



# EGI-InSPIRE

## PORTED APPLICATIONS WEBSITE

### EU MILESTONE: MS303

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#### Abstract

This document describes the current status of the EGI Applications Database (<http://appdb.egi.eu>) and the future steps to be taken to produce a full-fledged, community driven portal, which will act as a point-of-reference for scientific software and tools that are available in the EGI infrastructure, as well as a registry of persons who were involved of the development of these high level applications. The database serves as an important tool to promote the significance of EGI in e-Science and to facilitate the reuse of applications and expertise that is available in NGIs.



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## II. DELIVERY SLIP

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3.0	21/07/2010	Draft to review	Gergely Sipos, EGI.eu
4.0	30/07/2010	Review response modifications	William Vassilis Karageorgos, IASA Nafsika Zarife, IASA

## IV. APPLICATION AREA

This document is a formal deliverable for the European Commission, applicable to all members of the EGI-InSPIRE project, beneficiaries and Joint Research Unit members, as well as its collaborating projects.



## **V. DOCUMENT AMENDMENT PROCEDURE**

Amendments, comments and suggestions should be sent to the authors. The procedures documented in the EGI-InSPIRE “Document Management Procedure” will be followed:

<https://wiki.egi.eu/wiki/Procedures>

## **VI. TERMINOLOGY**

A complete project glossary is provided at the following page: <http://www.egi.eu/results/glossary/>.



## VII. PROJECT SUMMARY

To support science and innovation, a lasting operational model for e-Science is needed – both for coordinating the infrastructure and for delivering integrated services that cross national borders.

The EGI-InSPIRE project will support the transition from a project-based system to a sustainable pan-European e-Infrastructure, by supporting ‘grids’ of high-performance computing (HPC) and high-throughput computing (HTC) resources. EGI-InSPIRE will also be ideally placed to integrate new Distributed Computing Infrastructures (DCIs) such as clouds, supercomputing networks and desktop grids, to benefit user communities within the European Research Area.

EGI-InSPIRE will collect user requirements and provide support for the current and potential new user communities, for example within the ESFRI projects. Additional support will also be given to the current heavy users of the infrastructure, such as high energy physics, computational chemistry and life sciences, as they move their critical services and tools from a centralised support model to one driven by their own individual communities.

The objectives of the project are:

1. The continued operation and expansion of today’s production infrastructure by transitioning to a governance model and operational infrastructure that can be increasingly sustained outside of specific project funding.
2. The continued support of researchers within Europe and their international collaborators that are using the current production infrastructure.
3. The support for current heavy users of the infrastructure in earth science, astronomy and astrophysics, fusion, computational chemistry and materials science technology, life sciences and high energy physics as they move to sustainable support models for their own communities.
4. Interfaces that expand access to new user communities including new potential heavy users of the infrastructure from the ESFRI projects.
5. Mechanisms to integrate existing infrastructure providers in Europe and around the world into the production infrastructure, so as to provide transparent access to all authorised users.
6. Establish processes and procedures to allow the integration of new DCI technologies (e.g. clouds, volunteer desktop grids) and heterogeneous resources (e.g. HTC and HPC) into a seamless production infrastructure as they mature and demonstrate value to the EGI community.

The EGI community is a federation of independent national and community resource providers, whose resources support specific research communities and international collaborators both within Europe and worldwide. EGI.eu, coordinator of EGI-InSPIRE, brings together partner institutions established within the community to provide a set of essential human and technical services that enable secure integrated access to distributed resources on behalf of the community.



The production infrastructure supports Virtual Research Communities (VRCs) – structured international user communities – that are grouped into specific research domains. VRCs are formally represented within EGI at both a technical and strategic level.

## VIII. EXECUTIVE SUMMARY

The EGI Applications Database (henceforth also referred to as *AppDB* in this document) is the descendant of the EGEE Applications Registry [R 4] portal, which was initially developed by the IASA regional coordination team during the course of the EGEE-III project. It provides a catalogue of applications that have been ported, or are being ported, within the infrastructure [R 1]. As such it enables new communities to discover and reuse EGI applications, thus avoiding duplication of effort. By the reuse of ported applications one of the main barriers of grid adoption is eliminated.

At the time of writing, the first release of the EGI Applications Database portal is in production, and it provides read-only access to the hosted applications and people data. The next step is to finalize the developments on the read-write mode of the portal and to provide an authentication mechanism for users through the EGI Single Sign On (SSO) system. The next release of the AppDB with these features is expected to be in production in the middle of September 2010.



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## 1 INTRODUCTION

This document describes the current status of the EGI Applications Database (<http://appdb.egi.eu>) and the future steps to be taken to produce a full-fledged, community driven portal, which will act as a point-of-reference for scientific software and tools that are available in the EGI infrastructure, as well as a registry of persons who were involved of the development of these high level applications. The database serves as an important tool to promote the significance of EGI in e-Science and to facilitate the reuse of applications and expertise that is available in NGIs.



## 2 APPLICATIONS DATABASE

### 2.1 Introduction

The EGI Applications Database portal's [R 1] main goal is to provide all the necessary information about the applications running on the EGI Grid infrastructure thus enabling people to search for applications matching a pattern (such as scientific domain) – and also to contact the corresponding authors for guidance on application usage or further developments. Currently, it provides, among other information, the name, description, discipline and sub-discipline of applications, status, useful websites, abstract, scientific contact list, related publications and associated VOs. Moreover, since the EGI era started, the RESPECT [R 6] tools have also been registered in AppDB, making the database an even more valuable service for both application developers and end-users. Furthermore, during the EGEE to EGI transition process, the concept of storing personal profiles for each individual application developer and researcher was introduced, a feature that aims at simplifying the search for application developer experts who possess specialised knowledge.

By exploiting the above features, the portal aims to be community-driven, with information flowing inwards directly from involved individuals – NGI representatives, developers, and end-users alike. NGI representatives and developers on one hand should be responsible for keeping their applications' information up-to-date, while end-users on the other could contribute by sending valuable feedback to the developers, or by posting details of their experience with software on the EGI Wiki pages deployed for this purpose, which will be advertised through the portal. In order to create the vibrant user community needed to achieve this aim, various techniques may be employed, such as the use of informative mailing lists, RSS feeds, and messaging facilities. Moreover, integration with widely-used social networking sites could also be employed at some future point, in order to minimizing the effort needed by users to stay connected.

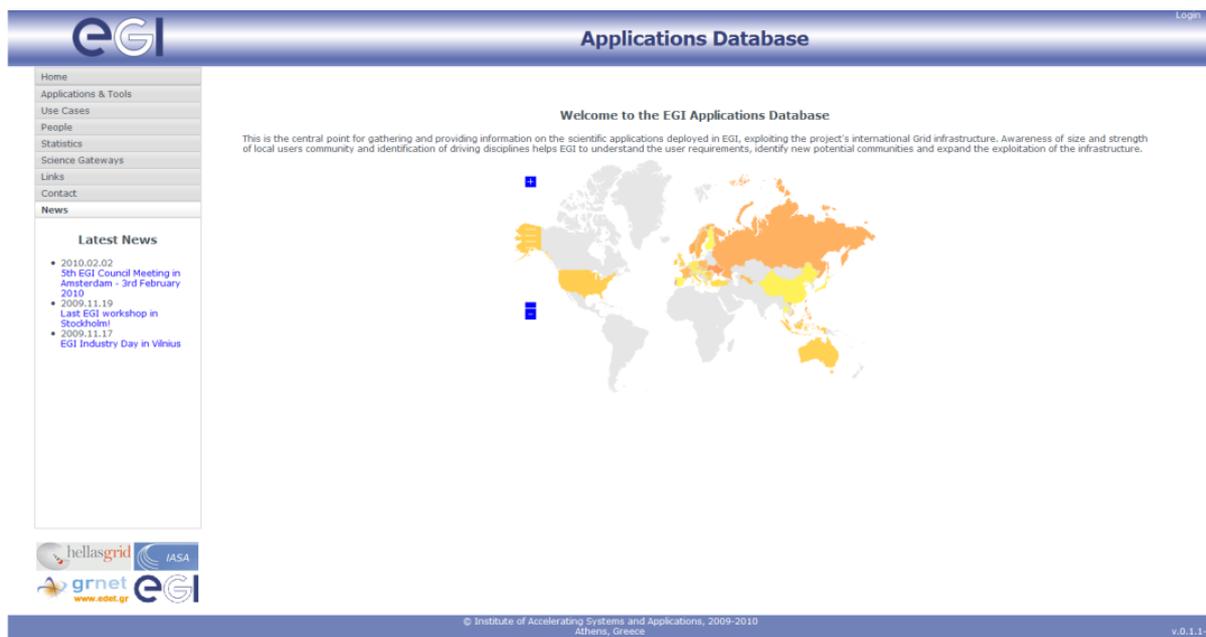
Apart from information flow, another important aspect is integrity and quality of information. Eliminating obsolete entries makes it easier for end-users to find what they want, while keeping a log of updates for each entry may give a quick picture of how active a certain application is. Such issues have been provisioned for and are due to appear in later versions. More specifically, NGI representatives could have the final say in marking orphaned entries as obsolete, and end-users may be able to view eliminated entries in a separate historical view.

It should be noted that the EGI Application Database portal is the descendant of the EGEE Applications Registry portal [R 4]. This portal was connected to a central database located at INFN. This database was also accessed by another portal interface [R 5] developed and provided by the INFN Catania application porting team. Both, the EGEE Applications Registry portal and the INFN's database remain accessible in read-only mode for historical reasons, until the users get used to the new portal.

The EGI Application Database portal, along with the physical database it is connected to, is developed, maintained and hosted by the Institute of Accelerating Systems and Applications, University of Athens (IASA).

## 2.2 Portal Navigation

The EGI Application Database user interface is divided in two main areas; a navigation pane on the left, and a data display pane on the right. Users can select the type of information they want to access from the navigation pane, which is subsequently displayed in the pane on the right.



**Figure 1. The main page of the AppDB portal, with the navigation pane on the left, and the data display pane on the right.**

The navigation pane contains the following categories:

- Applications and Tools: Allows access to the index of applications and tools, as well as the registration form for new entries [Fig. 1a]. Advanced and quick filters are located on the top of the page, assisting to user to find applications of interest based on his/her given criteria (i.e. discipline, sub-discipline, keywords, regionalized criteria etc.).
- Use Cases: A placeholder containing a link to the EGI Wiki portal, which may allow access to information on successful porting of individual applications in future releases [Fig. 1b].
- People: Allows access to the index of people profiles [Fig. 1c].
- Statistics: Allows access to statistics graphs about applications or people versus various parameters, such as disciplines, countries, etc. [Fig. 1d].
- Science Gateways: A placeholder for allowing access to existing or to be developed information portals within the identified scientific communities [Fig. 1e]. Please refer to section 2.5.2 for more information.

Moreover, there exists a few more tabs under the navigation pane, such as Links, Contact, and News, with self explanatory content. Further details about the features and functionality of the current version of the AppDB are provided in Section 2.3.

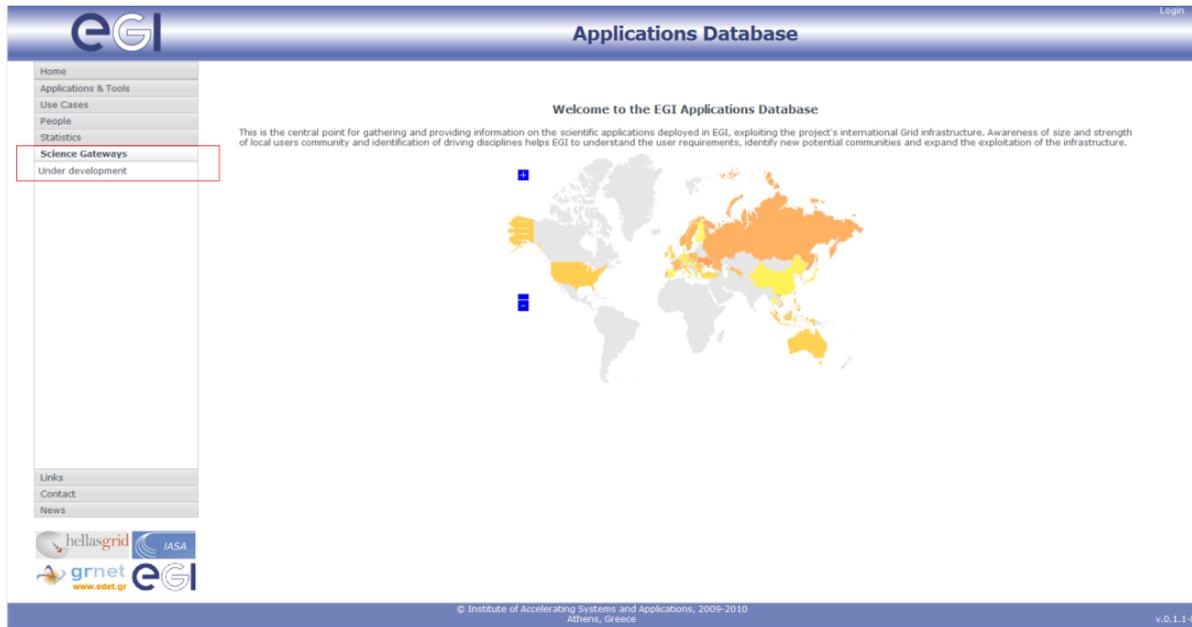
The screenshot shows the EGI Applications Database interface. The top header includes the EGI logo, the title 'Applications Database', and a 'Login' link. Below the header is a navigation pane on the left with tabs for 'Home', 'Applications & Tools', 'Use Cases', 'People', 'Statistics', 'Science Gateways', 'Links', 'Contact', and 'News'. The 'Applications & Tools' tab is active, displaying a list of applications and a 'Register Application' button. A filter dropdown is open, showing a list of disciplines such as 'Astronomy, Astrophysics, and Astro-Particle Physics (54)', 'Computational Chemistry (17)', 'Computer Science and Mathematics (30)', 'Earth Sciences (19)', 'Fusion (6)', 'High-Energy Physics (15)', 'Life Sciences (59)', and 'Others (57)'. The main display area shows a grid of application cards, each with a gear icon and a title. The cards include: 'hydrogen molecule model', 'Number DAta', '(no name yet)', '(no name yet)', '3D-H2+', 'AA-GISSmodelE', 'Abaqus by SIMULIA', 'ABC', 'ABC', 'ABINIT', 'ADAP', 'ADAT', 'aITALC', 'ALICE', 'AllRoot', 'ALMOST', 'AMBER', 'AMCBI', 'AMGA WI', and 'AMIAS'. The bottom of the page features logos for hellasgrid, IASA, grnet, and EGI, along with copyright information: '© Institute of Accelerating Systems and Applications, 2009-2010 Athens, Greece' and version 'v.0.1.1-8'.

Figure 1a. Applications index, with the navigation pane opened at the Applications and Tools tab. A toggle-able quick filter is also displayed in the display pane.

The screenshot shows the EGI Applications Database interface with the 'Welcome to the EGI Applications Database' message. The navigation pane on the left is open to the 'EGiWiki' tab. The main display area features a world map with colored regions indicating the locations of users or applications. The map shows high concentrations in Europe and Asia. The bottom of the page features logos for hellasgrid, IASA, grnet, and EGI, along with copyright information: '© Institute of Accelerating Systems and Applications, 2009-2010 Athens, Greece' and version 'v.0.1.1-8'.



**Figure 1d. Statistics pie chart sample, with the navigation pane opened at the Statistics tab. The export button is activated and shown on the right.**



**Figure 1e. Scientific Gateways opened at the navigation pane.**

## 2.3 Current Status

The AppDB service is in production status since May 2010 [R 1], but it only offers read-only access to the applications and people data. The most important features and functions that are already provided by the service are:

- Features related to Applications and Tools
  - Name, logo, description, discipline, abstract, status, countries, VO data, etc.
  - List of associated researchers and publications
  - List of URLs such as website, documentation, etc.
- Features related to People's profiles
  - Name, role, institute, country, contact information data
  - List of associated applications and publications (reverse lookup)
- User experience related features
  - people and application statistics graphs: Bar charts and pie charts of people or applications versus discipline, country, region, etc. [Fig. 4]
  - index page / statistics filtering: searching functionality is implemented through an extended data filtering mechanism

- toggle-able quick filters: for ease-of-use, some properties deemed more important are offered as quick filters located on the top of the page
- list of documents / publications for applications and people: documents are directly associated with applications, but reverse lookup is possible through people's profiles
- grid / list view for index pages: data index pages can be viewed in either a concise grid view, with an emphasis on the datum's logo/image [Fig. 2a], or a more detailed list view [Fig. 2b] where one can easily see more information about the datum without having to access the properties window [Fig. 3]. Views can be switched through the icon buttons located on the top-right edge of the page
- Data export features
  - XML/CSV export of applications and people data: Simple and concise CSV files, aimed towards human readability, and more detailed XML files aimed towards automated data exchange and analysis
  - PDF/JPG/PNG/SVG export of aforementioned statistics graphs: JPG/PNG formats for general purpose use, scalable SVG format for better presentation, and PDF format for ease-of-use with editors such as LaTeX.
- Other features
  - discrimination between applications and tools: Software packages aimed towards improving application performance and use – such those offered by the RESPECT program – and which do not lead directly to publications, are considered *tools* and are managed in a different way
  - application links to websites, documentation, etc.
  - manual registration of new applications through an according form offered for download (this is a temporary feature, until the read/write mode of the AppDB is ready for deployment).

As far as the current AppDB content is concerned, the data is the same as it has been migrated from the EGEE Applications Registry plus the webpage of the RESPECT program; this consists of 249 applications, 19 tools, (from the RESPECT program), and 494 people profiles. The Applications Database is publicly accessible at <http://appdb.egi.eu>, and is also linked from the User Support section of the EGI.eu website [R 3].

One may notice that there are almost twice as many people registered in the database than there are applications, and that most applications are from development teams based in Italy. The former observation is due to the fact that there is usually more than one person involved in the development of a grid application, and there aren't many applications registered yet from the same team. The large number of Italian applications can be attributed to the fact that the migrated data originating from INFN's database, which was mainly populated by INFN's staff. Both of these effects are expected to subside, once the write-enabled version of the AppDB is deployed and more data flows in by the developers, resulting in a better balanced view of applications.

Figure 2a. Application browser (grid view)

Figure 2b. Application browser (list view)

Application Details - 2D-MC-MOSFET

**Information** | Publications



ID: 110  
Name: 2D-MC-MOSFET  
Description: 2D Monte Carlo Doble Gate Silicon on Insulator MOSFET simulator  
Discipline: Computer Science and Mathematics  
Subdiscipline: Nanotechnology

[Website](#)

Monte Carlo simulations of semiconductor devices are computationally very expensive when a realistic simulation is required. This application simulates a 2D Double Gate Silicon on Insulator (DGSOI) MOSFET using the Monte Carlo method. The main motivation of this application is to reduce the execution time and to perform parametric computations over the grid. Therefore, thanks to grid computing we may perform a wide amount of important simulations to study physical characteristics of different transistors.

Country: Spain   
Region: SWE  
VOs: cesga  
Status: HandledByRS  
Added on 2010-04-29 20:54:33

**Scientific Contacts**

 <b>Huedo Eduardo</b> Regional Contact Universidad Complutense de Madrid	 <b>García Loureiro Antonio</b> Scientific Coordinator Universidad de Santiago de Compostela
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Figure 3. Application details card sample

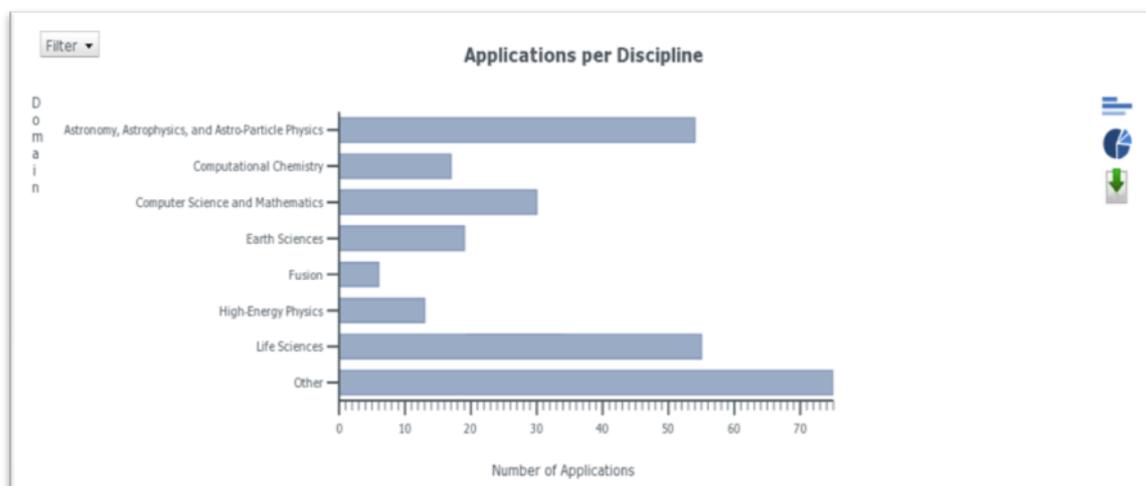
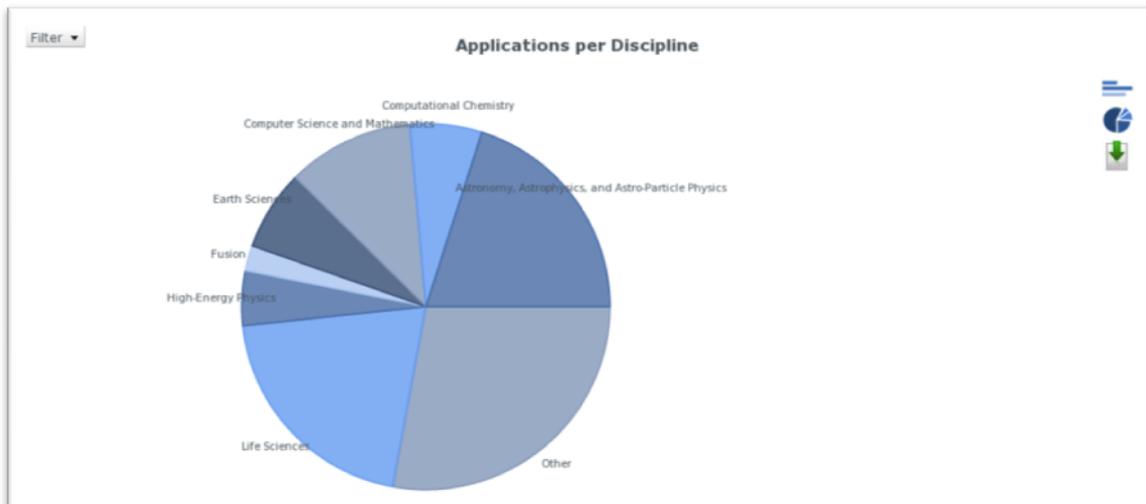


Figure 4. Statistics graph samples

## 2.4 AppDB Support Unit in Global Grid User Support (GGUS)

Communication with the AppDB support staff can be achieved in two ways:

1. Through the NGI based mailing list [appdb-support@hellasgrid.gr](mailto:appdb-support@hellasgrid.gr)
2. Through the AppDB Support Unit established in the Grid Global User Support (GGUS) system.

The main aim of the AppDB support unit is to deal with all kind of issues related to AppDB, such as issues concerning bugs, problems, requests for enhancements, requests for changes/modifications to the AppDB context etc.

In general, the contact procedure can be summarized in the creation of a ticket in GGUS, which gets assigned to the AppDB Support Unit, and an email notification which gets sent to the [appdb-support@hellasgrid.gr](mailto:appdb-support@hellasgrid.gr) mailing list.

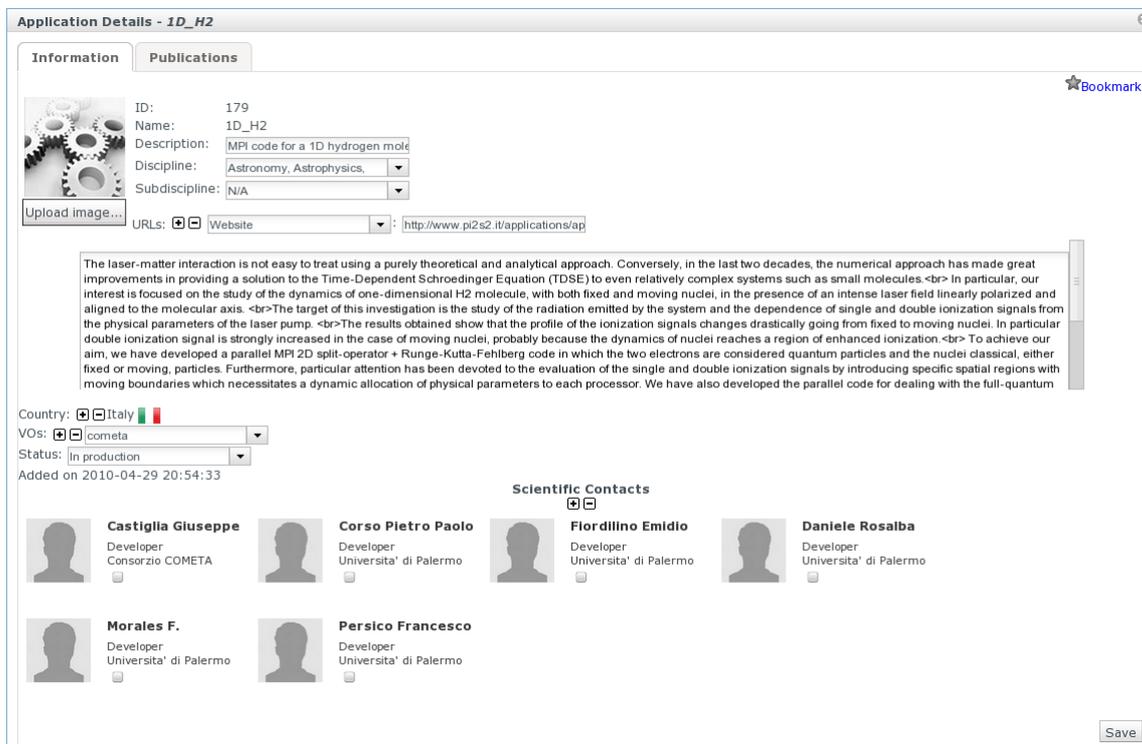
## 2.5 Next Steps

### 2.5.1 Upcoming version

The development of the AppDB are focused on the following objectives:

- Binding the AppDB with the EGI SSO system, and
- Enabling write mode of the AppDB to users with SSO account to:
  - Register new applications, instead of requesting that data be inserted for them by the AppDB support team
  - Edit existing application data and associate people with applications [Fig. 5, 6]
  - Edit their personal profiles
  - Bookmark applications
- Editing privileges based on users' role and additional permission granting based on a fine-grained control policy

These developments have already been initiated and are planned to be finalized no later than mid September, 2010. The prototype version of the new (upcoming) AppDB, can be accessed (upon request) at [R 2].



**Application Details - 1D\_H2**

Information | Publications

 ID: 179  
 Name: 1D\_H2  
 Description: MPI code for a 1D hydrogen mole  
 Discipline: Astronomy, Astrophysics  
 Subdiscipline: N/A

Upload image...  
 URLs: Website: http://www.pi2s2.it/applications/ap

The laser-matter interaction is not easy to treat using a purely theoretical and analytical approach. Conversely, in the last two decades, the numerical approach has made great improvements in providing a solution to the Time-Dependent Schroedinger Equation (TDSE) to even relatively complex systems such as small molecules. In particular, our interest is focused on the study of the dynamics of one-dimensional H<sub>2</sub> molecule, with both fixed and moving nuclei, in the presence of an intense laser field linearly polarized and aligned to the molecular axis. The target of this investigation is the study of the radiation emitted by the system and the dependence of single and double ionization signals from the physical parameters of the laser pump. The results obtained show that the profile of the ionization signals changes drastically going from fixed to moving nuclei. In particular double ionization signal is strongly increased in the case of moving nuclei, probably because the dynamics of nuclei reaches a region of enhanced ionization. To achieve our aim, we have developed a parallel MPI 2D split-operator + Runge-Kutta-Fehlberg code in which the two electrons are considered quantum particles and the nuclei classical, either fixed or moving, particles. Furthermore, particular attention has been devoted to the evaluation of the single and double ionization signals by introducing specific spatial regions with moving boundaries which necessitates a dynamic allocation of physical parameters to each processor. We have also developed the parallel code for dealing with the full-quantum

Country: Italy  
 VOs: cometa  
 Status: in production  
 Added on 2010-04-29 20:54:33

**Scientific Contacts**

 <b>Castiglia Giuseppe</b> Developer Consorzio COMETA	 <b>Corso Pietro Paolo</b> Developer Universita' di Palermo	 <b>Fiordilino Emidio</b> Developer Universita' di Palermo	 <b>Daniele Rosalba</b> Developer Universita' di Palermo
 <b>Morales F.</b> Developer Universita' di Palermo	 <b>Persico Francesco</b> Developer Universita' di Palermo		

Save

Figure 5. Application information editing card sample

Application Details - 1D\_H2

Information Publications

Title	Type	Conference Proceedings	Volume	Pages	Year	Publisher	ISBN
H2 Molecule Driven by a Laser Field	Full Paper	Grid Open Days at the University of Palermo, Palermo (Italy) the Symposium GRID Open Days at the University of Palermo		133 - 139	2008		978-88-95892-00-9
Bremsstrahlung from a repulsive potential: attosecond pulse generation	Full Paper						
Evidence of Nuclear Motion in H <sub>2</sub> -like Molecules by Means of High Harmonic Generation	Full Paper						
Control of Electron Motion in a Molecular Ion: Dynamical Creation of a Permanent Electric Dipole	Full Paper						
Hydrogene molecule in intense laser fields	Full Paper						
X-ray Emission from Protostellar Jets	Full Paper						
Parallel numerical simulation of a H <sub>2</sub> molecule in intense laser fields	Full Paper						
Harmonic Spectra in H <sub>2</sub> <sup>+</sup> in the Presence of a Laser Field	Full Paper	Grid Open Days at the University of Palermo, Palermo (Italy) the Symposium GRID Open Days at the University of Palermo		285 - 287	2007		978-88-95892-00-9
The Study of the Nuclear Motion in D <sub>2</sub> + Molecular Ion By Using the Harmonic Spectra	Full Paper	International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007)			2007		

**Edit publication data**

Title:

URL:

Conference:

Proceedings:

Volume:  Pages: From  To

Year:  Type:

Publisher:  ISBN:

Authors:

Figure 6. Publication editing card sample

## 2.5.2 Future versions

There are also plans to perform all the necessary enhancements and modifications needed in order to make the Applications Database also act as a registry for Science Gateways/Portals, which either exist, or will be developed within the identified scientific communities. For this purpose, an entry on the portal's navigation panel has been reserved. We are going to promote this kind of development to the communities of interest, in three main ways:

- In a "bulletin form", through announcements in the Applications Database portal.
- In a "periodic updates form", through periodic informative emails, using scientific contacts information contained in the database.
- In a "news form", through the creation of discipline-based RSS channels.

Another issue for future development is browser support for IE 8. Currently known supported browsers are Firefox 3.x, Google Chrome 5.x, Safari 5, and Opera 10.x, with the first two most thoroughly tested. At the time being, IE support is rather basic, due to technical reasons attributed to the browser's particularities. User requests and feedback will be evaluated and compared to the effort needed to implement IE support, in order to plan for its inclusion in future releases.

One more issue that needs to be evaluated and finally be covered in a future release of the AppDB, it is about the establishment of a review process for the applications/tools that already exists in the AppDB. For example, this procedure should cover the way that obsolete entries get removed from the AppDB.



### 3 CONCLUSION

At the time of writing, the EGI Applications Database consists of 249 registered applications, 19 tools (from the EGEE RESPECT program), and more than 490 people/scientists profiles.

The first release of the EGI Applications Database portal is in production since mid of May 2010 and provides read-only access to hosted application and people data. The next step is finalizing development on the write-enabled mode of the portal, as well as providing an authentication mechanism to registered users through the EGI SSO system. The next release of the AppDB is expected to be in production in the middle of September 2010.

## 4 REFERENCES

R 1	EGI Application Database (AppDB): <a href="http://appdb.egi.eu">http://appdb.egi.eu</a>
R 2	Prototype of the next release of AppDB (not publicly available): <a href="http://appdb-dev.marie.hellasgrid.gr/">http://appdb-dev.marie.hellasgrid.gr/</a>
R 3	User Support section of the EGI.eu website: <a href="http://www.egi.eu/user-support">http://www.egi.eu/user-support</a>
R 4	EGEE Applications Registry: <a href="http://appdb.egee-eu.org">http://appdb.egee-eu.org</a>
R 5	INFN interface to EGEE Application registry: <a href="http://grid.ct.infn.it/egee_applications">http://grid.ct.infn.it/egee_applications</a>
R 6	EGEE RESPECT program (Recommended External Software for EGEE Communities) <a href="http://technical.eu-egee.org/index.php?id=290">http://technical.eu-egee.org/index.php?id=290</a>