per number density (i.e. 1/cm³/s), so they can simply be scaled with the number density. Note that unless otherwise noted, log10(gamma) is given.</Comments>
      <Value units='1/cm³/s'>1</Value>
    </TotalNumberDensity>
  </Environment>
</Environments>
```

Again, additional environment sections were cut for brevity.

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