**Recommendations to improve the Applications Database   
and Operations Portal services to better serve scientific communities**

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In April 2012 EGI.eu opened an Application Expert secondment position for the NGIs. In May 2012 Jelena Tamuliené from the Lithuanian NGI has been selected for the position and she worked in the EGI.eu User Community Support Team between July-September. Jelena’s scientific background is in Computational Chemistry and one of her first tasks in the secondment position was to review the profiles of applications and tools that the NGIs offer in the EGI Applications Database (AppDB)[[1]](#footnote-1) for ‘Computational Chemistry and Material Sciences’ communities and to make suggestions on improving these application profiles, as well as the AppDB service itself for such communities.

The review of application and tool software entries of AppDB is reported in the first section of the document. The second section is a summary of the feedback that Jelena provided on the AppDB service itself, together with recommendations from the EGI.eu User Community Support Team on how to improve the AppDB and Operation Portal services in order to address the reported issues.

Although Jelena’s review was made from the ‘Computational Chemistry and Material Sciences’ perspective, her remarks could be made by the representative of any other scientific disciplines and therefore the suggestions of this document can help EGI improve the attractiveness of AppDB for researchers of other fields. In the future similar AppDB reviews should be made by other types of users, for example by software developers (software providers and integrators) and by dissemination/scientific writers.

1. **Computational Chemistry software review**

Most of the high level software services that NGIs offer for scientific communities are registered in the EGI Applications Database. Software within this database is categories by various parameters, including the scientific discipline. The below table provides a listing of software that are registered under the ‘Computational Chemistry and Material Sciences’ discipline within the database. Jelena’s review focussed on the accessibility of these software, i.e. is it visible within the database who and how is allowed to use these tools? If so, then is there any limitation for access, for example in respect to the nationality or location of the user?

For many of the software items the review pointed out that the method and conditions of access is undefined or unclear (Indicated as ‘unclear’ in the table). For these items:

1. The providers of those software need to be asked to complete/correct the registration.

and

1. The AppDB system itself need to be improved to systematically collect and present accessibility information about the registered items.

The second section of the document provides particular recommendations to AppDB for point 2. Once these recommendations are implemented by AppDB the software profiles that are registered in the system need to be systematically updated with information about accessibility. (to address point 1).

For some of the software items the table points out specific issues, such as being registered under the wrong scientific discipline, or displaying incoherent information in AppDB and the software native interface (e.g. a portal). These issues need to be dealt with on a one-by-one basis.

|  |  |  |
| --- | --- | --- |
| **Name of the registered software** | **Information about accessibility  by an external user** | **Additional remarks** |
| 3D-tdMC | VO cometa, **Unclear** |  |
| ABC | VO compchem, **Unclear** |  |
| ADF | VO vo.plgrid.pl, **Unclear** |  |
| Autodock VINA | **Unclear** | It is currently under ‘Computational Chemistry’ discipline. It can be relevant also to Bioinformatics, Life Science domains. |
| Autodock\_virtscreen | To use this application one needs to have a user account on the servers of CSC and must have access to the Finnish or Nordic grid environments. | It is currently under ‘Computational Chemistry’ discipline. It can be relevant also to Bioinformatics, Life Science domains. |
| COLUMBUS | VO compchem, **Unclear** |  |
| CANGRD | **Unclear** | To study interaction between turbulence and cavitation phenomena, and its effects on the development of the Diesel spray, i.e. it is not Computational Chemistry domain (probably engineering). |
| |  | | --- | | CPMD | | VO vo.plgrid.pl, **Unclear** |  |
| Crystal06 | VO balticgrid, **Unclear** |  |
| DeMon | VO balticgrid, **Unclear** |  |
| |  |  | | --- | --- | |  |  |   DL\_POLY | VO compchem, **Unclear** |  |
| DLPROTEIN | VO cometa, **Unclear** |  |
| |  | | --- | | FLUSS | | VO compchem, **Unclear** |  |
| GAMESS | VOs cometa, compchem, vo.plgrid.pl, **Unclear** | If you are a member of Gaussian VO, the application is available through InSilicoLab and that is mentioned on a profile of the portal. This is inconsistent with the VO list of the application. |
| |  | | --- | | Gaussian | | VOs vo.pllgrid.pl, gaussian  Registration in Gaussian VO is open for every userwho possesses a valid certificate from any CA recognised by EGI. The membership is valid for a period of one year. | The information is wrong because Gaussian is not available through InSilicoLab portal. |
| ggamess | VO compchem, **Unclear** |  |
| GriF | VO compchem, **Unclear** |  |
| GROMACS | VOs vo.pllgrid.pl, compchem, **Unclear** |  |
| |  | | --- | | InSilicoLab | | VOs vo.pllgrid.pl, gaussian  To register in gaussian VO (see above) |  |
| MCTDH | VOs compchem, **Unclear** |  |
| MOPAC | **Unclear** |  |
| MoSGrid | **Unclear** |  |
| NAMD | VOs compchem, **Unclear** |  |
| Octave | VOs prod.vo.eu-eela.eu, eumed, **Unclear** | It is a high-level interpreted language, nether a tool or an application. Consider to remove from AppDB or open a new category for these type of items. |
| RWavePR | VO compchem, **Unclear** |  |
| SC­IVR | VO compchem, **Unclear** |  |
| |  |  | | --- | --- | |  |  |   Serpens for Kepler | VO fusion, phys.vo.ibergrid.eu, vo.plgrid.pl, **Unclear** | To become member of chem.vo.ibergrid.eu the user should have an invitation from a member inside the VO.  It is not clear how to become the member of other VO. |
| SFS | VO SEE, **Unclear** |  |
| SIMAP | **Unclear** | It is currently under ‘Computational Chemistry’ discipline. It can be relevant also to Bioinformatics, Life Science domains. |
| SOMA2 | **Information in AppDb:** To use this service, an e-mail to grid-support@csc.fi must be send. This e-mail must include certificate's subject line.  **On web page of SOMA2:** requires an account from an institute in the HAKA federation. | The tool is not mentioned in the Computational Chemistry domain  (It is in discipline: Others).  Information provided in AppDb and on SOMA2 is incoherent. |
| SyMPoM | VO cometa, **Unclear** |  |
| VENUS96 | VO compchem, **Unclear** |  |

Some of the applications that are currently not classified under the ‘Computational Chemistry’ domain can be relevant to scientists within this domain thus should be made visible under this domain in AppDB. There is no objective answer on which one these tools and applications are because the boundary of the Computational Chemistry domain is fuzzy, but based on Jelena’s review the following applications and tools should be made visible under the Computational Chemistry domain: Abaqus by SIMULIA, ABINIT, ALMOST, AMBER, CB, Gromacs-WeNMR, JST, Migrating Desktop, RPA-MBS, SOMA2.

1. **Feedback and recommendations on the AppDB service**
2. Feedback:   
   AppDB presents applications, tools and Virtual Organisations (VO) in the highest level of the menu hierarchy. At the same time these services are not equally relevant for a scientific user:
   * Applications (e.g. Gaussian, Gromacs) are meaningful services to those researchers who want to use gridified applications.
   * Tools are meaningful services to those researchers who want to gridify custom applications.
   * VOs have secondary relevance in either cases, because the term ‘VO’ is not meaningful for a scientific user (VO is specific to grid in the AppDB context) and VO membership is often not even needed to use an application or a tool.

Recommendation:

1. Put software into the center of AppDB. (Any type of software in the broadest sense). Any other entity is ‘just’ meta-information about software that are stored in the system. The software and the meta-information should not be at the same level in the menus. (See how iPods use meta-information about an MP3 file for search and categorisation. For example Artists and Music are not at the same level in the menu of iPod.)
2. Feedback:   
   Information about the availability and methods of access of software is not available in application/tool profiles (Table 1.). Information and conditions are often missing for those applications software that are available for third party access (either by download or as an online service).

Recommendation:

1. Software profiles in AppDB need to be extended with information about software availability and access conditions:
   1. Available as an online service (no need to install, we operate it for you);
   2. Available for download and install (so you operate it);
   3. Not available for external users.

For option a. method of access can be one (or more?) of the following:

* + - * 1. Loginname and password required;

EGI SSO;

Other.

* + - * 1. Membership in an EGI Virtual Organisation is required;

VO X;

VO Y ...

* + - * 1. A personal grid certificate is required.

When an application profile is displayed, the availability and method of access must be very visible and AppDB should simplify getting access (especially to online services) as much as possible – e.g. by proving link to EGI SSO; link to the registration page of VO X, VO Y, ...; link to the visitor’s CA (based on his/her IP).

1. Feedback:   
   One of the most important information about a VO for potential users is whether the VO can accept new members or not, and, if it does then what are the conditions to join and how can one join? This information is not available in either the Applications Database, or in the Operations Portal. It is available for some VOs on their own website, but getting to this information is often complicated or impossible.

Recommendations:

1. The Operations Portal need to store information about the conditions and the methods of joining the VO if VO membership is necessary to use a particular software. Related fields need to be added to the VO ID Cards, and a campaign needs to be run with the VO Managers to fill and keep the new fields up to date.
2. If a VO is not open for external users then the AppDB should display the same information (i.e. not available for external users) about every application that runs on that VO and only on that VO.
3. Feedback:   
   The search does not seem to search in the discipline field, causing confusion to those who want to get a list of for example every software that has something to do with Computational Chemistry. These users will see only those software that include the word ‘Computational Chemistry’ in their description but will not see those that are under the ‘Computational Chemistry and Material Sciences’ category without the explicit mention of this word in the description.

Recommendation:

1. Extend the search to the discipline field and clarify in the manual how search works.
2. Feedback:   
   Those software that has anything but not “Production” status in their profile makes the user question the relevance of the software for use. Software should become production as soon as possible, the time that software spend in non-production statuses should be minimal.

Recommendation:

1. AppDB should send reminders to owners of applications that are not in production status and remind them the importance of publishing production applications in AppDB, asking them to update the status as soon as possible.
2. Feedback:   
   A software can have various different contacts being associated with it in AppDB. (For example developer, scientific coordinator, etc.) The meaning of these roles is not evident for a user, and the most important contact – the person who should be asked if one wants to get access to the software – is not highlighted.

Recommendation:

1. Review and rethink the AppDB user role structure and the software contact structure. Merge these as much as possible and use categories that are meaningful for external users and are independent from EGI-specific roles (e.g. do not display NIL as a role, display national contact instead).
2. Feedback:   
   The meaning of ‘related countries’ in software profiles is fuzzy. What does ‘related’ mean in this context? One can easily associate to the country where the software can be used, assuming that users from other countries are not allowed to access the software. This assumption is often false and related often means that the developers are from the ‘related countries’ or users exist in the ‘related countries’. In these are users from other countries welcome to join?

Recommendation:

1. The most important information to a user about countries of an software are:

* What are the countries where the software can be used? 🡪 Can I use it or not?
* What are the countries where software-specific user support exists? 🡪 Who could I talk to in case I have a question?
* What are the countries where the software is already used? 🡪 Who could provide feedback about his/her experience with the software?

The different types of country relationships should be distinguished on the software profile page instead of blending these into the single ‘related countries’ relationship.

1. Feedback:   
   The contact information part in some of the personal profiles are not filled, making it impossible to get in touch with the person for example to ask for access, clarification or feedback concerning the software they are linked to. (Examples: A. Zengin, P. Orviz, O Gervasi)

Recommendation:

1. Identify all those personal profiles that have incomplete contact information and using Google, NILs and institutional EGI contact points get in touch with them and ask them to fill the contact part or delegate the ownership of the software to a colleague of them.
2. Feedback:   
   Some of the VOs that are listed in AppDB have no software associated with them. Having these listed confuses the user.

Recommendation:

1. Do not display VOs that have no software associated with them.
2. Feedback:   
   Some of the stored items do not have their ‘Subdiscipline’ field filled and for these their profile include a “Subdisciplines: “ line. This is misleading as one thinks that something is missing here, so it’s a bug in the system.

Recommendation:

1. For those software that have no subdiscipline specified for them do not display this field, or display it as “Subdisciplines: Not specified”.

1. EGI Applications Database: <http://appdb.egi.eu> [↑](#footnote-ref-1)