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Abstract:

This deliverable provides the results of the validation of the reference communities, which were mainly obtained by means of the interoperability demo carried out by the project during the EGI Technical Forum 2012. To get there, several previous advances were achieved, mainly the collaboration with the scientific communities addressed by CHAIN and the use of the Science Gateway platforms.

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Table of contents

1. Executive Summary

During the two-year lifetime of the project, CHAIN has performed a study of the state-of-the-art in Grid developments across the world regions and their relation to the European Grid Initiative. Such a study has been undertaken on a three-fold basis: consolidation of the state-of-the-art (interoperability and interoperation aspects included), e-Infrastructures and Virtual Research Communities (VRC). With respect to the latter, two kinds of deliverables have been produced during last 24 months, i.e. those devoted to describe the trans-continental scientific and technical communities that have been collaborating with CHAIN (D3.1 and D3.3) and those assessing the proposed road-map of trans-continental e-infrastructures for virtual communities (D3.2 and D3.4).

In this document, the results of the validation of the reference communities, which were mainly obtained by means of the interoperability demo carried out by the project during the EGI Technical Forum 2012, are presented.

To obtain such results, the first successful action has been the continuous collaboration with the following VRCs: We-NMR, WRF4G, jModelTest, INDICATE, DECIDE, LSGC, Climate Change and SuperB. These collaborations have been nourished by continuous exchange of information and by attendance to most of the events organised by CHAIN.

The second action has been the adoption of the Science Gateway platform. Such paradigm collects in some way most of the recommendations listed in the road-map of trans-continental e-infrastructures for virtual communities, and due to the platform being based on the use of standards, it has demonstrated the effective employment of several and different e-Infrastructures and can be accessed by a much easier method than the previously adopted one based on personal Grid certificates.

In what regards the results themselves, it can be mentioned that they can be grouped in three main areas:

- The strengths enhanced by the collaboration between VRCs and CHAIN, which can be summarised into exchange of best practices, tools and users interested in the deployed advances, training activities and international coordination.
- The "Quality Metrics" assessment set up within the project, the numbers of which have been six (6) VRCs officially supported (MoUs), fifteen (15) applications deployed on the participating regional e-Infrastructures and three (3) new applications with respect to those already deployed in the Regional projects.
- The CHAIN Worldwide Interoperability Demo, which was a success since it could fulfil all of its objectives: easy and unattended access to the infrastructures, submission of jobs of several different codes, and use of several e-Infrastructures with different technical characteristics and middleware.

2. Introduction

EC has pushed e-Science over the last decade in Europe; besides, it has supported its development in Africa, Asia and Latin America and has tried to be coordinated with other Regions such as USA or Japan. This effort has covered as many aspects as possible: different layers of e-Infrastructures, computing platforms, human power, etc.

Thus, even when supercomputers have maintained a leading role, Grid emerged as a valid option for producing e-Science in those scientific fields and economic scenarios where the first could not be feasible. Then, the coordination of these world-wide efforts is a must that CHAIN project has been devoted to.

The CHAIN project started on December 1st, 2010 and has been working on coordinating and leveraging the efforts made over the past 6 years to extend the European e-Infrastructure (and particularly Grid) operational and organisational principles to Africa, Asia and Latin America. Now that the project is almost over, it can be mentioned that this vision has been structured in several lines of performance: study of the state-of-the-art of the current e-Infrastructures and e-Science status per region, needs and commonalities of these computing platforms, and VRCs requirements and services. In this sense, several results are available to the community by means of the public CHAIN deliverables which can be consulted at http://www.chain-project.eu/status.

CHAIN WP3 'Present and emerging needs of trans-continental scientific communities' devotes its framework to the study of VRCs. A trace of its work can be found in the two kinds of deliverables that has been produced during last 24 months, i.e. those devoted to describe the trans-continental scientific and technical communities who have been collaborating with CHAIN (D3.1 and D3.3) and those assessing the proposed road-map of trans-continental e-infrastructures for virtual communities (D3.2 and D3.4).

Thus, a coordinated data collection on the existing Grid state-of-the-art across the world was carried out. Such a work was summarised in D3.1 'Trans-continental scientific and technical communities'[1] and its follow-up D3.3 'Transcontinental scientific and technical communities Updated'[2], which focused on the description of the results related to VRCs obtained up to the sixth (May 2011) and to the eighteenth (May 2012) month of the project respectively. On both documents, the communities who have been collaborating with CHAIN were described.

In addition, a study on the requirements and services of interest for the VRCs that had to be offered by the infrastructure providers was documented in D3.2 'Road-map of trans-continental e-infrastructures for virtual communities'[3] and also its follow-up D3.4 'Road-map of trans-continental e-infrastructures for virtual communities Updated'[4].

As a consequence, it would be of outmost importance to check if the work carried out by the Work Package, also supported by the project as a whole, could be evaluated in a specific and concrete result. Then, three different scenarios could be used to check and validate such results:

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[1] CHAIN D3.1, http://documents.ct.infn.it/record/500/files/CHAIN-D3.1-V06.pdf
[2] CHAIN D3.3, http://documents.ct.infn.it/record/525/files/CHAIN%20D3.3-V05.pdf
[3] CHAIN D3.2, http://documents.ct.infn.it/record/525/files/CHAIN%20D3.3-V05.pdf
[4] CHAIN D3.4, http://www.chain-project.eu/status

- The strengths enhanced by the collaboration between VRCs and CHAIN
- The "Quality Metrics" assessment set up in the project DoW, and
- The CHAIN Worldwide Interoperability Demo

All of them offer different and complementary approaches for the community in order to assess if the WP has fulfilled all its objectives beyond the submission of deliverables or the achievement of milestones.

To obtain these results, and mainly those devoted to the CHAIN Worldwide Interoperability Demo, the adoption of the Science Gateway paradigm and its key role have been the solid basement to build on.

2.1. Purpose

The aim of this deliverable is to demonstrate the achievements provided by the CHAIN project as a result of the validation of the reference communities. Such achievements are the consequence of the work carried out along 24 months which can be summarised as a close collaboration between the identified and lately official VRCs associated to CHAIN and the initiative itself.

In this sense, it is the aim of this document to demonstrate that:
- there has been a 'symbiotic', continuous and fruitful exchange of information between the VRCs and CHAIN
- the Quality Metrics set up in the DoW have been fulfilled
- the CHAIN Worldwide Interoperability Demo, which was showed during the EGI Technical Forum 2012, has collected most of the requirements that VRCs demanded to Infrastructure providers, validating in that way the information collected in D3.4 'Road-map of trans-continental e-infrastructures for virtual communities Updated'.

2.2. Glossary

CHAIN	Co-ordination and Harmonisation of Advanced e-Infrastructures
DCI	Distributed Computing Infrastructure
DoW	Description of Work – Annex I to the GA
EC	European Commission
EGI	European Grid Initiative
EGI-InSPIRE	European Grid Initiative-Integrated Sustained Pan-European Infrastructure
EPIKH	Exchange Programme to advanced e-Infrastructure Know-How
FP6/FP7	European Commission's Framework Programme Six / Seven
GA	Grant Agreement
HEP	High Energy Physics
HPC	High Performance Computing
JRU	Joint Research Unit
KoM	Kick-off Meeting
MoU	Memorandum of Understanding

MS	Milestone
NREN	National Research and Education Network
OLA	Operating Level Agreement
ROC	Regional Operation Centre
PMB	Project Management Board
SLA	Service-Level Agreement
VO	Virtual Organization
VRC	Virtual Research Community
WP	Work Package

3. Brief summary of WP3 activities during the CHAIN lifetime

CHAIN's first action was to deliver the Regional and National versions of the WP2 questionnaire, the analysis of which can be consulted in D2.2 'Interoperability and interoperation guidelines'[5] and D4.1 'Specificities of the various regional e-Infrastructures'[6]. Both surveys contained a specific section where questions devoted to VRC topics were present; such list can be consulted in D3.1 'Trans-continental scientific and technical communities'[1].

Later on, the first contacts with the VRCs were established. As a result, 'MS05 Call for interest for reference communities'[7] was published in the project web page, followed by 'MS06 Shortlist of reference communities ready'[8] and 'MS07 Agreements with reference communities signed'[9]. Even though this latter milestone was to be fulfilled in M09 with the signature of two MoUs, WP3 has been working on the same topic through the whole lifetime of the project. Thus and only regarding agreements with scientific communities, CHAIN counts on six (6) official VRCs: We-NMR; WRF4G, jModelTest, INDICATE, DECIDE and LSGC. With the Climate Change and SuperB communities there has been a deep collaboration, but with no signature of a MoU. A detailed description of all the work jointly performed with them can be found in the already published WP3 deliverables.

During this second year of the project, the VRC related part of the National survey was delivered again in order to acquire updated information about the advances made on scientific aspects in the Regions of interest to CHAIN. In addition to the questionnaire submitted to the national representatives, the link to D3.2 'Road-map of trans-continental e-infrastructures for virtual communities'[3] was included in the text of the e-mail and the section containing the specific information about the road-map in such deliverable was attached. This has been the primary source of information for updating and improving the first version of the road-map of services requested by the VRCs. The second one has been the aforementioned collaboration with the coordinators of all the VRCs, due to them making comments and suggestions about the road-map bearing in mind their experience in their specific domains.

As a complementary action, during the two years of the project, Distributed Computing Infrastructure providers and scientific communities have met several times by means of the events organised by CHAIN[10]. These meetings, as well as those attended by WP3 in major conferences, have been an outstanding source of information for improving the quality of the work done by the Activity.

Most of that work has crystallized in D3.4 'Road-map of trans-continental e-infrastructures for virtual communities Updated'[4].

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[5] CHAIN D2.2, http://documents.ct.infn.it/record/506/files/CHAIN_D2.2_V1.8.pdf

[6] CHAIN D4.1, http://documents.ct.infn.it/record/499/files/CHAIN_D4.1%20V1.3.pdf

[7] CHAIN milestone MS05, http://www.chain-project.eu/news/-/asset_publisher/W5vf/content/preliminary-call-for-interest-for-reference-communities?redirect=http%3A%2F%2Fwww.chain-project.eu%2Fnews%3Fp_p_id%3D101_INSTANCE_W5vf%26p_p_lifecycle%3D0%26p_p_state%3Dnormal%26p_p_mode%3Dview%26p_p_col_id%3Dcolumn-1%26p_p_col_count%3D1

[8] CHAIN milestone MS06, http://www.chain-project.eu/news/-/asset_publisher/W5vf/content/shortlist-of-reference-communities-ready?redirect=http%3A%2F%2Fwww.chain-project.eu%2Fnews%3Fp_p_id%3D101_INSTANCE_W5vf%26p_p_lifecycle%3D0%26p_p_state%3Dnormal%26p_p_mode%3Dview%26p_p_col_id%3Dcolumn-2%26p_p_col_pos%3D1%26p_p_col_count%3D3

[9] CHAIN MoUs, http://documents.ct.infn.it/collection/CHAIN%20-%20MoUs?ln=en

[10] CHAIN events, http://agenda.ct.infn.it/categoryDisplay.py?categId=79

At this point, it is worth mentioning the excellent work done by CHAIN WP5 on implementing in the webpage of the project the 'Knowledge base' and 'Applications' sections. These web pages have been very useful for providing information not only to the rest of the project Activities, but also to the general public and for sure that they will keep on working in the future.

4. The Science Gateway paradigm: an actor for the validation model

Science Gateways have risen as an ideal option for using Grid. This is so because the technology underneath has provided four key points:

I. Easy access by the users to the Grid
II. Unattended use of the available codes
III. Employment of standards for the technological implementation, and
IV. Interoperability and interaction among different infrastructures (middleware)

With all of them, it has been possible to join in a common framework most of the requirements compiled in D3.4 which were requested by the VRCs to the DCIs. As a summary of all of them, it can be mentioned that, by means of SG, it is possible with an identity provision (point I), which is usually provided by academic institutions or even social networks, to simply simulate the desired phenomenon updating the input file and clicking on a "Run" bottom (II) and retrieve the results as fast as possible since there exists a bigger pool of resources belonging to different infrastructures (III and IV). As it can be easily inferred, this process can be done by a non-ICT skilled person.

This previous goal that has been finally achieved was firstly identified because it was demonstrated that using Grid was not straightforward. There can be found several barriers, but undoubtedly, one major drawback is the difficulty to be used in the beginning due to the required ICT skills and to the way to accessing it (authentication & authorisation). Users have to cope with complex security procedures, execution scripts, job description languages, command line based interfaces and lack of standards. This makes the learning curve very steep and keeps non-IT experts away.

TeraGrid project defined a Science Gateway (SG) as a community-developed set of tools, applications and data that is integrated via a portal or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community. In this manner, it will be possible to abstract the final user from the technological complexity that would be underneath.

The second step is to gain easier access to the SG. The adoption of robot-certificates for managing the jobs to be executed and the authorisation to access the SG by means of Identity Federations (see for example eduGAIN[11]), which count on millions of users (so, for example, any researcher belonging to a R&D Centre or to a University can immediately login by his own credentials), is an outstanding asset for this paradigm.

Last action is then to develop a computational framework where available and new developments could be coupled (added) as independent linked modules. Doing so, it will be easier to integrate new applications and codes in the framework.

Because of all the above reasons, SG is supposed to provide a short term answer to interoperability when several different e-Infrastructures have to cooperate in order to fulfil the requirements of intercontinental VRCs and is being proposed and fostered by CHAIN.

The framework for SG is fully web-based and adopts official worldwide standards and protocols, through their most common implementations. These are:

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[11] eduGAIN, http://www.geant.net/service/edugain/pages/home.aspx

- The JSR 168 and JSR 286 standards[12] (also known as "portlet 1.0" and "portlet 2.0" standards)
- The OASIS Security Assertion Markup Language[13] (SAML) standard and its Shibboleth and SimpleSAMLphp implementations
- The Lightweight Direct Access Protocol and its OpenLDAP implementation[14]
- The Cryptographic Token Interface Standard[15] (PKCS#11) standard and its Cryptoki implementation, and
- The Open Grid Forum (OGF) Simple API for Grid Applications[16] (SAGA) standard and its JSAGA implementation

In addition, SG is built using the Liferay portal framework and can be downloaded and installed by a virtual machine containing the development environment and examples of basic template portlets that can be customised to integrate specific applications. A schematic view of the proposed model is depicted in Fig. 1.

More detailed technical information about SG and its current status about connections to different middleware and integration in initiatives can be found in Subsection 4.5 of D4.2[17]**Error! Bookmark not defined.**. Besides, the CHAIN web page offers continuous updated information about all these topics through its "Applications" section[18].
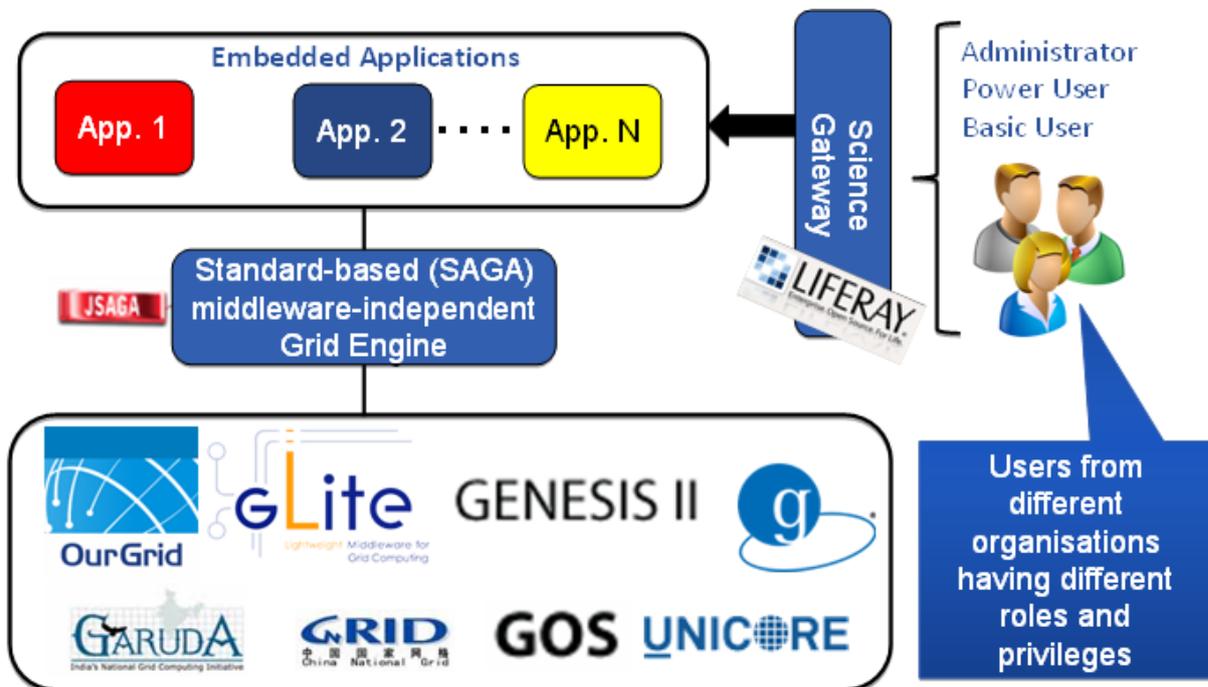

Figure 1. The Science Gateway model.

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[12] JSR 168 and JSR 286, http://developers.sun.com/portalserver/reference/techart/jsr168/

[13] SAML, N. Ragouzis *et al.*, Security Assertion Markup Language (SAML) V2.0 Technical Overview. OASIS Committee

[14] OpenLDAP, B. Arkills, LDAP Directories Explained: An Introduction and Analysis. Addison-Wesley Professional. (2003)

[15] PKCS#11, http://www.rsa.com/rsalabs/node.asp?id=2133

[16] SAGA, https://forge.ogf.org/projects/saga-rg/

[17] CHAIN D4.2, http://documents.ct.infn.it/record/515/files/CHAIN_D4.2%20V1.pdf

[18] "Applications" Section in the CHAIN webpage, http://www.chain-project.eu/applications

5. Results of the validation model

In this Section, more detailed information about the three levels of action that CHAIN has identified to assess its validation model will be presented.

5.1. Strengths enhanced by the collaboration between VRCs and CHAIN

During the two-year lifetime of CHAN, there has been a continuous exchange of information between the associated VRCs and the project. A deeper explanation about this can be found in the WP3 deliverables, where information about the procedures, requirements and vision of the communities that have been notified to CHAIN are detailed as well as the different actions carried out by the project in order to improve the initiatives impact. Nevertheless, all of them can be summarised in Fig. 2, where such exchange is depicted.
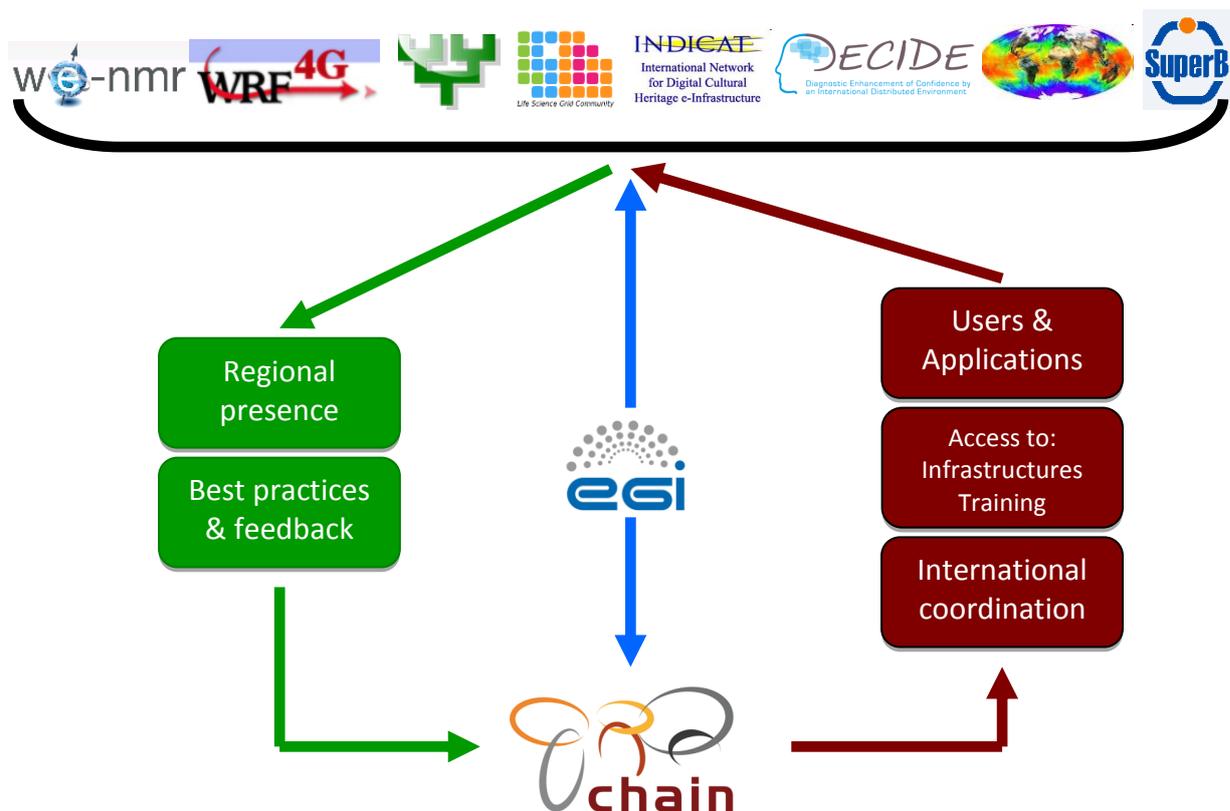

Figure 2. Schematic transfer of knowledge and collaborative work produced between the associated VRCs and CHAIN during the lifetime of the project.

As it can be seen, CHAIN has provided the VRCs with:

- New users all around the world (for example in Burundi, China, Costa Rica, Cuba, India for the WRF4G case, see D3.3[2] for the rest)
- New codes of interest to the communities (for example, jModelTest and ProtTest3 distributed versions to jModelTest initiative)
- Access to infrastructures by means of the interoperability demo
- Access to training activities with the collaboration and support of EPIKH[19] project (see the CHAIN training agenda[20]), and

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[19] The EPIKH project, http://www.epikh.eu/
[20] CHAIN training activities, http://agenda.ct.infn.it/categoryDisplay.py?categId=81

- Information about the different actions that have been running worldwide, mainly in the Regions targeted by CHAIN (for example, the one provided in the CHAIN events)

On the other hand, the VRCs have provided CHAIN with very valuable information in:

- Regional presence and impact of the different communities (for example, information on WeNMR users in African, Asian, Latin American and Oceania countries)
- Best practices and requirements (for example, presentation of the VRCs in the CHAIN workshops at EGI series of conferences), and
- Feedbacks about the CHAIN published information (for example, the suggestions received to the road-map of services appearing in D3.2[3], which was updated with them in D3.4[4])

In an equidistant point or, in other words, a two-way channel, the relationship with EGI and EGI-InSPIRE can be mentioned, since we have tried to coordinate all the challenges we had in accordance to the European initiative and, at the same time, VRCs have made their best in order to produce their e-Science in this defined technological framework.

5.2. "Quality Metrics" assessment

As part of the validation model, the Quality Metrics[21] assessment is also of help. With regards to WP3, this is the status as of November 2012:

Project Key Indicator	Metric	Target (Nov 2012)	Current status (Nov 2012 - M24)
PKI WP3.1	Number of VRCs officially supported (MoUs)	2	**6** (WeNMR, WRF4G, jMT, LSGC, INDICATE, DECIDE)
PKI WP3.2	Number of applications deployed on the participating regional e-Infrastructures	2 (1 per scientific discipline)	**15** (ProtTest, Octave, jModelTest, Astra, Specfem3d, RCSA, R, Me-mls, Industry@grid, Gromacs, Gate, Ga_dppm, Clustalw, Phylogenetics, Cmsquares)
PKI WP3.3	Number of new applications with respect to those already deployed in the Regional projects	1	**3** (ProtTest, jModelTest, Gromacs)

Table I. Quality Metrics related to WP3 in the CHAIN DoW at the end of the project.

As it can be seen, the different thresholds that were set up for the different metrics have been reached.

It is important to point out that the applications in Table I appear as final and definitive ones since they have already been integrated in the SG paradigm. In addition, it is also worth mentioning that the figures appearing in the third column, 'Current status (Nov 2012)' have been extracted from the CHAIN applications webpage (http://www.chain-project.eu/applications), those related to PKI WP3.2 are the codes deployed on the participating regional e-Infrastructures and those regarding PKI WP3.3 are the applications available through the CHAIN SG portal.

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[21] CHAIN Quality Metrics, http://www.chain-project.eu/quality-metrics

5.3. The CHAIN Worldwide Interoperability Demo

During the EGI Technical Forum 2012 held in Prague, CHAIN performed its Worldwide Interoperability Demo[22]. It was specifically showed as part of the 'CHAIN Interoperability Workshop'[23], but also on a continuous basis in the CHAIN booth that was permanently open during the whole duration of the Forum.

The main aim of the demo was based on the project vision about a world-wide DCI that can address big scientific challenges that are not manageable with departmental computing systems. Counting on it, VRCs can transparently access different kind of resources: scientific applications, tools, and/or data repositories. The vision is that of VRCs using resources ubiquitously across different administrative domains, this is, VRC-specific applications can be submitted from anywhere and run everywhere. In this sense, regional e-Infrastructures should be made interoperable among each other, i.e. interoperability should be addressed.
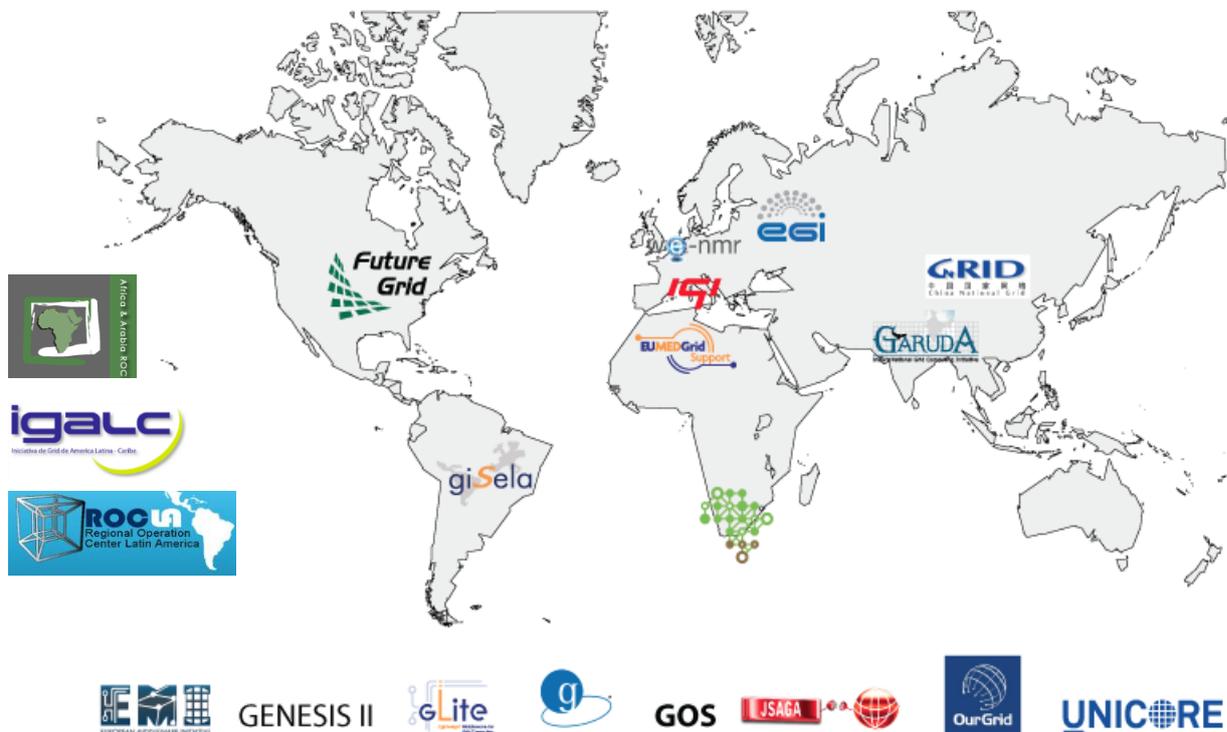

Figure 3. CHAIN Worldwide Interoperability Demo infrastructure contributors.

In order to achieve the above goal, some requirements were set-up:
  i. The user interface must be only web based
  ii. Users must be transparently authenticated & authorised on all e-Infrastructures without any additional human/machine intervention
  iii. There must be the smallest possible interaction with both site managers and e-Infrastructure operators, and
  iv. No modification whatsoever of the various middleware should be required to their developers

These requirements were fulfilled by means of:
  • The Science Gateway paradigm (i and iii)
  • Identity Providers authentication and authorisation (ii), and

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[22] CHAIN Worldwide Interoperability Demo, http://science-gateway.chain-project.eu/
[23] CHAIN workshop at EGI TF 2012, http://agenda.ct.infn.it/conferenceDisplay.py?confId=816

- Implementation of JSAGA adaptors and portlets (iv)

In the demo, several contributors were present in addition to CHAIN:
- e-Science projects/initiatives: CNGrid, EGI-InSPIRE, EUMEDGrid Suuport, Future Grid, GARUDA, GISELA, SAGrid and WeNMR
- Middleware developers: EMI, GENESI II, gLite, GOS, JSAGA, OurGrid and UNICORE
- ROCs: Africa & Arabia ROC, EGI associated ROCs, IGALC, ROC-LA
- And the applications that could be executed were:
- ASTRA
- GROMACS
- jModelTest
- Octave
- Parallel 'Hello world'
- ProtTest3
- R
- Sequential 'Hello world'
- Sonification

The middleware associated to these codes can be consulted in the demo applications full list[24].

A snapshot of the running sites at the time when the demo was performed, September 17th-21st, 2012, can be found in Fig. 4.
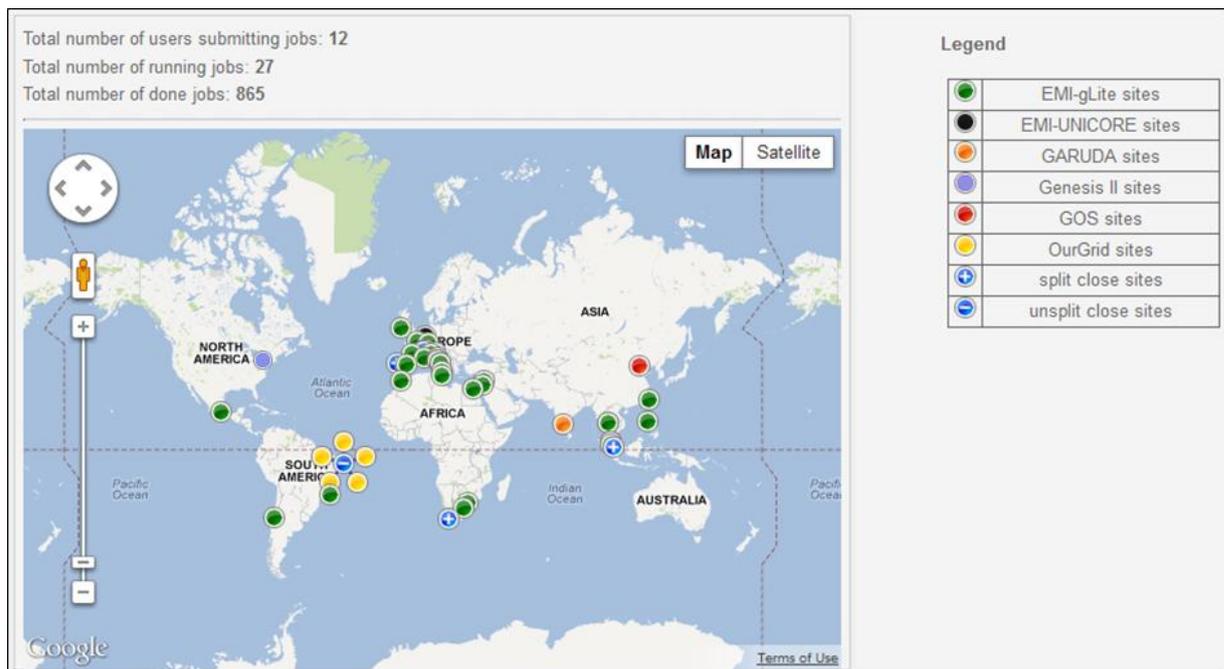

Figure 4. CHAIN Worldwide Interoperability Demo status (at one time of the Sep. 17th-21st, 2012 week).

The demo was a success and it could run different kind of jobs on different infrastructures by means of different middleware. In addition, and as a key point, it was run with a user's complete unattended control, who simply selected the input and submitted the job by clicking on a "Run" icon. Consequently, several conclusions can be drawn:

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[24] The demo applications full list, http://science-gateway.chain-project.eu/general-overview

- The CHAIN worldwide interoperability program demonstrated that users can access global e-Infrastructures in a seamless and ubiquitous way independently of the underlying middleware
- The Science Gateway framework, with support for Identity Federations and Social Networks, can change the manner Grid infrastructures are used, hugely widening their potential user base across the continents, especially non-IT experts and the "citizen scientist", yet keeping the required security
- The adoption of standards (JSR 286, SAGA, SAML, etc.) represents a concrete investment towards sustainability
- The collaborative scenario between VRCs and DCIs is strengthened

Thus, the proposed model that the SG paradigm has provided to the scientific community can be considered as a proof of concept that validates most of the recommendations (the other ones are related to different topics such as training or technical aspects for administrators) that appear in the road-map of trans-continental e-infrastructures for virtual communities.

6. Conclusions

CHAIN has been working in consolidating the state-of-the-art (interoperability and interoperation aspects included) of e-Science (mainly Grid), coordinating the efforts and advances made by the e-Infrastructures and promoting the liaison with the VRCs. Then, after two years of work, it is time to analyse the results of the validation of the reference communities, which were mainly obtained by means of the interoperability demo carried out by the project during the EGI Technical Forum 2012.

To obtain such results, the first successful action has been the continuous collaboration with the following VRCs: We-NMR, WRF4G, jModelTest, INDICATE, DECIDE, LSGC, Climate Change and SuperB.

The second one has been the adoption of the Science Gateway platform. Such paradigm collects in some way most of the recommendations that are listed in the road-map of trans-continental e-infrastructures for virtual communities, due to the platform being based on the use of standards, it has demonstrated the effective employment of several and different e-Infrastructures and middleware and can be accessed and managed by a much easier method.

In what regards the results themselves, they can be evaluated in three main areas:
- The strengths enhanced by the collaboration between VRCs and CHAIN, which can be summarised in exchange of best practices, tools and users interested in the deployed advances, training activities and international coordination.
- The "Quality Metrics" assessment that was set up within the project, the numbers of which have been six (6) VRCs officially supported (MoUs), fifteen (15) applications deployed on the participating regional e-Infrastructures and three (3) new applications with respect to those already deployed in the Regional projects.
- The CHAIN Worldwide Interoperability Demo, which was a success since it could fulfil all of its objectives: easy access to the infrastructures, unattended submission of jobs of several different codes and use of several e-Infrastructures which different technical characteristics and middleware. The demo was executed by means of the SG paradigm, so, to some extend, by the adoption of recommendations proposed by CHAIN in D3.4.

Bearing in mind these three areas, it can be considered that the proposed model of the reference communities has been comprehensively validated.