Jointly exploiting data and distributed computing eInfrastructure

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Abstract

CHAIN-REDS promotes and supports technological and scientific collaboration across different e-Infrastructures established and operated in various continents. To this, it has included data related capabilities so any user can search, retrieve and easily use datasets in a specific application. After two years of work, specific results on data handling (use, management, exploitation, interoperability) and their exploitation on distributed computing infrastructures are presented in this work.

Keywords: CHAIN-REDS, Data Repositories, Distributed Computing Infrastructure, Linked Data, Semantic Web

1. Introduction

CHAIN-REDS (www.chain-project.eu) is a project co-funded by the European Commission within its Seventh Framework Program with a consortium made of ten renowned organisations in the field of e-Infrastructures, representing Europe and most of the world regions (Africa, Asia, Latin America and the Caribbean, and the Middle-Eastern and Gulf Region). Its vision is

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to promote and support technological and scientific collaboration across different e-Infrastructures established and operated in various continents in order to facilitate their uptake and use by established and emerging Virtual Research Communities (VRCs), but also by single researchers, promoting instruments and practices that can facilitate their inclusion in the global e-Science and e-Research.

To fully exploit those eInfrastructure, it is necessary to count on active VRCs, which, many times, need to access, use and easily store data. In this paper, the Data Accessibility Reproducibility and Trustworthiness (DART) workflow is presented, which represents the CHAIN-REDS vision about data management, use, and persistent identification and storage.

2. Technological pillars

Data accessibility reproducibility and trustworthiness is a goal that needs previous technological developments to properly work. In this sense, CHAIN-REDS defined a road-map devoted to address the following objectives:

Obj1. Extend the CHAIN Knowledge Base (KB) with Data Infrastructure. During the CHAIN project lifetime, the consortium made a big effort in implementing a KB that contained detailed information about the different Grid initiatives around the world. This information could be displayed in the CHAIN webpage (see [1]) in a three-fold basis: Country, DCI Site and DCI Table views. In the former, the user could search on a worldwide map their country of interest and click on it, so that information about their domestic Grid status was displayed. In the DCIs views, information about the Distributed Computing Infrastructures per site geographically displayed on a map or per country showed in a table could be retrieved. For CHAIN-REDS, the KB is being enhanced with information related to Data infrastructure.

Obj2. Support the study of data infrastructures for a few VRCs. Use cases aforementioned should count on a community of users (VRCs) who would test and give feedback about the solutions proposed by CHAIN-REDS related to interoperability aspects of data infrastructures. In this sense, the project will support these VRCs in the process of learning (if any), implementation (if any) and final validation.

Obj3. Promote trust building towards open scientific data infrastructures across the world regions. Trust building is of outmost importance for users from different groups to be able to access data previously stored by different researchers in different world regions relying not only on their accuracy, but also on their computational format i.e. these users are retrieving the information they are looking for.

Obj4. Study the opportunities of data sharing across different e-Infrastructures and continents. For achieving such a goal, it is necessary to survey different sources of information in order to look for synergies that could be exploited: groups of researchers (VRCs) who could make use of big amount of data in the countries belonging to the continents targeted by CHAIN-REDS; DCIs that could report on the users who usually transfer big amount of data too; and, on-going well-established data initiatives.

Obj5. Provide proof-of principle use-cases for data sharing across the continents. Select among the identified candidates those who present promising opportunities for data sharing in terms of standards and good practices selected by CHAIN-REDS.

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To achieve Objective 5, several actions have been carried out:

- Analyse which standards are most used and, as a consequence, extended worldwide and accordingly propose best-practices to the communities to be approached (i.e. achieve Obj3);
- Define in what terms the CHAIN-REDS KB should be improved in order to firstly collect and lately display, in a dynamic way, information related to data infrastructures (Obj1);
- Analyse which repositories and what related scientific fields are of interest to CHAIN-REDS according to Action1 and Action2 (Obj2 & Obj4);
- Survey the different countries and DCIs of interest to CHAIN-REDS and the well-established data-related initiatives in order to get their feedback about their usage of the identified standards and the computational platforms that are being utilised (Action2) and about the groups that are profiting from a huge employment of data and belong to the identified scientific fields (Action3). In addition, propose to the latter the CHAIN-REDS support for adopting the proposed standards (Obj2-Obj4);
- Analyse the results of the survey (Action4) and focus the project efforts on two or three scientific communities in order to efficiently perform data sharing in terms of some standards and good practices (Obj5). This action have counted on the support from CHAIN-REDS in order to implement or adopt some standards if necessary, the collaboration of the identified communities by means of MoUs which would rule the scientific liaison and the support of DCIs for making the real demonstration of data interoperability.

In order to work on any action or goal, the first key point is the definition of the way in which it is expected to be achieved. In CHAIN-REDS, this meant to select the standards that would be fostered by CHAIN-REDS and, hopefully, adopted by the collaborative VRCs (if necessary).At the same time, it is of outmost importance that such standards have a wide presence worldwide because of the intercontinental scope of CHAIN-REDS.

Thus, after a deep analysis on the best practices that on-going data initiatives were carrying out, the following standards were selected by the project for pursuing trust building:

- OAI-PMH [2] for metadata retrieval.
- Dublin Core [3] as metadata schema.
- SPARQL [4] for semantic web search.
- XML [5] as potential standard for the interchange of data represented as a set of tables.
- Persistent Identifiers (PID) [6] as a tool to know where and how data and metadata are stored, which is of importance for retrieving the required data successfully. Strictly talking, PID is not a standard yet, but it is becoming the de facto tool for uniquely identifying any kind of document resources.

With this selection in mind, a work plan for improving the CHAIN-REDS KB by adding new functionalities was also planned. As a result, the following developments have been implemented:

- Integration of the KLIOS [8] services inside the KB in order to extend its functionalities. Knowledge linking and sharing in research domains (KLIOS) is a project for developing small research projects and implement them in real-life use cases related to data sharing by means of metadata harvesting.
- Dynamically include in the KB Data Repositories (DRs) and Open Access Documents Repositories (OADRs) worldwide by using the already defined standards. The information related to these repositories should be presented to the user in the same way as the already available DCIs one.
- Take this integration as a proof-of-principle for demonstrating the work carried out. Repositories containing documents (articles, proceedings, books, etc.) were selected in principle for testing and depurating the KB functionalities with the aim of improving its characteristics to other fields and data (see items below).
- Provide the KB with the following capabilities, so that further extraction and exploitation of raw data by any user could be performed: semantic web enrichment; semantic search engine; and, a tool for extracting the data associated to the repositories.
- Start working with some specific communities on a strategy for demonstrating data trust building, i.e. the access by a user of data already stored in order to extract them and employ them as input in a scientific application for reproducing and/or extending the results of a given research. The new data and, may be, the new paper will be lately stored on the Data Infrastructure and will be easily found by the people belonging to the same domain (see DART challenge below).

New tools have been provided on the CHAIN-REDS website that are of interest to Data Infrastructures and User Communities. They actually are the backbone that is being used by the DART challenge to achieve data trust building and are the basis for several of the use cases provided by the project. These tools based on the previous mentioned standards are:

- The Knowledge Base is one of the largest existing e-Infrastructure-related digital information systems. It currently contains information, gathered both from dedicated surveys and other web and documental sources, for more than half of the countries in the world. As of today, the KB contains about 2,500 OADRs and 600 DRs. The total number of resources that are indirectly included in the KB is well above 30 million.
- The CHAIN-REDS Semantic Search Engine (SSE), which semantically enriches the OADRs and DRs, gathered in the KB for relating linked data. The multi-layered architecture of this engine provides the results of a given query displayed on the webpage and ranked according to the Ranking Web of Repositories. Visitors can also access the detailed view of the resource and its reference in Google Scholar, access the document specific link and, if existing, the corresponding dataset, and select one or more of the resources found and get a graphic view of the semantic connections among Authors, Subjects and Publishers. Thus, if new links appear, users can infer new relations among resources, thus discovering new knowledge.
- The Science Gateway, which is a friendly front-end that allows users to submit jobs seamlessly and unattendedly to be run on Grid, Cloud and HPC infrastructure

independently of the middleware they were using. This Science Gateway can be accessed with the user's Identity Federation credentials.

In September 2013, and also as part of EGI Technical Forum, the demo 'Managing and using interoperable DCIs through a standard-based Science Gateway' was successfully performed. It was planned to both demonstrate interoperability (by allowing a scientist to seamlessly run applications on HPC machines, Grids and Clouds) and interoperation (by allowing a cloud-tenant of a real or virtual organisation to seamlessly and easily manage Cloud resources pledged by providers owning/operating infrastructures based on different middleware stacks). Logging into the user-friendly CHAIN-REDS Science Gateway using his/her federated credentials; the user could select an application from a menu and transparently execute it on HPC machines, Grids and Clouds. It is also worth mentioning that the fractions of executions on the three different platforms could be adjusted to simulate the need to "boost" the resources in case of temporary peaks of activity.

3. DART: Data Accessibility, reproducibility and Trustworthiness

By using metadata standards already implemented in the project Knowledge Base) and the Semantic Search Engine, any user can find repositories including a term and lately retrieve the raw data for performing a new calculation. The latter, is executed on distributed computing infrastructures, including Grid, local clusters and Clouds, using OCCI and SAGA as standard interfaces and the CHAIN-REDS Science Gateway as a virtual research environment. Last, the obtained results (raw data and publication) are able to be stored again in a way that they are searchable again.

In this sense, this workflow is a step forward in the previous interoperability actions already achieved by CHAIN-REDS and provides scientists with a powerful tool. The standards on which DART is based on are the ones mentioned in the previous section.

DART demonstrates the achievability of the following vision:

- A scientist can search on a wide plethora of resources for a specific term, subject, author or publisher (those already integrated in the CHAIN-REDS Knowledge Base by using the project Semantic Search Engine).
- He/she can discover new knowledge by linking the retrieved results via a semantic enrichment.
- He/she can retrieve the article and associated raw data of interest and either replicate the previous experiment or perform a new study with those data.
- He/she can seamlessly run applications on HPC machines, Grids and Clouds compatible with those retrieved data;
- The cloud-tenant of a real or virtual organisation can seamlessly and easily manage Cloud resources pledged by providers owning/operating infrastructures based on different middleware stacks.
- The new produced data (and publication) can be stored again using the same standards and being assigned to a specific Persistent Identifier (PID) so the cycle can be initiated again.

The previous items above were initially addressed by using the CHAIN-REDS tools already integrated in the project website and by accessing current repositories already hosted by

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initiatives such as Zenodo. First tests of DART were done with a portlet that makes use of a chemical physics code that obtains molar absorption coefficients from molecular gaseous cross sections (Molon [8]). Such portlet can upload the input file in a three-fold basis: from the local computer where the user is working, introducing the dataset assigned PID, or directly introducing the associated web address of the dataset. The latter two input formats can be obtained from a search on the CHAIN-REDS KB and/or SSE. Then, the user has to simply click on the "Run" bottom of the portlet webpage to start the calculation.

Once this is completed, the user can retrieve the final results and, if desired, assign a PID, so the cycle can be restarted again by any other user who would search for them. For the sake of completion, Molon can use a cross section of datasets from the MPI-Mainz UV/VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest [9].

At this point, it is worth mentioning that the PID can simply assign a permanent reference to a digital object or include also some additional parameters required by the user. At the same time, it can identify a simple raw data or a whole experiment (input and output data, application used).

A demo of the DART workflow was shown at the EGI Community Forum 2014 in May 2014 in Helsinki. In addition, CHAIN-REDS has recorded two videos of this demo as well as a technical tutorial, which are available at the CHAIN-REDS webpage and the project YouTube channel [10].

4. CHAIN-REDS application use cases

A number of proposed use cases have been analysed and supported by the project. All of them make use of the e-Infrastructure services promoted by CHAIN-REDS in the different regions, but they cover different and complementary aspects of users' characteristics.

Of special interest in the African region is the APHRC case. The African Population and Health Research Centre (APHRC) [11] undertakes research in a wide range of topics related to societal health and well-being. APHRC runs around 60 projects, publishes around 60 papers, and trains more than 150 fellows per year. To do so, it counts on 18 donors and 51 partners. This use-case is mainly devoted to assign Persistent IDentifiers (PIDs) to the wide plethora of datasets that APHRC manages and curates. This is of utmost importance due to these datasets are widely used by almost every country in Africa in order to improve societal health and well-being. APHRC and CHAIN-REDS have firstly identified which repositories must be catered for and defined a road-map for making this assignment. The PIDs are being assigned to an entire data set at the top-level. The software being used to document the data is Nesstar [12].

Due the significant development of the ab initio calculations especially the Density Functional Theory (DFT) in the fields of quantum chemistry and the physics of materials, the calculations in those areas become vital. Therefore the idea of introducing a powerful code such as ABINIT [13] within the Grid computing paradigm comes to ease the task of researchers. There is a strong group of users in Algeria who are also training new scientists in the field. The aforementioned versions have been installed in 6 European and Arab sites and the required portlet for job submission has been implemented; such a work will be extended to Latin America in the near future. The portlet has been integrated in the CHAIN-REDS Science Gateway [14] and in the Algerian one [15].

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Also in the Arab region it is worth mentioning the CMSquares usage, which looks for Magic Squares. The goal of this application is to generate all natural magic squares of order 6 with predefined restrictions, like having the four corner property or being semi pan-diagonal magic squares. A huge amount of computing resources related to the CMSquares code are being exploited in Jordan via the CHAIN-REDS Science Gateway of this code [16] and this use case is a clear of example of how the project can also support the so-called "long tail" of users, i.e. those that do not belong to a big community.

Outside Africa, several use cases are being promoted by CHAIN-REDS as well. The Latin America Giant Observatory (LAGO - first known as Large Aperture Gamma Ray Observatory) [17] project is a recent collaboration that counts on Water Cherenkov Detectors in 9 Latin American countries, more than 80 Latin American researchers and a close collaboration with European teams such as IN2P3 in France and INFN in Italy. LAGO use-case success story is based on the DART challenge. The consortium maintains a repository of astrophysics interest that is based on DSpace and uses the Corsika code [18] to study the astroparticle clusters. The LAGO repository has been integrated in the CHAIN-REDS Knowledge Base and the Semantic Search Engine. Also, LAGO is currently analysing with the project which is the best strategy for assigning PIDs to the current datasets and to the new data produced as a result of the Corsika executions via the project Science Gateway [14]. LAGO will address three different phenomena thanks to the CHAIN-REDS DART workflow.

Knowing the protein structures is essential for a complete understanding of life processes at the molecular level. Threading is the leading method for protein structure prediction, and it is exceedingly time-consuming. The TreeThreader code [19] uses a new practical threading program, which can take pairwise interaction into consideration. TreeThreader can run on a Linux platform and on a volunteer computing e-Infrastructure using the CAS@home BOINC client and consuming around 6 million of CPU hours a year. The code is already available to the desktop computing community, and is now made available on a full-blown e-Infrastructure: virtual machines launched from physical servers belonging to the China ROC and managed with OpenStack. For making as easy as possible the use of the new pool of computing resources (BOINC and cloud) to scientist, all TreeThreader jobs can be submitted both within China and Europe.

Researchers are trying to observe molecular activity of various bio-molecules using Molecular dynamics simulation approach. GROMACS software package [20] is used for molecular dynamics simulation. These kinds of studies present a huge computational demand. That is the reason why GROMACS version to be used in this use-case success story is v4.6.5 due to its full-blown MPI capabilities. Fourteen European, Arab and Indian Grid sites have already been enabled with GROMACS version with two flavours: both an installation package and a Science Gateway portlet. In addition, new services related to eTokenServer, GridEngine and wiki pages have been created as well.

5. Conclusion

CHAIN-REDS is supporting and promoting several application use cases in the regions of interest. Among them, the APHRC and ABINIT use cases are currently being developed in Africa; other application use cases supported by the project are LAGO in Latin America, TreeThreader in China and GROMACS in India.

CHAIN-REDS also supports single users who need a massive use of distributed computing infrastructures. In this regard, it is worth mentioning the CMSquares application that is being exploited in Africa as well.

All these use cases profit from instruments and practices that can facilitate their inclusion in the community of users. In concrete, they have been promoted and several standards have been adopted. Based on them, several useful tools have been implemented such as the Knowledge Base, the Semantic Search Engine and the Science Gateway

Doing so, CHAIN-REDS facilitates the e-Infrastructures uptake and their final use by established and emerging Virtual Research Communities (VRCs), but also by single researchers. These communities can now easily access the project Knowledge Base, which provides direct link to more than 30 million of documents that can be also semantically searched and accessed.

Biography

Dr. Rafael Mayo García (male) is Senior Researcher at CIEMAT and earned his PhD in Physics from the Universidad Complutense de Madrid (2004). From 2006 he has also been Adjunct Faculty and Honorary Fellow at the same University in the Physics of Materials Department. He has been involved in many experiments in Bulgaria, Sweden and Ireland (funded, among others, by the European Commission with a Marie Curie fellowship). He has also obtained a postdoctoral fellowship in the Spanish Juan de la Cierva Programme. He is author of 29 scientific articles published in international JCR referenced journals (being cited 180 times) and more than 70 proceedings (being cited 308 times in Google Scholar). He is project coordinator of 2 Spanish R&D IT initiatives and has been involved in several European and National projects working on ICT scientific developments (EGEE-III, EUFORIA, EFDA-ITM, Spanish e-Science Network) and even on managerial activities as Work Package Manager and/or member of Executive Boards (EELA, EELA-2, EPIKH, GISELA, CHAIN, CHAIN-REDS, BETTY). He also has served to several institutions as evaluator for their competitive calls, European Commission included.

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