The Astro-WISE datacentric information system

K. Begeman · A. N. Belikov · D. R. Boxhoorn · E. A. Valentijn

Abstract In this paper we present the various concepts behind the Astro-WISE Information System. The concepts form a blueprint for general scientific information systems (WISE) which can satisfy a wide and challenging range of requirements for the data dissemination, storage and processing for various fields in science. We review the main features of the information system and its practical implementation.

Keywords Data grid · Grid computing · Information system · Middleware

1 Introduction

Digital astronomical catalogues have been built from the very first moment information technology enabled this, e.g. the first Abell catalogue of clusters of galaxies was digitally prepared and printed in the days minus signs were not available in print [1]. As soon as digital scanning devices became available photographic material was scanned and first large image surveys were digitally published, such as ESO-LV [2] and the digitized sky surveys like DPOSS [3],

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succeeded by the Palomar-Quest Survey [4], in the 90’s followed by CCD-based surveys such as the 2MASS survey [5], the Sloan Digital Sky Survey SDSS [6].

The rapid accumulation of astronomical digital data and its public dissemination was, compared to other disciplines, achieved at an early stage, thanks to an open and collaborative astronomical world community who adopted the FITS image data format as early as 1979 [7].

The CDS, initially Centre de Données Stellaires and later renamed into Centre de Données astronomiques de Strasbourg took the lead in Europe to collect and disseminate the ever growing data sets of a zoo of astronomical observatories and projects. VizieR webservice nowadays provide access to over 9,000 catalogues. Numerous astronomical data centers followed, developing specialized services, for example, the Infrared Processing and Analysis Center and the bibliographical SAO/NASA Astrophysics Data System.

In the early 2000’s it was realized that the ever growing data volumes require new approaches: the community becomes the data provider and the International Virtual Observatory and its European branch, the European Virtual Observatory, developed standards and interfaces to allow individual data centers to publish their catalogues and images in a common framework providing worldwide access to users who can query, cross-match and visualize multiple databases via the internet. A highlight formed the overplotting of data from different experiments, like X-ray satellites and optical ground-based observatories with some keystrokes on the Aladin interactive software sky atlas.

While the Virtual Observatory focused on the dissemination of published data it was also realized in the early 2000’s that the upcoming data deluge required a new approach to the handling of the data stream from the telescope to the science-ready result. Modern experiments not only involve more data, but also require increasing precision on the various calibrations. The dependency of the final result (sometimes only a few numbers, like cosmological parameter values) on time-variable calibrations of very large data sets, involving the evaluation by large research teams distributed in smaller groups over various sites sets the basic requirements to the system handling the data. While in classical systems data is delivered in various releases to the public, often re-processing the whole set with higher versions of the code, the high data rates of modern experiments require an alternative approach, where the up-to-date result is derived on demand by the user.

Thus, we set out to design and implement an integrated datacentric system Astro-WISE in which the processing, storage and administration is integrated in a single environment, providing a living system to both the data producers and the customers. Early reports of this development and implementation have been given in [8, 9]. To reach this goal, traceability of each individual data item handled by pipelines or any piece of code is carefully maintained, every data item beyond pixel value is kept as Metadata and made persistent and distributed in a relational database with an object-oriented view, mapping all the dependencies.
2 Datacentric approach to data processing

The datacentric approach makes it easier for scientists to cooperate in data analysis and mining by means of the internet, nowadays referred to as e-science. The Astro-WISE information system connects to an own developed distributed grid processing system (based on Distributed Processing Unit, DPU), but has also been connected to the EGEE/EGI/BiGGrid-Grid [10], particularly for the operations of the Lofar radio telescope. Nowadays, this aspect of the system is referred to as cloud computing, but the Astro-WISE datacentric approach at the same time facilitates the sharing and web hosting of all the data handled by the system.

Today, we are just taking the first small steps towards the development of approaches and systems who could handle the upcoming data deluge. The way of managing and administrating the data will be key, and will require ever improving, refining and self-organizing approaches. The key notion is that a fruitful approach towards handling the data deluge focuses on the administration, modeling, standardizing and tracking of the data rather than on the processing of the data by CPUs. This is a datacentric approach, in which the design of operational systems is driven by data management and data standard issues rather than data processing/cpu/pipelining issues. Processing systems turn into information systems. First attempts to combine archiving and processing in the 1980s include ESO’s MIDAS Table File System [11], integrating common tables both accessible in source code and by user interfaces like the MIDAS monitor/prompt. The MIDAS Table File System allows both users and programmers to change its content and also registering the modifications in table keywords leading to archives ready for further review and (trend) analysis. Its development was essential for the production and photometric calibration of the images of the ESO-LV galaxies. However, the 600,000 foreground and background objects visible on the images, stars and galaxies, could only be handled with great difficulties inside the system, the response times running into hours per operations, demonstrating the importance of built-in scalability.

This MIDAS Table File System marked a stepping stone to current data-centric approaches which are enabled by the introduction of modern object-oriented programming languages, data modeling tools like UML and XML and relational databases.

We have combined these views, systems and requirements in order to design and build integrated information systems which have the potential for self-organizing and enrichment with new data. Both self-organizing and enrichment are processes in time. In fact, the datacentric approach implies the detailed modeling and awareness of how things change in time. Important changes range from

I. new data entering the system (ingest) to
II. new or modified source code handling these data. In turn, the new data entering the system might be
III. subject to physical changes (e.g. the gain of a sensor), while source code is often modified on the basis of

IV. advancements of human understanding of the physical changes—our model of the world also changes (e.g. the cause and modeling of the gain variations of the sensor).

The ideal information system would seamlessly cope with all these changes in time, thus creating a living long term digital preservation environment. Astrowise is one of the first systems attempting to reach this goal.

For several years many authors predicted the upcoming data avalanche due to the advancements in digital sensor technology. Obviously, this has now started, both scientific experiments such as LHC and LoFAR are running into the tens of Petabytes data acquisition regimes, while text, imaging, genome and internet gathered data collections like e-Bay are exceeding these volumes. This triggered the development of Grid infrastructure that is able to handle Petabytes of data [12, 13].

All this has happened in an approximate 20 year time span when the first large digital imaging collection was published, ESO-LV [2], containing scans of 32,000 galaxy images, 4 Gbyte of data filling a room full with tapes and populating the very first version of optical media.

By now, the data avalanche is multidisciplinary and worldwide and involves all aspects of our society, from science to commerce, public services and health care. Digital data is gathered, processed, distributed and accessed at a continuously growing rate. And this is only the beginning: in, say, two decades, the same room full with 4 Gbyte of tapes 20 years ago, and 40 Petabyte of tapes today could possibly contain 40 Zetabytes (40 million Petabytes) of data. The growth of the data volume produced by various types of sensor networks met with the growth of disk capacity and search for new methods to increase memory storage density (see [14]). In order to be useful all this data has to be organized, administrated, managed and distributed.

It took a billion years for cells to develop into extremely complex information systems around the DNA; it has resulted into systems and approaches with an incredible complexity with memory mapping, copying, filtering and distribution mechanisms of data including feedback. Compared to this, our present data organizing mechanisms in IT are still very simple and rudimentary and we are just making the first steps to living self-organizing systems and archives required to deal with and optimally use the ocean of digital data to come.

However, also in the cell stochastic processes are important, and the absence of organization “from above” is countered by survival of the fittest type of mechanisms, which appear as self-organizing. Also in human endeavored IT, standards seldom come from above, an exception being the ASCII character standards, mandated in 1968 by U.S. President Lyndon B. Johnson to be used in all computers purchased by the United States federal government.

I have also approved recommendations of the Secretary of Commerce regarding standards for recording the Standard Code for Information Interchange.
on magnetic tapes and paper tapes when they are used in computer operations. All computers and related equipment configurations brought into the Federal Government inventory on and after July 1, 1969, must have the capability to use the Standard Code for Information.

In practice, standards are often invented by companies or scientific communities which are discriminated in a complex survival of the fittest battle, which involves that many factors that it appears stochastic.

The view, or better requirement, for future self-organizing information systems and its archives is that it organizes itself for all these changes in time. It could be seen as a step towards the extremely complex and self-organizing information systems in a cell.

The core problem for the definition of an information system is the definition of information itself. The information can be an input data flow from sensor detectors, an archive of transactions, trends deduced from the analysis of some data and even results of the data modeling or simulations. As a result, information systems will host a variety of subsystems defined by its purpose. Examples are a Decision Support System gathering and analyzing trends for a specific business use case (see [15]) or Geographical Information Systems with focus on geospatial data analysis and visualization of the data.

Nevertheless, it is possible to define primary components of any information system following simple requirements on storage, processing and sharing data. Such a system should include a data model, storage and data processing facilities together with user interfaces. In Astro-WISE we have decided to separate and store all data beyond pixel/measurement data in a database and all pixel/measurement data in files on independent storage media.

This paper does not touch details of the implementation of the Astro-WISE information system which are described in other papers but describes the general outline of the Astro-WISE information system and specifies features which make Astro-WISE unique. For the more in-depth review of particular aspects of Astro-WISE we recommend to read corresponding papers on the optical pipeline implemented in Astro-WISE [16], quality control realised in Astro-WISE [17], the system of user interfaces and services [18], and the hardware solution for Astro-WISE and information systems created on the basis of Astro-WISE [19].

3 Building a scientific information system

The development of the Astro-WISE information system, the first one which implemented WISE technology, started from the very practical challenge: enable a community of researchers distributed over the world to process the data of astronomical imaging survey of the OmegaCAM 256 Megapixel camera on ESO’s VST telescope at Cerro Paranal (Chile). These scientists should be able to evaluate the quality of the data, apply a number of calibrations, share the data within the team and employ distributed resources on a Petabytes scale of data storage and Teraflops capacity in data processing.
From this our basic requirements on the system are derived:

* Scalability of the system. Any part of the system, i.e., data storage, data processing, metadata management, should be scalable with the increase of incoming data and a number of users involved in the data processing. The system should be scalable with respect to the data processing algorithms and pipelines, allowing the implementation of new pipelines and derive improved results from the same raw or intermediate data with new algorithms. The scalability of data mining should be possible, i.e., the system should satisfy all possible kinds of requests; from the retrieval of a single data item by identifier to a complicated archive study involving multiple complex queries.

* Distributed system. Any derivation of a result or search for a result should be possible by different users at different sites where the system is implemented. This makes it possible to optimally use shared resources.

* Traceability. All activity in the system should leave a clear footprint so that it will be possible to trace the origin of any changes in the data and find an algorithm, program and user who created a data item. This allows expert knowledge to be shared amongst all users of the system.

* Adaptability. It should be possible to adopt the system for a number of different scientific use-cases, providing resources, pipelines and expertise to perform data processing according to a user's interests in the same data set.

The most general requirements listed above result in a set of more detailed and specific requirements to different components of the information system. First, the ability to share data among a number of users becomes more valuable when all these users are working with the same set of standards for the data. Second, the requirement to trace any changes in the data processed by different users with different programs and pipelines implies that the system has a common approach to treat the data items in different stages of the data processing and keeps records of changes in the data. As a result the basic requirements to the system dictate the use of a common data model and the common standards for the data storage. Below we will describe the common data model features defined from the requirements to the system.

**Requirements to the data model**

- Petabyte systems can not work when anarchy is allowed at the data acquisition. Users should operate with the same standards as for the raw measurements data acquired at the experiment. Moreover, this implies a careful definition of the data taking scenarios, observing templates in astronomy, scan scenarios on sensor systems both for the scientific measurements data and for the calibrations. The raw data ingested in the system should be fully and completely described in the system so that users
do not need to involve detailed knowledge about the acquired data and can share it with other users of the system. **The data model must provide complete data provenance**, i.e., both external data ingested into the system and the data derived inside the system should be described with sufficient level of detail to be able to rederive them in the environment external to their original one.

- The data model should describe all the data products, on all stages of the data processing. For the user it should be possible to understand the origin of each data item and to trace the data item back to the raw data. **The data model must provide full data lineage**, i.e., each data product and literally each bit of information must be traced back to the origin and creator of the information.

- The model should match all scientific use-cases and should allow the flexibility to modify source code without changing the model as long as this makes sense. Obviously, here boundaries will have to be determined by means of inside, thus human, knowledge. This is the most tedious part in the design of the information system, but in practice it turns out that the various processes are well defined and dictated by physics. **The data model must be flexible to the changes in the data processing.**

- Requirements to trace changes in the data triggered by different versions of the processing software and the necessity to repeat the data processing due to the changes in the pipeline implies that all parameters that affect the derived result must be preserved in the system. The user should be able to reproduce the data item and to find a trend in the data due to the changes in the processing parameters or algorithm. At the same time the user should be able to reproduce already existing items to ensure the preservation of the data and software used previously. **The data model must allow both data reprocessing and data reproduction**, and the reprocessing should be done with the preservation of the previously produced versions of the data.

When properly defined the data model allows to code, instantiate and trace the data processing for all scientific use-cases.

Also, the data model should allow to accommodate external data, as well as provide necessary comparison and checking with these external data sets. When the data model is carefully defined our approach is to convert this into a pipeline model, in turn translated into a hierarchy of Classes. These Classes are then mapped into a database. We originally did this with object-oriented databases like Objectivity, but currently we do this in a relational database and build an object oriented view in order to maintain transparency in the class model, and its dependencies.

**Requirements to infrastructure** The data model should be shared among geographically remote sites of the system, as research groups at various locations are collaboratively adding and extracting data from the distributed system. The basic requirement is that in fact any component (database, file system,
code base, CPUs) should possibly be present at different sites, for a number of reasons:

- hardware resources between the sites can be shared,
- avoiding single centralized components prevents an overload of resources and duties at that node,
- redundancy of the system to overcome single-site malfunctions,
- sharing of resources between partners allows to reduce the overall cost of the system.

For example, the data ingestion to the system can be done in Garching, Germany, the data processing in Groningen, The Netherlands and the image analysis in Napoli, Italy.

Requirements to the user interfaces

The user should be able to trace the data processing, to retrieve data items and identify all its dependencies on other items (mostly calibrations) in the system, to initiate data processing of particular data items and to find a quality estimation for the data.

As we can see, all these requirements put together are more challenging than requirements on common business information systems. The key difference is that we allow everything, including the code base to change in time.

In the following chapter we outline how our requirements formed a layout for a scientific information system capable of sharing a huge data volume, to process these data and fulfill scientific use-cases for a number of users.

4 WISE concepts

First of all we have to clearly distinguish between two classes of data storage systems in Astronomy: proper archives containing fixed published data and information systems. For an archive stored data is a stable entity which is provided to the user as it is, meanwhile an information system allows the users to modify their own data creating user-specific versions of an archive and share versions with other users.

The Astro-WISE approach, and its general multi-discipline WISE approach implements a scientific information system.

The usual approach to building an information system is to perceive three components: the data layer, business rules and the interfaces (see Fig. 1). In our case, we separate the data layer in two parts: the pure measurement data layer, hereafter data layer, and everything beyond that, hereafter Metadata layer, ranging from file sizes, to statistics of pixel values and detected events in the measurements (galaxy, particle, word). The Metadata layer allows to implement a data model, the data layer allows to store the data as files in a standard format, while business rules implemented in Python classes bind the metadata and the data layers. Interfaces provide user access to both the business rules and the data. In the case of Astro-WISE business rules are
Fig. 1 Top-level definition of Astro-WISE information system with the specification for each layer

present in the Metadata layer (Data Definition Language used to create a data model), data layer (the on-the-fly compression of the data on data storage grid) and—the most apparent to the user—in a number of pipelines and programs which the user defines to process the data. This last part of business rules components we will call data processing layer.

To implement Astro-WISE we use abstractions of storage, processing and database capabilities as a basis for the infrastructure for each of the layers of the system. The metadata layer is realized in a relational DBMS through an abstraction of the required database functionality, the data layer is put on the Astro-WISE data storage grid through an abstraction of storage and the processing grid is used to connect the user with the data and metadata layers by a number of interfaces for the data processing layer. Separation of these three infrastructures plays a key role in the flexibility of the system, as we will see below.

The metadata layer implements a list of necessary functionalities:

1. **Inheritance of data objects.** Using object-oriented programming, all objects within the system can inherit key properties of the parent object. All these properties are made persistent.

2. **Full lineage.** The linking (associations or references, or joins) between object instances in the database is maintained completely. Each data item in the system can be traced back to its origin. The tracing of the data object can be both forward and backward. For example, it is possible to find which raw frames were used to find magnitudes, shapes and position for this particular source and, at the same time, which sources were extracted from that particular raw frame.
3. **Consistency.** At each processing step, all processing parameters and the inputs which are used are kept within the system. Astro-WISE keeps the old versions of all data items along with all parameters used to produce them and all dependencies between objects.

4. Embarrassingly parallel and distributed processing, the administration of asynchronous processing is recorded in the metadata layer in a natural way.

Our requirements on distribution and multiple users propagate as key principles of the realization of metadata and data layers and business rules which form the core of the WISE approach:

1. **Component based software engineering (CBSE).** This is a modular approach to software development, each module can be developed independently and wrapped in the base language of the system (Python) to form a pipeline or workflow.

2. **An object-oriented common data model used throughout the system.** This means that each module, application and pipeline will deal with the unified data model for the whole cycle of data processing from the raw data to the final data product.

3. **Persistence of all the data model objects.** Each data product in the data processing chain is described as an object of a certain class and saved in the archive of the specific project along with the parameters used for data processing.

The Astro-WISE system is realized in the Python programming language. It allows one to wrap any program into a Python module, library or class. The use of Python also allows to combine the principles of modular programming with object-oriented programming, so that each package in the system can be built and run independently with an object-oriented data model serving as glue between modules. At the same time, the logic behind pipelines and workflows in Astro-WISE allows the execution of part of the processing chain independently from the other parts. We will describe this approach in more detail in the example of optical image processing in Section 4.1.

The conceptual difference between Astro-WISE and other existing systems is that Astro-WISE moves from the usual for astronomy processing-centric approach to a datacentric approach. The data processing itself becomes an integral part of the archive.

The typical solution for the data processing and storage for Astronomy handles the data processing and the final data product delivered to the user as two completely separated entities. The data product usually is a result of the processing for the whole survey with fixed processing parameters used for the whole set of images. The user has access to reduced images and the catalogue, where both kinds of data products are stable within a “release”, which usually refers to the sky coverage performed by the survey.

In this way the survey data center provides the user with a specific version of the data product that will not change over time, which covers most of the science use-cases.
Nevertheless there are a number of use-cases which cannot be satisfied by the “standard” version. For example, in the search for objects like brown dwarfs or quasars it is important to lower the detection threshold which implies the reprocessing of the data. The user himself has to care about such reprocessing thereby reinventing the whole data processing system for the survey and involving his own resources. The Astro-WISE system allows to work on any use-case using the standard pipelines and performing programming on a minimal level—if this is necessary at all.

Figure 1 shows the principles of WISE concepts in binding together all layers of the information system. Data processing pipelines define use-cases and a data model for the system, which is implemented in the Python classes which wrap pipelines and define the common persistent data model objects. The data layer uses this data model, and interfaces are providing access to the system by users. The common data model effectively brings together all layers of the information system.

The common data model can be modified by a mutual agreement of all users of the system. Any user can propose changes in the data model, and, if changes were accepted, the system administrator implements these changes in corresponding Python classes and in the database scheme.

In the next sections we will review in detail the infrastructural layers of Astro-WISE and their implementation.

4.1 Metadata layer

The bulk of the data stored in Astro-WISE is stored in files of some format (FITS). Each file is registered in the Astro-WISE metadata database with a unique filename. Apart from just registering each file in the system the metadata database implements the important part of WISE approach—the common data model.

Figure 2 shows the general outline for all data models implemented in information systems based on WISE concepts. Two core classes DBObject and DataObject are parent classes for the classes which store metadata persistently and the classes which store the data in a file. These classes include interfaces to the metadata database and the data storage, the physical implementation of the metadata database and the data (files) storage can be different for different systems.

Let us suppose that we wish to use Astro-WISE for the data processing of optical images. Figure 3 shows typical classes of data items used by the optical data processing pipeline to reduce the data from raw images to the final science ready catalogue. This data model, deduced from the pipeline (Fig. 4) and enhanced keeping in mind possible scientific use-cases, is a central part of the metadata layer.

The data model is implemented both in the relational database (currently Oracle 11 g RAC is used) and in the hierarchy of Python classes. All core classes are made persistent, i.e., any change in the object is mirrored in the
corresponding tables of the database. The method used for the implementing the data lineage is the Persistent Object Hierarchy (Fig. 2). According to this method objects of Astro-WISE are made persistent recursively, all operations and attributes of the object are saved in the metadata database.

As an example let us explore the data reduction task—we will create a reduced image from the raw image on one CCD chip. First of all, we will select an image we wish to process:

```python
awe> raw = (RawScienceFrame.filename == 'WFI.2000-01-01T08:57:15.410_3.fits')[0]
```

The image is selected by browsing the metadata database for an object of class `RawScienceFrame` with filename `WFI.2000-01-01T08:57:15.410_3.fits`. The returned object `raw` was retrieved from the metadata database with all attributes. In the next step we will retrieve from the database all necessary calibration objects. The logic in the function `select_for_raw` allows to take the calibration files for the same night of observation (2000-01-01T08:57:15.410) or closest to this night.

```python
awe> hot = HotPixelMap.select_for_raw(raw)
awe> cold = ColdPixelMap.select_for_raw(raw)
awe> flat = MasterFlatFrame.select_for_raw(raw)
awe> bias = BiasFrame.select_for_raw(raw)
```
Fig. 3 A set of dependent Astro-WISE classes for an optical data processing pipeline with references to each other. Each class is a persistent one stored in the metadata database and linked to the file stored in Astro-WISE system.

Now we can instantiate a new object—our target—a reduced image which will be based on all the images above:

```python
awe> reduced = ReducedScienceFrame()
awe> reduced.raw = raw
awe> reduced.hot = hot
```
Please, note that all images which will be used to create a new reduced image are referenced through attributes of the new image. This new image should get a unique ID, which is a name of the file where the image will be stored.

Now the image can be created invoking the make() method of the ReducedScienceFrame class.

The make() produced a file with a new image which will be stored on one of the dataservers of Astro-WISE (see Section 4.2):

Finally, the metadata database will be updated and the new image will become a part of the metadata layer.

The sequence described above is a general way to create a new data entity in Astro-WISE: to combine a set of references to entities which will be used to create a new one, to invoke a pipeline or a part of pipeline which will generate a new entity, save the created data in the data layer, commit a new data entity to the metadata layer. The processing parameters, for example, the method used for the overscan of the image, will be saved as a persistent attribute of the new data entity as well.

An important feature of keeping the full data lineage in the system is the ability to avoid unnecessary reprocessing. The execution of the make() method of reduced object actually will start with the search in the metadata database for an object with the same attributes, and if such an object exists (and the user is allowed to retrieve it according to the user’s permissions) the user will be redirected to an already existing object and the processing part of the method will be skipped. The data lineage makes it possible to avoid unnecessary reprocessing as well as to use forward and backward chaining in the dependencies of the data items in the system.

Objects can be deleted from the database under the following restrictions: every user can delete the data he created at the privileges level 1 (see Section 4.5). For higher privileges levels only the project manager is allowed to delete. To delete a data object myobject from the database Context class is used (see [16] for the full description):

```python
awe> Context().delete(myobject)
```
Objects can be deleted if they are not referenced by other data objects. If they are, it might be desirable to invalidate the object, so that the object will stay in the system but will not be used for the data processing (unless the user specifically ask for invalidated objects). The user-friendly service for the validation of data objects is described in [17].

4.2 Data layer

Each data entity in Astro-WISE has two parts: a data part which is stored in a file and a metadata part in the form of a metadata database and which keeps all dependencies of the data entity. The data part of the entity is stored as a file on one of the Astro-WISE dataservers. The predefined file format can be changed, but for most files the format is FITS. Nevertheless the dataserver is not limited to a single file format and can store files of any type. The dataserver is a specific solution which in its functionality is closest to the storage element of the Grid.

The main requirement on the dataservers as storage space is, apart from the safety, scalable size. The size should be scalable at the Terabyte level allowing to increase the storage volume from a few Terabytes to almost a Petabyte (this is the typical scale for the KIDS data archive from a few raw images at the beginning of the survey to hundreds of Terabytes with all intermediate data products at the end of observations).

Dataservers are organized in geographically close clusters, within each cluster all dataservers know about the existence of all other dataservers in the cluster. A dataserver in one cluster can contact other clusters via at least one dedicated dataserver in another cluster (see Fig. 5). All communications are done using a standard HTTP protocol. Following types of requests are available: retrieve a file, store a new file, locate a file and delete a file.

The unique name of the file is used as a unique identifier and this unique name is stored in the database as part of the metadata.

The user of the system does not know the actual location of the file on the underlying file system and operates with the URL of the file only. The URL has the form http://<data_server_address>/<file_name>. Each Astro-WISE service has pre-defined dataservers which are used to retrieve data. Usually the administrator of the local Astro-WISE node assigns this dataserver selecting “geographically closest” dataserver. The user can change this assignment and use the dataserver the user prefers.

On request from the user to retrieve the file the dataserver can then either return the requested file or redirect the client to the dataserver that has the file. Each dataserver has a permanent data storage and a cache, the last one is used to temporarily store a file retrieved from the other dataserver. By user request, for example, http://ds.astro.rug.astro-wise.org:8000/WFI.2000-09-28T02:22:37.466_8.fits the dataserver ds.astro.rug.astro-wise.org will check its cache space for the file WFI.2000-09-28T02:22:37.466_8.fits. If the file is not found, the dataserver will check its own permanent storage space, and if there is no such file, all dataservers in a “local” cluster
Fig. 5 Data storage network of Astro-WISE. Dataservers are grouped geographically with one dataserver dedicated to the external data exchange. The user requests a file from a local dataserver and, if the file is not found in the local group, the local dataserver will request the file from the other dataserver groups. As soon as file is found it is copied to the dataserver that the user contacted and provided to the user.

(astro.rug.astro-wise.org) will be requested. If there is still no file found, all other clusters will be requested, and as soon as the file is located it will be copied to the cache of the ds.astro.rug.astro-wise.org and returned to the user. In addition, a file can be compressed or decompressed on-the-fly during retrieval, and a slice of the data can be retrieved by specifying the slice as part of the URL.

The dataserver is written in Python and can be installed on any operating system and underlying filesystem that can support long case-sensitive filenames. For the Astro-WISE Linux filesystems, XFS and GPFS are currently in use.

4.3 Processing layer

The example in Section 4.1 involves the processing facilities of Astro-WISE, which are distributed and combined from processing facilities of all Astro-WISE partners. The user has the choice to send the job to one of the processing elements of Astro-WISE (including Grid computing elements) or to use the processing power at the user’s disposal, for example, a PC or notebook.

In the core of the processing layer of Astro-WISE is a Distributed Processing Unit (DPU). This middleware consists of three components, which are DPU server, DPU client and the so called DPU runner. The DPU server is a front-end to any processing system and interacts with the processing...
system’s native queuing system, allowing the user to submit jobs to this particular queuing system, inspect or cancel them. The DPU client includes all functions and methods the user can call to interact with DPU server. The DPU runner is a program which is run on the remote processing facility and checks availability of all necessary software to run an Astro-WISE job, installing required packages if needed. The system runs on openpbs or under its own queue management software. The DPU itself allows synchronizations of jobs as well and can also transfer parts of a sequence of jobs to other DPUs.

In the case of a Grid computing element the DPU server will check a user’s identity and will use the user’s credentials (Grid certificate) to mediate with the Virtual Organization Management System. Currently OmegaCEN is using omegac Virtual Organization with an ability to submit jobs to Grid computing elements in Amsterdam and Groningen.

4.4 Interfaces

The description of the Astro-WISE system would be incomplete without the description of a number of interfaces provided to the user. The user can write his own applications in the Python language calling Astro-WISE libraries or can involve Astro-WISE services. The first case requires the use of the Astro-WISE Command Line Interface called AWE (Astro-WISE Environment), which can be installed at any site, on PC or notebook.

The Command Line Interface—CLI—supposes that the user writes his own programs using Python, but to browse the data or even to process observations there is no need to use the CLI. All operations required to perform these activities are possible with a set of standard web services of Astro-WISE. Of course, the use of the CLI gives to the user much more freedom in data processing. The CLI is more useful for experienced users working on a particular use-case, meanwhile web services are developed for routine operations during the data processing of the surveys.

The web interfaces are divided into two types: data browsing/exploration and data processing/qualification. The first group includes:

* dbviewer\(^1\)—the metadata database interface which allows browsing and querying of all attributes of all persistent classes stored in the system,
* Quick data search\(^2\)—allows querying on a limited subset of attributes of the data model (coordinate range and object name), and provides results of all projects in the database,
* Image cut out service\(^3\) and color image maker\(^4\)—these two services are for the astronomical image data type and allow to create a cut out of the image

\(^1\)http://dbview.astro-wise.org/  
\(^2\)http://gowise.astro-wise.org/  
\(^3\)http://cutout.astro-wise.org/  
\(^4\)http://rgb.astro-wise.org/
or to create a pseudo-color RGB image from three different images of the same part of the sky,
* GMap\textsuperscript{5}—exploration tool of the Astro-WISE system using the GoogleSky interface.

Data processing/qualification interfaces are:

* Target processing\textsuperscript{6}—the main web tool to process the data in Astro-WISE. This web interface allows users to go through pre-defined processing chains, submitting jobs on the Astro-WISE computing resources with the ability to select the computing node of Astro-WISE,
* Quality service\textsuperscript{7}—allows to estimate the quality of the data processing and set a flag indicating the quality of the data,
* CalTS\textsuperscript{8}—web interface for identifying and qualifying calibration data.

All web services are built using a set of Python classes developed for Astro-WISE as a basis and uses a modular principle, which allows to create a new web service using components of older ones.

4.5 Authorization and authentication system

Astro-WISE is a multi-user system which must accommodate sharing data between scientists and at the same time protect the private data of each user. Each user in the Astro-WISE system has an identity protected by a password, and, optionally, if the user wants to submit job to Grid resources he has to get a Grid certificate.

The authorization and authentication system is implemented on the level of the metadata database. As soon as a user logged in with his username/password, the user’s privileges are checked in the database, allowing the user to browse the data according to the user’s privileges while obeying the privileges of other users. The data in the metadata database are grouped by projects. A Project is a collection of resources which is associated with a group of users who can access these resources, usually one of these users has the role of Project Manager who has privileges to include new users, remove users and publish the data to the wider community.

Access to the data is granted based on three attributes which any data entity in Astro-WISE has: user, project and privileges. The first one identifies the user that created the data entity. The second one defines to which project the data entity belongs, the third one defines who is able to use this data entity. All

\textsuperscript{5}http://skymap.astro-wise.org/
\textsuperscript{6}http://process.astro-wise.org/
\textsuperscript{7}http://quality.astro-wise.org/
\textsuperscript{8}http://calts.astro-wise.org/
Table 1 Privileges system of Astro-WISE

| Privileges | Scope                  | Visible to                          |
|------------|------------------------|-------------------------------------|
| 1          | Private                | The creator only                    |
| 2          | Project                | Users of the project                |
| 3          | Astro-WISE             | Authorized users of Astro-WISE      |
| 4          | World                  | Anonymous users of Astro-WISE       |
| 5          | VO                     | Published in Virtual Observatory    |

these attributes are initialized the first time the data entity is made persistent in the Astro-WISE system (including the case that the entity is created by one of the Astro-WISE pipelines) and they are all persistent attributes, i.e., stored in the metadata database.

Table 1 shows the range of values for the privileges attribute. In the case of \( privileges = 1 \) only the creator of the data item can see it, the creator can raise privileges to \( privileges = 2 \), in this case all the users within the project will be able to browse this data entity. Raising privileges to 3 the user makes the data item accessible for all Astro-WISE users in all projects, and with \( privileges = 4 \) the anonymous user (a user with minimal read-only privileges in the system) can see it as well. Finally, with \( privileges = 5 \) the data item is accessible via Astro-WISE Virtual Observatory interfaces.

The special Python class Context was created to handle authorization and authentication. The Context allows to change privileges of all user’s data items, during the change Context is checking for dependencies to prevent inconsistency in the dependencies due to the different privileges of data items. For example, if the raw image was published by the user to the project scope and some other user has created a reduced image from this raw image, the original user will not be able to downgrade privileges on the raw image to the private data scope.

4.6 WISE architecture

We described above three infrastructural components of Astro-WISE: the relational DBMS (the metadata layer), dataserver (the data layer) and DPU (the processing layer). Combined with user interfaces these components build an Astro-WISE node—a detached Astro-WISE site which can operate independently from other sites. Multiple nodes can be combined to form a distributed system. Each node is independent from others in the sense that it is administered independently and can handle both the data distributed over other nodes and the data restricted to this node only and shielded from other nodes.

Figure 6 shows the elements of the node:

* Data storage servers (dataservers).
* A metadata database to store a full description of each data file with links and references to other objects.
Fig. 6 Present-day Astro-WISE nodes with a typical composition of a node in a full deployment node

* Astro-WISE programming environment (CLI) along with web services which give the user an ability to access the stored data and launch a data processing.
* Computing nodes for the data processing with DPU servers on top of their queueing system.
* A version control system for developers to include new modules, classes and libraries into the system.

All these elements are optional, an Astro-WISE node can be installed without dataservers (dataservers from other nodes are used), metadata database or processing facilities. In fact an Astro-WISE node can be installed on a notebook as an Astro-WISE environment only giving the user access to the system—if the user is not satisfied with web services on the remote nodes.

Presently Astro-WISE includes sites at Groningen University, Leiden University and Radboud University Nijmegen (The Netherlands), Argelander-Institut für Astronomie, Bonn and Universitäts-Sternwarte München (Germany) and Osservatorio Astronomico di Capodimonte, Napoli (Italy).
5 Astro-WISE: migration to other systems

The WISE concepts for an information system are principles described in Section 4. Astro-WISE is the first system which realizes these concepts and serves as a basis for the further development of information systems. In this section we describe the adaptivity of the parent system to new tasks and challenges on the example of the LOFAR Long Term Archive and the Molgenis system.

The importance of the LOFAR Long Term Archive (LTA) for the development of WISE concepts is the necessity to use an external infrastructure which should be included in the architecture to form a complete information system. We preserved all principles of Astro-WISE adding storage and processing which is not controlled by the system itself (BiGGrid\(^9\)). Additionally we integrated three different systems of authorization and authentication to make it possible for the LOFAR observatory to create new users and control resources in the system. The LOFAR LTA design is described in [20] and the architecture and infrastructure in [21].

Another significant development was achieved with the adaptation of Molgenis.\(^{10}\) Molgenis is a framework written in Java to build user interfaces and databases from definitions that are written in XML. From these definitions the database tables and webserver are generated. Its origins lie in biomedical applications. Historically Molgenis focused more on interaction with the user to streamline the “protocols” (recipes for analysis) of researchers to keep track of analyses of results. On the other hand, the WISE technology focused more on results from a processing perspective. This lead to the idea to combine the strengths of both frameworks and use some models that already existed in XML for Molgenis to generate a datamodel in Python for Astro-Wise. Then Molgenis could be extended to use the WISE infrastructure for distributed storage and processing.

The existing Molgenis XML model is organized in a common fashion through “module”, “entity” and “field” where each field has a type of \texttt{int}, \texttt{float}, \texttt{str} or can be a reference type such as \texttt{mref} or \texttt{xref}. Most of these have counterparts in the WISE framework which made it possible to write a conversion tool.

The webserver that is generated by Molgenis has to communicate to a database that it usually creates itself. However, in this case the database had to be generated by Astro-WISE because the frameworks did not have a backend for a common database (Oracle vs. Non-Oracle). Instead of writing a new database backend for either framework it was decided to write an \texttt{xmlrpc} interface to encapsulate database queries and return their results. Since client software for all database flavours does not have to be present this functionality can be extended, e.g., since this is \texttt{xmlrpc}, a programming

\(^9\)http://www.biggrid.nl/

\(^{10}\)http://www.molgenis.org/
language independent implementation could also use the database in a way that the WISE framework dictates.

The approach developed and tested in the case of Molgenis allows to create a new information system based on Astro-WISE with all services starting from the data model coded in XML and to do this automatically. This approach allowed to decrease the time and resources spent for the development and implementation of a new system significantly.

The next system which will be created with the approach tested on Molgenis is a data processing system for Multi Unit Spectroscopic Explorer\textsuperscript{11} (MUSE).

6 Conclusion and future work

The Astro-WISE information system, the first information system in Astronomy, proved to be a reliable and flexible tool for the data processing. Originally developed to process the data of KIlo Degree Survey (KIDS\textsuperscript{12}) it triggered development of the unique approach to the architecture of scientific information systems (WISE approach).

Both Astro-WISE and the WISE approach are living systems which are open to improvements. For the last 2 years further development of the WISE approach is hosted by Target Holding.\textsuperscript{13} Target Holding is an expertise center in the Northern Netherlands which is building a cluster of sensor network information systems and provides cooperation between a number of scientific projects and business partners like IBM and Oracle. Target creates and supports a hardware infrastructure for hosting tens of Petabytes of data for projects in astronomy, medicine, artificial intelligence and biology.

In this development the WISE approach was used to create new information systems extending the original Astro-WISE on new data models, new data storage and processing capacities and new fields.

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\textsuperscript{11}http://www.eso.org/sci/facilities/develop/instruments/muse
\textsuperscript{12}http://www.astro-wise.org/projects/KIDS/
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