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Feeding an astrophysical database via distributed computing resources: The case of BaSTI

G. Taffoni [b,*], E. Sciacca [c], A. Pietrinferni [a], U. Becciani [c], A. Costa [c], S. Cassisi [a], F. Pasian [b], D. Pelusi [a], C. Vuerli [b]

[a] *INAF - Astronomical Observatory of Teramo, Via M. Maggini, s.n. 64100, Teramo, Italy*

[b] *INAF - Astronomical Observatory of Trieste, Via G.B. Tiepolo 11, 34143, Trieste, Italy*

[c] *INAF - Astrophysical Observatory of Catania, Via S. Sofia 78, 95123, Catania, Italy*

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ABSTRACT

Stellar evolution model databases, spanning a wide ranges of masses and initial chemical compositions, are nowadays a major tool to study Galactic and extragalactic stellar populations. The Bag of Stellar Tracks and Isochrones (BaSTI) database is a VO-compliant theoretical astrophysical catalogue that collects fundamental datasets involving stars formation and evolution. The creation of this database implies a large number of stellar evolutionary computations that are extremely demanding in term of computing power. Here we discuss the efforts devoted to create and update the database using Distributed Computing Infrastructures and a Science Gateway and its future developments within the framework of the Italian Virtual Observatory project.

1. Introduction

The availability of large sets of stellar evolution models spanning a wide range of stellar masses and initial chemical compositions is a necessary prerequisite for any investigation aimed at interpreting observations of Galactic and extragalactic, resolved and unresolved stellar populations. In the last few years, thanks to the new developments in various fields of Physics, our understanding of the structure and evolution of stars improved and consequently the stellar evolution models also increased in complexity and completeness.

Pietrinferni et al. (2004) built a database of evolutionary predictions: The Bag of Stellar Tracks and Isochrones (BaSTI, see Pietrinferni et al., 2004, 2006, 2009, 2013; Cassisi et al., 2006; Cordier et al., 2007). The database collects the results of a large number numerical simulations based on Frascati Raphson Newton Evolutionary Code (FRANEC) (Pietrinferni et al., 2004) and it is specifically devised for population synthesis studies of resolved and unresolved stellar populations.

BaSTI relational database archives a large number of parameters such as chemical composition coverage, improvements in the model input physics and bolometric corrections/colour transformations, coverage of physical parameters, reproduction of empirical constraints, ease of interpolation and inclusion in population synthesis codes. For this reason it is considered as one of the most complete stellar libraries (Conroy, 2013; Gallart et al., 2005; Marín-Franch et al., 2010).

The Database has been designed to account the following main criteria for a reliable and homogeneous stellar evolution library:

1. the input physics employed in the model computations is the most up-to-date;
2. models for all initial chemical compositions are computed with the same evolutionary code and the same physical framework;
3. models and isochrones reproduce a large array of empirical constraints obtained from observations of single stars and local resolved stellar populations.
4. All results have to be easily available to the potential users.

Recently BaSTI has been expanded by adding new important quantities evaluated during the key points of stellar evolution to allow a fast visualisation of these phases. A particular effort has been devoted to port BaSTI to a VO-compliant environment (see Pietrinferni et al., 2014, for more details) and to develop a new simple and user-friendly web interface (Pietrinferni et al., 2014).

From a computational point of view, to populate the BaSTI database with a new isochrone it is necessary to execute a large number of FRANEC runs that are extremely demanding in terms

* Corresponding author.
E-mail address: taffoni@oats.inaf.it (G. Taffoni).

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of CPU time. New runs are necessary to update, maintain and extend the database and to keep the accuracy, homogeneity and completeness of the data. Extensions are often requested by Astronomers who need new data for their scientific activities.

To carry out this large set of simulations we need an extremely high computational power, Taffoni et al. (2010) showed that a Distributed Computing Infrastructure (DCI) can be successfully used to address this problem. However, even today's most powerful DCI such as Grid or Cloud computing infrastructures still have limitations, especially due to the design of the user interfaces. Many sophisticated tools are command line driven and are complex to use. As a consequence, new users have to become familiar, not only with Astrophysical methods and theories, but also with the use of new codes and with the handling of complex computing resources. In order to hide this complexity, it is common to adopt Science Gateways (SG) technologies (Raicu et al., 2006; Wilkins-Diehr et al., 2008a) powered by a workflow management systems to distribute computation on various computing infrastructures (Belloum et al., 2011; Deelman et al., 2009; Barker and van Hemert, 2008; Curcin and Ghanem, 2008).

A SG or portal is defined here as a community-developed set of tools, applications, and data that are integrated via a portal customised to meet the needs of the Astronomical community. The computational processes supported by SGs are organised as scientific workflows that specify dependencies among underlying tasks for orchestrating DCI resources (such as clusters, grids or clouds). SG technologies allow the scientific research community to create a web-based working environment where researchers can concentrate on scientific problems without facing the complexities of computing, data and workflow infrastructure.

In this paper we discuss the design and development of a SG that allows to execute different types of FRANEC runs giving the Astronomers the possibility of updating the BaSTI database or to make on demand simulations of synthetic stellar evolutionary tracks. In the next section we discuss the physics inputs adopted in the updated version of FRANEC and we describe the global properties of the code. In Section 3 we present the SG technology adopted to develop a FRANEC SG that allows to execute FRANEC runs on local clusters, Grid or Cloud infrastructures. In Section 4 we present the FRANEC SG. Finally we compare this approach with the use of DCI previously adopted by Taffoni et al. (2010). We also discuss the "connection with the virtual observatory". Final remarks and a short discussion concerning the planned developments in the context of Euro-VO will conclude the paper.

2. FRANEC evolutionary code

BaSTI has been computed by using a new version of the FRANEC evolutionary code.

FRANEC is a Fortran 77 code, that simulates the evolution of a star on the basis of a number of different physical inputs and parameters. Almost all the adopted physics inputs have been updated in the new version as well as numerical scheme for treating the nuclear burnings and the accuracy of the numerics. The nuclear reaction rates have been updated by using the NACRE compilation (Angulo et al., 1999), with the exception of the $^{12}C(\alpha, \gamma)^{16}O$ reaction, that comes from Kunz et al. (2002). As for the Equation of State (EOS), we employ the new EOS by A. Irwin (Cassisi et al., 2003), that covers the full structure of the models along with all the relevant evolutionary stages.

All stellar models have been computed by fixing the extension of the convective core during core H-burning both classically (Schwarzschild criterion) and considering a non-negligible overshooting beyond the Schwarzschild boundary. This latter choice reproduces empirical constraints coming from intermediate-age cluster Color-Magnitude Diagrams (CMDs) and field eclipsing binaries.

We have also accounted for mass loss by using the Reimers formula (Reimers, 1975) with the free parameter η (estimate of the mass loss) set to zero (no mass loss), 0.2 and 0.4, respectively.

A single run of FRANEC produces one synthetic model (SM). A model evolves from the Pre-Main Sequence phase up to the C-ignition, or until the first thermal pulses along the asymptotic giant branch. A SM run (SMR) is a very simple pipeline consisting of 2 different software (SW) modules: the FreeEoS code and FRANEC. It can last from 1 h up to several hours according to the value of the initial mass and metallicity.

To compute an isochrone (Full Isochrone Run, FIR), it is necessary to execute a large number of SMR varying initial mass and metallicity. The calculations cover 13 different metallicities, namely $Z = 0.00001, 0.0001, 0.0003, 0.0006, 0.001, 0.002, 0.004, 0.008, 0.01, 0.0198, 0.03$ and $0.04, 0.05$, with two different heavy element distributions each: a scaled-solar (Grevesse and Noels, 1993) and an α-enhanced (Salaris and Weiss, 1998) one. We adopted a cosmological He mass fraction $Y = 0.245$ (Cassisi et al., 2003), and a helium-to-metal enrichment ratio $\Delta Y/\Delta Z \approx 1.4$, fixed by the initial solar metal mass fraction obtained from the calibration of the standard solar model.

For each chemical composition it is also necessary to compute additional He-burning models with He-core mass and envelope chemical profile fixed by a Red Giant Branch (RGB) progenitor having an age of $\sim$13 Gyr at the RGB tip, and a range of values of the total stellar mass. These Horizontal Branch (HB) models ($\sim$30 for each chemical composition) constitute a valuable tool to perform synthetic HB modelling, and to investigate pulsational and evolutionary properties of different types of pulsating variable stars.

Data obtained by the simulations is then post-processed and correlated to compute the isochrones. Different isochrones are calculated making different FIR varying other physical parameters as the EOS or the heavy element distribution.

During a FIR a single EOS is shared by a number of independent FRANEC runs. Data produced is then processed to compute the isochrone. Fig. 1 displays some tracks and isochrones for $Z = 0.002$, $Y = 0.248$ and scaled-solar mixture of BaSTI DB. Luminosities and effective temperatures of the models produced by the code should be transformed to magnitudes and colours for several photometric filters – see Table 1 – by using colour-T_{eff} transformations and bolometric corrections obtained from an updated set of calculations of stellar model atmospheres and spectra.

The accuracy of theoretical predictions archived in BaSTI DB, have been extensively tested by employing comparisons with Color Magnitude Diagrams (CMDs) of field stars and a sample of stellar clusters with empirically established parameters like distance, [Fe/H] and reddening (Percival et al., 2009; Cordier et al., 2007; Pietrinferni et al., 2004, 2006).

On the other side, the BaSTI theoretical framework has been used by several authors to perform their scientific investigations (Skillman et al., 2014; Calamida et al., 2014; King et al., 2012; Monachesi et al., 2012; Milone et al., 2012; Cassisi et al., 2008; Piotto et al., 2005, 2007; Recio-Blanco et al., 2005).

Different isochrones are calculated making different FIR varying other physical parameters as the EOS or the heavy element distribution.

During a FIR a single EOS is shared by a number of independent FRANEC runs. Data produced is then processed to compute the isochrone (eg. Fig. 1).

The BaSTI DB includes the metadata of the simulated stellar files and is hosted on an Oracle 10g SQL server, its actual size is $\sim$200 GB.

To populate the BaSTI DB with a new isochrone it is necessary to execute a large number of FRANEC runs (typically more than 100) exploring large number of different parameters. This type of

Table 1
The main characteristics of the *BaSTI* archive.

Mixture	Scaled-solar					α-enhanced			
η	0.0	0.2		0.4		0.2		0.4	
λ_{OV}	0.2	0	0.2	0	0.2	0	0.2	0	0.2
N^O tracks	20	20	20	40	20	20	20	40	20
$M_{min}(M_\odot)$	0.5	0.5	1.1	0.5	1.1	0.5	1.1	0.5	1.1
$M_{max}(M_\odot)$	2.5	2.4	2.4	10	10	2.4	2.4	10	10
N^O isoc.	44	63	44	54	44	63	44	54	44
Age_{max} (Gyr)	9.5	19	9.5	14.5	9.5	19	9.5	14.5	9.5
Photometric system	UBVRIJKL–ACS HST–Strömgren–Walraven Sloan–WFC2–WFC3 (UVIS, IR)								

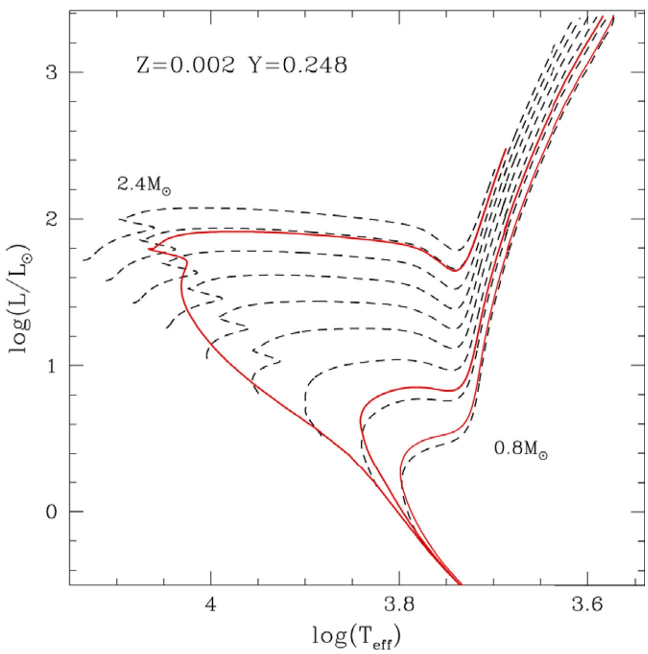

Fig. 1. HR diagram for a sub-sample of tracks (black dashed lines) from $0.8M_\odot$ to $2.4M_\odot$ ($\Delta M = 0.2M_\odot$) and isochrones (red solid lines) with age equal to 0.5, 5.0 and 12.0 Gyr (from left to right) for $Z = 0.002$, $Y = 0.248$ and scaled-solar mixture.

runs are commonly called parameter-sweep jobs. Each FRANEC run produces about 150MBs of outputs (EoSs, evolutionary tracks, logging information), typically the addition of a new set of models (stellar evolutionary tracks plus isochrones) implies an increase of the database size of the order of a few Gigabytes.

The whole computing process to obtain a single evolutionary track can require a time interval since a few hours up to about 10 h depending on the stellar mass and final evolutionary stage to which one is interested. The whole computing time for obtaining an isochrones set can be of the order of a few days up to a couple weeks on a single server. Once the simulations are completed and all the data is available, the addition of the new set of models into the database requires just a few minutes, so it represents a negligible fraction of the overall execution time and does not produce any performance issue.

The production of new isochrones is a CPU bound process: to carry out this large set of simulations we need an extremely high computational power. In a DCI, tasks with different initial parameters can be executed simultaneously on distinct computing resources so drastically reducing the computing time.

This transparent access to resources and data allows Astronomers to test extensively the parameter space, either by simulating and storing data or by retrieving information already produced and eventually re-processing it.

3. Science gateways and workflow technology

To develop FRANEC SG it is necessary to identify a framework that simplifies the web interface design, that allows to easily configure the access to DCIs or local clusters and enables to implement user defined SFR and FIR workflows.

Scientific workflows have become an effective programming paradigm to compose complex computational modules for scientific simulations such as FRANEC. A workflow is a formal specification of a scientific process, which represents, streamlines and automates the analytical and computational steps that Astronomers need to go through from computation and analysis to final data presentation and visualisation. A workflow system supports the specification, modification, execution, failure recovery and monitoring of a workflow using a workflow engine.

The SG technology used to develop the FRANEC gateway is based on gUSE/WS-PGRADE (Kacsuk et al., 2012). gUSE/WS-PGRADE[1] is a collaborative and community oriented web application development environment based on the Liferay[2] portal framework. gUSE/WS-PGRADE computational processes are natively organised as workflows.

WS-PGRADE is the workflow engine (Kacsuk, 2011), it offers generic services to handle distribution, monitoring and fault-tolerant distributed computing in various types of platforms (e.g. web services, grids and clouds); automatic capture of provenance of the involved processes and data; workflow composition and progress monitoring (see e.g. Kozlovszky et al., 2012).

gUSE is a resource virtualization environment providing a large number of high-level DCI services. These services include a workflow storage, an application repository, an information system, and a monitoring system. Several types of DCIs are supported for the submission of workflows like grid and cloud infrastructures, batch systems, and desktop grids (e.g., UNICORE, EMI, BOINC).

Moreover, gUSE/WS-PGRADE is integrated with SHIWA[3] workflow interoperability platform, that grants workflow developers the freedom to choose their preferred workflow system for development, whereas enabling the execution of all these workflows expressed in different languages within WS-PGRADE engine.

gUSE/WS-PGRADE framework is a widely adopted robust technology. A number of scientific communities are using this framework to build their SG (e.g. CancerGrid gateway, ProSim gateway, Amsterdam Medical Centre gateways and the MosGrid gateway) as discussed by Kacsuk et al. (2012). About 50 production gateways based on gUSE/WS-PGRADE are actually available. The Framework is distributed as an OpenSource software and supported by a community of developers, this should also guarantee a long term availability and constant upgrades for the users.

1 http://www.guse.hu.
2 http://www.liferay.com.
3 http://www.shiwa-workflow.eu.

4. The distributed computing infrastructure

The gUSE environment allows to implement different gateway back-ends where actual computations are executed. In the case of FRANEC we identify two different resource: the European Grid Initiative (EGI) grid and a local computing cluster.

4.1. EGI grid environment

EGI developed a DCI based on the EMI Grid middleware (Aiftimiei et al., 2012). EMI middleware builds upon standard open source solutions like Condor (Frey et al., 2001), Globus (Foster et al., 2001), gLite (Laure et al., 2006), extended by the European Middleware Initiative.[4] This middleware provides the user with high level services for scheduling and running computational jobs, accessing and moving data, and obtaining information on the Grid infrastructure as well as Grid applications.

Workload Management System (WMS) is responsible for the distribution and management of tasks across Grid resources, in such a way that applications are efficiently executed. The computation tasks are described through a CONDOR ClassAds-based Job Description Language (JDL). Each JDL file specifies both the binary to execute (the processing to perform) and the input/output files (the data to process) either directly (explicit mention of the input and output data files) or indirectly (through the job input sandbox, command line parameters).

Data Management System (DMS) takes care of file I/O, mass storage and data access and replication. Each file stored in the grid has a Unique IDentifier (GUID). To make the file accessible also to a human user it is possible to assign one or more Logical File Names (LFN) to the same GUID. A LFN is a human readable string. Starting from the GUID or LFN it is possible to find the physical location of the file (SURL) and the transport protocol to use in order to move the file or to download it. EMI DMS is based on LFC File Catalogue. LFC maps LFNs or GUIDs to SURLs. LFC exposes to the user a set of commands that allow to manage files in the Grid.

gUSE can be configured to interact with both high level services (WMS) and low level resources (the computing elements of each grid site) thanks to a software components called *DCI bridge*. Once gUSE is properly configured the workflow developer can decide which resource is more appropriate to execute workflow tasks that the DCI Bridge expresses in terms of JDL jobs. Additionally gUSE is able to manage input data and output data via LFC distributed file system.

4.2. EGI.eu grid and astrophysics applications

The grid infrastructure, currently in use for production purposes, is strongly computing-oriented, suitable for scientific communities whose applications require intensive computation and distributed data storage. EGI.eu grid have been designed to support high throughput computing where uncorrelated tasks are executed in a large amount of computing resources and largely used by the High Energy Physics community, in particular the Large Hadron Collider data analysis (Bird, 2011).

Grid computing is not commonly used by the Astronomy and Astrophysics community (A&A) except for some Astroparticle Physics experiments (e.g. MAGIC telescope, the Auger Observatory, the LIGO project), in fact the grid computing model is not optimal to address the computational needs of A&A, for example: data reduction and analysis tasks, interactive jobs, visualisation of complex datasets, hydrodynamic simulations For these reasons, the A&A community usually relies on national and/or local computing centres or on large HPC facilities offered by super computing centres.

However, the FRANEC application is a good example of a code that fits perfectly with the grid computing paradigm, moreover in the last decade there was an investment for a National Grid Infrastructure in Italy where A&A community was strongly involved. While the BaSTI collaboration has not access to any suitable local or national cluster, an A&A Virtual Organisation (that provides ∼5000 cores and 40TB of distributed storage) is available to execute FRANEC jobs. Moreover, we have a long experience in grid services and in porting applications on grids (Taffoni et al., 2007, 2008, 2010) that allow us to overcome the initial complication in using a grid environment. Finally, we start our development activity from the grid enabled framework developed by Taffoni et al. (2010) that provides a prototype of computing service for BaSTI.

The other aspect to take into account when approaching grid computing is the stability and reliability of the infrastructure. Grid infrastructures and middleware stacks encounter reliability problems proportionally to their complexity and scale. When first implemented, users of the EGI.eu infrastructure reported high error rates, up to 30% in some cases, regularly more than 10%. These result in non negligible amounts of failed tasks and in high and unforeseeable delays in the tasks management time (see e.g. Lingrand et al., 2009). As discussed by Montagnat et al. (2010), today the reliability increases and the expected job failure is much less that 10% (commonly around 3%). Those results are in line with the ones we experienced testing the grid infrastructure in Taffoni et al. (2010) and the ones presented in Section 5.1.

To improve the reliability it is crucial to provide an application environment able to automatically check the jobs status, kill and resubmit non-finished jobs (pending forever), and resubmit failed jobs. This is one of the main challenges when developing a DCI enabled SG. The gateway may take decisions on file replication, resource provisioning, and task scheduling on behalf of the user. Performance optimisation is a target but the main point is to ensure that correctly-defined executions complete, and that misbehaving runs (e.g. failures coming from user errors or unrecoverable infrastructure downtimes) are quickly detected, stopped and resubmitted.

5. FRANEC science gateway

FRANEC Science Gateway[5] is a grid portal that is wrapped around WS-PGRADE providing the execution of a set of FRANEC runs from a simplified web interface (see Fig. 2).

A FRANEC workflow (as depicted in Fig. 3) has been developed using WS-PGRADE native workflow language (Balasko et al., 2010). Moreover, we decided to adopt a modular architecture, each module is a workflow task that can be reused to build other workflows. We developed 7 modules as shown in Fig. 3. In particular:

- **EOS** module provides the Equation of State in tabular form. The input values are the Metallicity Z and the type of mixture (combination of chemical elements heavier than helium).
- **OPACITY** module produces a table of Opacity from pre-calculated tables. Given the Metallicity value Z and the type of mixture it obtains a new table of opacity which is interpolated from the pre-calculated ones.
- **FRANEC** is the core module of the workflow. It produces the models of stellar evolution starting from the output of the two modules EOS and OPACITY and a set of input parameters given by the user to perform the evolution. It produces a set of parameter values varying in relation to time, quantities varying in relation to the radius of the model, the chemical composition of the core (vs. time), surface chemicals (vs. time), and energy resolution Flows(vs. time).

4 http://www.eu-emi.eu.

5 http://starnet.oa-teramo.inaf.it:8081.

Fig. 2. FRANEC Science Gateway home page.

- **TAR** produces an archive of the main outputs.
- **GNUPLOT** produces the output plots.

The dependencies between different modules are explicitly defined by the workflows visualisation and design interface. In Fig. 3 we present the workflow used to execute SFR. The nodes of the graph, represented by boxes, are the modules and denote the activities related to individual computations. Each module is actually a job to execute on the DCI. Each job communicates with other jobs within the workflow through job-owned input and output ports. An output port (small grey boxes) of a job connected with an input port (small green boxes) of a different job is called channel; these are directed edges of the graph. A single port must be either an input, or an output port of a given job.

The FIR workflow is a parameter sweep workflow (Kacsuk et al., 2008) where SIR workflows are executed in parallel sharing the same EOS module.

The simulations of stellar models produce simulation output files with a set of associated metadata. Such metadata are linked to all parameters concerning the numerical evolutionary code. In this way it is possible to store and easily search and retrieve the obtained data by many set of stellar simulations, and also get access to a huge amount of homogeneous data such as tracks and isochrones computed by using FRANEC.

A portlet has been developed to allow the configuration of the workflow execution (see Fig. 4).

This customised web interface (Fig. 4) has been developed to allow users to execute a SFR or a FIR. It is a portlet that allows to run the workflow on a DCI and to configure the workflow execution specifying input parameters for the star such as: the initial mass (in solar unit), the metal content, the initial helium abundance, the mixing-length value, the efficiency of the mass loss and of the overshooting.

The access to this portlet (i.e. web page) is restricted only to authenticated users. In fact security is a critical issue in developing a SG in particular when SG's resources are not entirely dedicated to the SG and managed by it, but they are DCIs shared with other communities. In this case it is necessary to implement an efficient user authentication and authorisation service. FRANEC SG supports user authentication for personalisation, managing user information across sessions, tracking usage, and providing authenticated access to external resource.

The portal implements a login module based on user name and password and a role-based authorisation modules. Roles allow to identify differ users profiles that allow to give access to different applications and resources. Currently we define three roles: standard user, advanced user and administrator.

Guests are not provided with an account for the SG and they have access only to information about FRANEC and the features offered by the gateway. A new account can be created by a standard user or by exploiting credentials from already created Facebook or OpenId accounts.

Standard users are allowed to access the web interface to FRANEC runs. They are also allowed to change input and relevant parameters, to invoke and monitor workflows.

Advanced users can access additional features to create and change workflows and to set configurations of grid infrastructures.

The gateway implements some data management services by means of a graphical environment. A Data Management portlet (see the left portlet on Fig. 4) allows users the recycling of their private staging area within the system for managing their datasets as well as images produced from such datasets (see Fig. 5). All the evolutionary predictions generated by workflows are stored in a local file system or in an LFC distributed file system. The data management service is able to browse the two filesystems and gives the possibility to move upload and download user data from the web interface. Files can also be converted in VO-Tables, this allows to use VO tools like TOPCAT,[6] to analyse the simulation data, and to easily compare the theoretical predictions with observational counterparts and to import easily in the BaSTI database.

All the implemented portlets are developed with the Java Vaadin web Framework.[7] This open source framework has been employed to implement server side Java Servlet based web applications using the full power and flexibility of Java without taking care of the client side since it compiles the Java source code to JavaScript which can then be run on browsers.

5.1. Testing the science gateway

To verify the stability of the SG and of the DCI and the gain in performances when the number of jobs to process is close to a real production case, we set up a set of tests that involved the whole computing power and data storage offered by the A&A Virtual Organisation.

We submitted 100 concurrent FIRs (using the same set of parameters) with 10 portal users with the only requirement of finding enough free disk space to save the output on the close Storage

[6] http://www.star.bris.ac.uk/mbt/topcat/.

[7] http://www.vaadin.com.

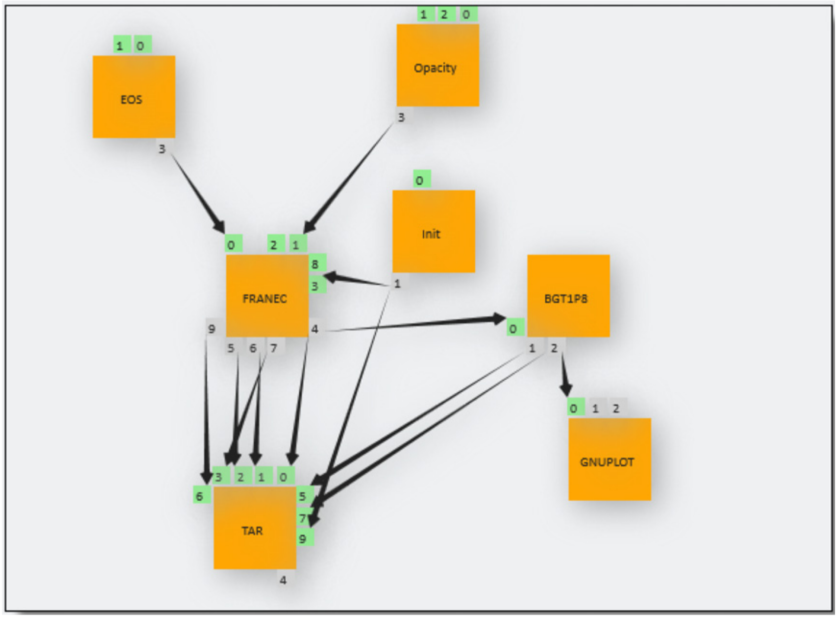

Fig. 3. FRANEC workflow.

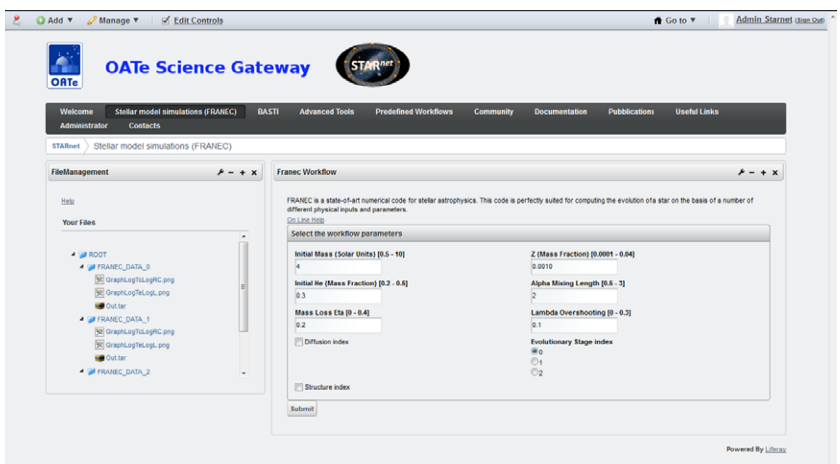

Fig. 4. FRANEC portlet (on the right) and Data Management portlet (on the left).

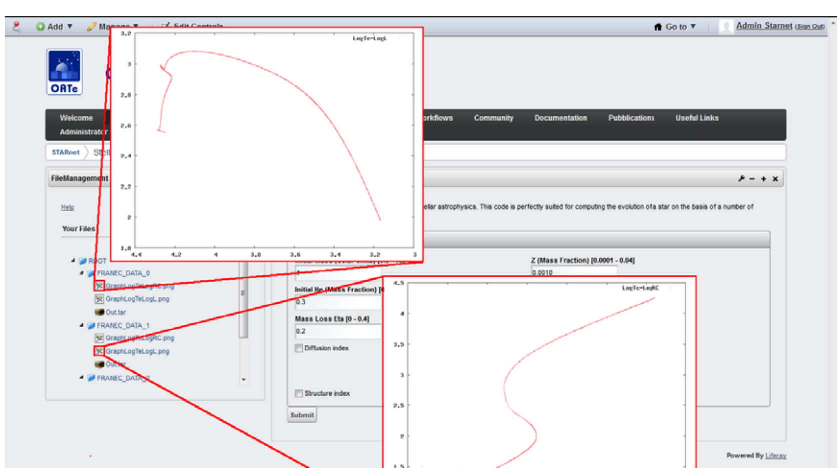

Fig. 5. Data Management portlet (on the left) allows users to visualise graphs produced by FRANEC Workflow.

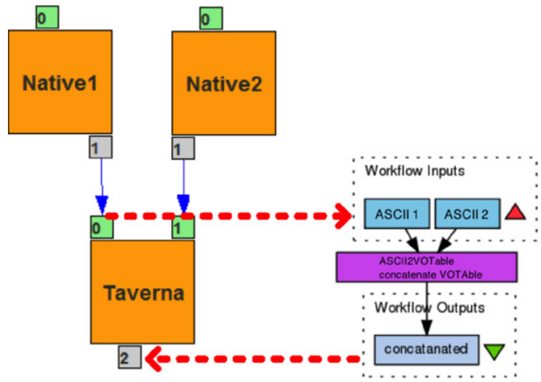

Fig. 6. Example of a workflow that is designed using two native modules and one Taverna2 AstroTaverna module that manipulate the output.

Element. Actually, during the test a number of jobs were scheduled and queued waiting for a free resource for their execution. The whole test lasts for about 4 days and was repeated different times with different load of the EGI grid with no significant change in the results. On average, the FIR is completed in ~80 min, which include: job scheduling, FIR execution (14 SMR), and the output data handling.

The SG was able to handle the tests with no particular performance issue, all the task where submitted, monitored and the data collected.

Finally, we noticed that ~3% of the jobs are lost. They are jobs that actually start but end with unpredictable errors (and they are not resubmitted by the WMS) or that last on the WMS queue. To solve this problem we introduced a time-to-live (ttl) parameter for each job in the DCI Bridge configuration. If the job is still scheduled when its ttl expires it is cancelled and resubmitted by the application specific services.

5.2. Science gateway and VO standards

In the framework of the Workflow4Ever project,[8] the Astrophysics community has developed more than 50 workflows using Taverna (Oinn et al., 2006) and the AstroTaverna plugin (Schaaff et al., 2012). AstroTaverna integrates existing Virtual Observatory web services as first-class building blocks in Taverna workflows (e.g. to search a registry, add found services to the workflow, manipulate data in form of VOTables, and convert coordinates).

Those *Data-oriented* workflows are used to interact with data, being mainly designed to search and get data in distributed database systems, manipulate data or perform simple data analysis tasks. Each of these "Atomic" operations are implemented by an individual simple workflow module. These workflow modules are simple to operate and do not demand large computing effort, so they are executed using the Taverna Desktop environment, by an astronomer. The data tasks run locally or on clusters using IVOA standards to access computing resources.

gUSE/WS-PGRADE technology allows to import and execute non-native workflows. A non-native workflow is a module in a WS-PGRADE workflow, which executes a workflow of some other workflow engine (e.g. a Taverna workflow). In this way it is possible to create a so called meta-workflow, which consists of a mixture of native and non-native workflows embedded within WS-PGRADE. Thanks to this capability we are able to embed AstroTaverna workflows as simple module to find and manipulate data and to access BaSTI database using IVOA standards directly from the gateway (see Fig. 6). In particular we use modules to create VOTables from ASCII files, manipulate VOTables for visualisation and search data in BaSTI archive.

8 http://www.wf4ever-project.org.

5.3. Science gateway development: lesson learned

Developing a SG poses some important challenges, in particular: the adoption of a suitable technology, the DCI access and the user authorisation and authentication.

Although the gUSE/WS-PGRADE technology offers a valid framework to develop SGs, it also presents some significative drawbacks. gUSE/WS-PGRADE project is continuously developed and the developer community is extremely active, therefore new framework versions are released frequently (a new one each month) and upgrades are often required (in particular security patches). The upgrade procedure can only be performed from one release to the next one and it consists of a list of commands to execute manually on the server. Since no automatic procedure is available the update/upgrade process is error-prone and requires a full science gateway (re)configuration.

Upgrade manuals are available for each release, but the administrator must get acquainted with the procedure. FRANEC SG is installed on a virtual machine, that simplify software upgrades and gateway maintenance.

Developing this gateway required Astronomers to create a precise list of requirements the gateway must meet, and a gateway developer to implement the framework, user interface and to link it to the workflow system to run these workflows. A SG expert profile is mandatory for successfully configure the system. This profile is related to the installation, configuration and maintenance of the portal (the operator), as well as to the design and implementation of graphical web user interfaces to configure, submit, monitor and access the results of application (the developer).

Programming (mainly web programming) and system administration skills are required to install, operate and customise the gUSE/WS-PGRADE framework. In particular, to customise the gateway, it is required to learn the basics of portlet development (mainly based on Java Server Pages) and the Application Specific Module (ASM) API. However, once the programmer implement the first portlet and struggle with the first issues (regarding for example the gUSE web service connection or the proper usage of the ASM API) the portlet can be used as template to build new portlets. Nevertheless an example portlet and ASM usage manuals can be downloaded from the gUSE/WS-PGRADE sourceforge page and a forum is available to discuss any issue in using the technology.

The access to DCI resources was another challenge to face in developing this SG. The *DCI Bridge* component was configured in order to access EGI.eu grid, the configuration file consists of two set of parameters: a DCI specific (e.g. the Virtual Organisation, the WMS, the LFC) and a gUSE specific (that influence the portal behaviour). While the first set of parameters is easy to define, the second one is more complex to tune. In fact, the default configuration does not turn on any job control feature and our first tests resulted totally unsatisfactory: more that 50% of the jobs failed. Tuning the configuration parameters and in particular the *retry_count*, enables the job control and automatic resubmission in case of failure, improving the stability and reliability of the service.

6. Discussion

In the last years, the BaSTI stellar evolution database has been largely used as a test-case for the integration and interoperability between VO and DCI facilities (see e.g. Taffoni et al., 2010). Nowadays BaSTI provides, not only a database of stellar evolutionary tracks, but also a set of tools that facilitate the analysis of observations of stellar populations, providing "on demand" stellar evolution predictions thanks to a SG.

To provide an efficient "on demand service" for the Astronomical community and to feed the BaSTI database with new data, it is necessary to use an infrastructure able to execute a large number of numerical simulations. The vast number of simulations required can be generated by computational resources that exceed what the single institution can offer and for this reason DCI solutions are extremely useful. Moreover, the adoption of a web interface can increase the number of Astronomers that benefit of this service and provides effective usage of the e-infrastructures.

The adopted SG technology requires to build workflow-oriented gateways. A workflow-oriented gateway enables scientists to share their workflows and to identify best practices for investigating their datasets. However, in this specific implementation, we are not profiting of the overall workflow capabilities, FRANEC is a simple application with three main software components easily interconnected, and it could be designed also as a single application. The goal of our work was the development of a stable and reliable SG. Using a workflow-oriented gateway we also benefit from some previously designed workflow components (e.g visualisation components, and data management components) and we automate workflows for repeating computations varying input parameters (parameter-sweep jobs). Moreover, future developments will increase the complexity of the FRANEC application that, being designed as a workflow, will be easily integrated with new components and with already available ones (e.g. the AstroTaverna components to access VO services).

In this paper we discuss the use of a SG as an effective tool to profit of a DCI grid environment in running FRANEC jobs. The approach we propose here is an improvement with respect to a previous work of Taffoni et al. (2010) where a complex script-based environment was developed to allow Astronomers to execute FRANEC jobs on the Grid.

The use of a SG framework based on gUSE/WS-PGRADE has some main advantages:

- It speeds up the SG design and development. We focus our development activity on the design and implementation of the workflows and workflow modules, and on the web portlets used to configure and execute the SFR and FIR (Fig. 4). All the implementation aspects, in particular the ones related to the interface towards the DCI, are built-in the gUSE/WS-PGRADE gateway framework and only need to be properly configured. The gateway framework offers the possibility to use different gateway's back-ends at the same time, so we are not limited in using only the grid infrastructure. Advanced users and developers can configure workflows or even workflow components to run on local linux clusters or on other DCIs.
- It offers an easy interface for Astronomers. A gateway may offer a simple web user interface that allows to configure and execute simulations, visualise the results and access to simulated data.
- It offers rapid prototyping of web user interfaces and strong support for parameter-sweep jobs.
- It offers a framework to integrate IVOA tools and services. The gUSE/WS-PGRADE technology is able to run workflows written using differ workflow languages requiring different workflows management systems (non-native workflows) for example Taverna, Kepler, Moteur (Terstyanszky et al., 2014). A meta-workflow is a workflow that involves both native and non-native workflows as its constituent parts. The ability to design and execute meta-workflows is a peculiar characteristic of gUSE/WS-PGRADE that can be used to re-use AstroTaverna workflows to access VO services directly from the portal.

This SG will be maintained by the Italian Virtual Observatory initiative VObs.it and by the Italian National Institute of Astrophysics. The planned future improvements of the FRANEC SG are the following:

1. We wish to include a TOPCAT visualisation portlet on the SG and to implement SAMP (Taylor et al., 2012) technology to make the SG communicate directly with the TOPCAT installed in the user desktop when available;
2. We wish to improve the graphical treatment of the stored data by providing new and more efficient tools for improving the access to the data as well as the interoperability among various (theoretical and observational) resources;
3. We wish to implement IVOA Theory access protocols and standards. This effort is a fundamental requirement to facilitate and improve the inclusion of micro-simulations data inside the VO.
4. We wish to make use the IVOA Parameter Description Language to facilitate the implementation of FRANEC software components in to workflows components. Actually, we are using a custom shell artefact to create the FRANEC workflow components, however using the PDL we will use a standard approach that will facilitate also the re-use of modules in other contexts.
5. We wish to implement an interface towards the VOSpace to manage the results of the workflows execution also in a VO distributed storage environment.

7. Conclusions

We have received a positive feedback from the BaSTI users, reinforcing our belief that SG technology is a good approach for offering on-demand services to Astronomers. An effective SG framework is crucial to offer an efficient, extensible and maintainable service and we think that our results show that gUSE/WS-PGRADE is a good technology to develop a workflow-based gateway.

Even if extremely successful for FRANEC, according to our experience high level of technical competence is still necessary to set up and run calculations efficiently on a grid infrastructure and consequently an investment in terms of human resources to provide support for porting applications. For this reason we do not recommend the use of this approach unless already familiar with it.

The gUSE/WP-PGRADE framework help to avoid lock-in to particular computing and storage DCI by flexibly abstracting the resources; this should allow to migrate in an almost seamless manner from one underlying technology or provider to another modifying only the gUSE configuration. Our next step will be to migrate from the grid DCI to a cloud approach. In particular, we are planning to use the EGI Federated Cloud[9] that offers a general academic Cloud Infrastructure.

The cloud e-infrastructures has been already successfully implemented by other projects in A&A (see e.g. Gaudet et al., 2010) and they represent the natural evolution for FRANEC SG.

The development of this gateway results as collaboration between Astronomers and a SG expert. Also in the Teragrid and XSEDE science gateway initiatives, the infrastructure providers identify the roles of scientists and science gateway experts (Pierce et al., 2010; Wilkins-Diehr et al., 2008b). According to our experience this workflow-oriented gateway technology is not particularly complex to setup and maintain and also teams that are not familiar with it will be able to develop SG with a few efforts. Moreover the use of workflows will give more flexibility to the gateway, even if it implies a small overhead in learning the framework and implementing the gateway respect to other technologies.

FRANEC gateway is also one of the partners of STARnet gateway federation. STARnet Gateway Federation, is a federation of Astronomy and Astrophysics oriented SG designed and implemented to support the Astronomy and Astrophysics community and its peculiar needs (Becciani et al., 2014).

STARnet envisages sharing a set of services for authentication, a common and distributed computing infrastructure, data archives and workflows repositories. Each gateway provides access to specialised applications via customised workflows, the first

9 https://www.egi.eu/infrastructure/cloud/.

implementation of STARnet provides workflows for cosmological simulations, data post-processing and scientific visualisation. These applications run on local or shared computing infrastructures thus guaranteeing resources availability and they can be shared between the different communities of the federation, published worldwide for dissemination purposes or kept local for privacy issues.

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