**EGI-InSPIRE**

SUSTAINABILITY PLANS FOR THE ACTIVITIES OF THE HEAVY USER COMMUNITIES

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| Abstract   |  | | --- | | The Heavy User Community activities are planning for a sustainable future – either within their own community, as part of the generic production infrastructure, or through some other mechanism. This annual report exposes the sustainability plan for each task within the SA3 activity and assesses the progress made to date towards sustainability.  **This is the final SA3 sustainability report and updates and replaces D6.2 (2011) and D6.5 (2012).** | |

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1. 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.

1. 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:  
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1. Terminology

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

1. 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.

1. EXECUTIVE SUMMARY

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| --- |
| The Heavy User Community activities are planning for a sustainable future – either within their own community, as part of the generic production infrastructure, or through some other mechanism. This annual report exposes the sustainability plan for each task within the SA3 activity and assesses the progress made to date. This is the final SA3 sustainability report and updates and replaces D6.2 (2011) and D6.5 (2012).  The basic model for sustainability of the solutions and services that are currently supported by SA3 is that of collaboration development. This isolates individual projects from funding changes at individual participating institutes, but cannot easily cater for significant reductions in funding, such as that which will occur when SA3 terminates in April 2013.  However, as the main objective of the work package has been to ensure a smooth transition from previous projects and to prepare for the longer term by identifying commonalities as well as other synergies, the work package can be considered to have met its main objectives.  The primary goal of the final project year for this work package has therefore been to complete any remaining development and ensure that any tools / services are adequately documented and that the support is passed over to the units that will carry it on in future years. This has been successfully achieved and is described in detail below. |

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# Introduction

The SA3 activity within EGI-InSPIRE provides continued support for activities previously supported by

EGEE while they transition to a sustainable support model within their own community or within the production infrastructure by:

1. Supporting the tools, services and capabilities required by different Heavy User Communities (HUCs);
2. Identifying the tools, services and capabilities currently used by the HUCs that can benefit all user communities and promoting their adoption;
3. Migrating the tools, services and capabilities that could benefit all user communities into a sustainable support model as part of the core production infrastructure;
4. Establishing a sustainable support model for the tools, services and capabilities that will remain relevant to single HUCs;
5. As a further step, seeking additional areas of commonality that would result in lower on-going support costs through reduced diversity.

All of the above mentioned tasks aim to reduce the cost of new development and support, and have as a common objective improving the sustainability of the model. Working towards sustainability is therefore a key element of the strategy of this activity and this document describes the progress to in achieving throughout the duration of the work package.

The document is organised by HUC – a description of the communities involved is given in the section below.

## SA3 Sustainability Workshop

The EGI Technical Forum 2011 was held in Lyon from 19-23 September 2011. The event was hosted by EGI.eu, the Computing Centre of the National Institute of Nuclear Physics and Particle Physics (CC-IN2P3) and France Grilles, the French National Grid Initiative. For the Heavy User Community (HUC) workshop, each community was asked to come prepared with answers to three questions regarding the sustainability of their respective discipline, Distributed Computing Infrastructure (DCI) and the support the community received. Below is a table summarising the key points that were highlighted by each community.

|  |  |  |  |
| --- | --- | --- | --- |
| **HUC** | **SUSTAINABILITY OF:** | | |
| **DISCIPLINE** | **DCI** | **SUPPORT** |
| Life  Sciences | Life Sciences is a very broad “discipline”.   * Ranging from fundamental research to direct clinical applications. * Every potential patient may be interested: really everybody. * Strong societal impact. | Foundation of the Life Sciences Grid Community.   * <http://wiki.healthgrid.org/LSVRC:Index> * 5 NGIs (Dutch, French, Italian, Spanish, Swiss). * 5 VOs (biomed, lsgrid, medigrid, pneumogrid, vlemed). * 2 projects (EGI-InSPIRE, Lifewatch ESFRI). | Services:   * LSGC dashboard and support team. * Hydra encryption / decryption service. * GRelC database interface service. * Taverna workflow manager. * EBI core databases. |
| Astronomy & Astrophysics | * Worldwide, distributed community that operates large experiments and observing facilities. * Observation-driven science based on national and international ground and space-based observatories. | * A&A Grid/DCI community funded so far through short/medium term national and international projects (e.g. EGI-InSPIRE and former EGEE projects) and funds typically from Europe and national governments. | * The most relevant SA3 tool directly provided by A&A is VisIVO. |
| Earth Sciences | Fundamental topics:   * Understanding of the Sun-Earth system. * Societal needs. * Civil protection. * Natural resources identification / exploration. * Reaction to natural and human-induced changes. * Long-term Climatology * Multi-disciplines: to observe and interpret one event. * Cross scientific domains: Physics, chemistry, fluid mechanics. * International societies and programs. | Resources:   * Resources from ES related sides directly at NGIs. * Resources are not only by EGI. * Support * Community building. * Community tools. * Publications: see actual papers from e.g. climate, hydrology, and satellite data exploitation. | Services:   * Organisational: achieved collaboration e.g. with GENESI-DR or ESGF –on-going applications. * Software. * Generic VO and services. |
| High Energy Physics | * HEP is clearly a long term effort, the main experiments are becoming bigger and bigger. | * Grids have become integral part of HEP computing. * WLCG has a MoU with long term financial commitments by the participating countries. | * A strategy following multiple paths. * More commonality = Lower maintenance burden. * HEP experience is a key resource here. |

Table 1 - Sustainability of HUC Communities

## EGI Sustainability Workshop

In January 2012 a series of workshops were held in Amsterdam – organised by EGI.eu – to cover sustainability of EGI, of NGIs and of user communities. From these workshops it became clear that even the long (medium) term support of the basic middleware was not assured: NGIs and communities such as WLCG were called upon to make statements about their willingness and ability to make contributions to this support. Given this situation, it became clear that objective 3 above (Migrating the tools, services and capabilities that could benefit all user communities into a sustainable support model as part of the core production infrastructure) was no longer an option and that any ongoing support would have to be organised by the community or communities concerned.

**This is the strategy that has thence-forth been adopted.**

# Heavy User Communities

Heavy User Communities (HUCs) are Virtual Research Communities (VRCs) that have been using EGEE and now EGI routinely and thus have become more structured and advanced in terms of their grid usage. These communities focus on domain specific issues, such as how to access High Energy Physics (HEP) applications on EGI, how to enable new physics experiments on EGI and so on.

On the one hand these teams are operated by external projects, such as the Worldwide LHC

Computing Grid (WLCG), but on the other hand have members in the SA3/WP6 work package of EGInSPIRE. The effort of the distributed WP6 team of EGI-InSPIRE is targeted towards the provision of shared services that will ease the porting of new applications from these scientific domains to the wider grid by detecting and exploiting commonalities between virtual organisations (VOs) and driving the implementations to a generic direction.

At the same time inter-VO collaboration typically not only result in more powerful solutions, but also saves significant amounts of manpower in the long run. Such benefits would be unlikely to be achieved with generic support structures, both for individual large communities such as HEP (which could otherwise develop multiple similar solutions to basically common problems), as well across disciplines (e.g. the usage of Dashboards [DASHBOARD], Ganga [GANGA] and HammerCloud [HAMMERCLOUD] across communities).

In conclusion HUCs can offer benefits not only to new adopters of grid technology but also to each other. This continues to be demonstrated, both by the adoption of tools initially developed for one community spreading to others, as well as at the conceptual level: which offers a more pragmatic solution for existing communities.

# High Energy Physics

## Introduction

The Services for High Energy Physics (HEP) task continues to focus primarily but not exclusively on the 4 LHC VOs (experiments) centred at CERN: ALICE, ATLAS, CMS and LHCb (and hence for and via the WLCG project and collaboration). Services and tools developed or extended by these VOs are also used by other HEP experiments and/or are under consideration for the future.

On July 4th 2012, to a packed audience at CERN and via webcasts worldwide, ATLAS and CMS presented their results in the search for a Higgs boson – the key missing element of the “standard model” of particle physics. Aside from the scientific significance of such a discovery, the Director General of CERN concluded that to be successful in such a search three things were required: the accelerator, the experiments (including both the detectors as well as the large distributed collaborations of physicists) and Grid Computing. Whilst the distributed computing infrastructure that the LHC experiments use will continue to evolve in the future, it will still satisfy Ian Foster’s legendary 3-point checklist.

HEP is clearly a long term effort, the main experiments are becoming bigger and bigger, with additional institutes joining the LHC experiments. A number of these institutes are proposing to setup “Tier1” sites which would bring significant additional computing and storage resources to the supported VOs. Similarly, the number of countries wishing to apply for membership of CERN continues to grow. Furthermore, given the exciting results that have so far been achieved at the LHC and facilitated by grid computing, the medium-term future would appear to be in good shape.

**The strategy for particle physics – including computing-related aspects – was discussed at a workshop in Krakow in September 2012. The results of this workshop will eventually be formally endorsed by the appropriate policy making and funding bodies, but can be expected to enshrine the following key components in terms of computing for HEP:**

* **The importance of embracing standard, open interfaces where possible;**
* **The necessity of collaboration with other sciences, facilitated by the above;**
* **The need for support for heterogeneous devices, backed by a “computing and storage cloud”;**
* **The continued requirement for “a grid” – much favoured by the funding bodies in that it enables the use of resources local to participating sites.**

In conclusion, some level of funding is expected to be available long term. The community of physicists is well connected and organized at the national and international level even when different “data producing” labs are used. However the HEP computing community has in the last 10 years counted on projects (EU and others) for gaining extra funds and for sharing the development and maintenance effort with other communities within and outside HEP.

The timeline of the LHC and related accelerators / colliders is given in the two figures below. The first shows a tentative programme lasting for the next quarter of a century that is obviously subject to funding and approval. However, the WLCG Virtual Research Community and / or its successors will need to be sustained for at least this duration, followed by up to a decade of further analysis that typically follows after the machine has finished its exploitation phase. The second figure shows a more detailed picture of the coming years and in particular the Long Shutdown (LS1) that is expected to start around March 2013 and last for up to two years. During this period, whilst there will be on-going activity not only to (re-)analyse data such as that used to produce the Higgs result mentioned above, but also additional data acquired during 2012 and distributed to the sites but for which there were insufficient resources to process in-line with data taking.

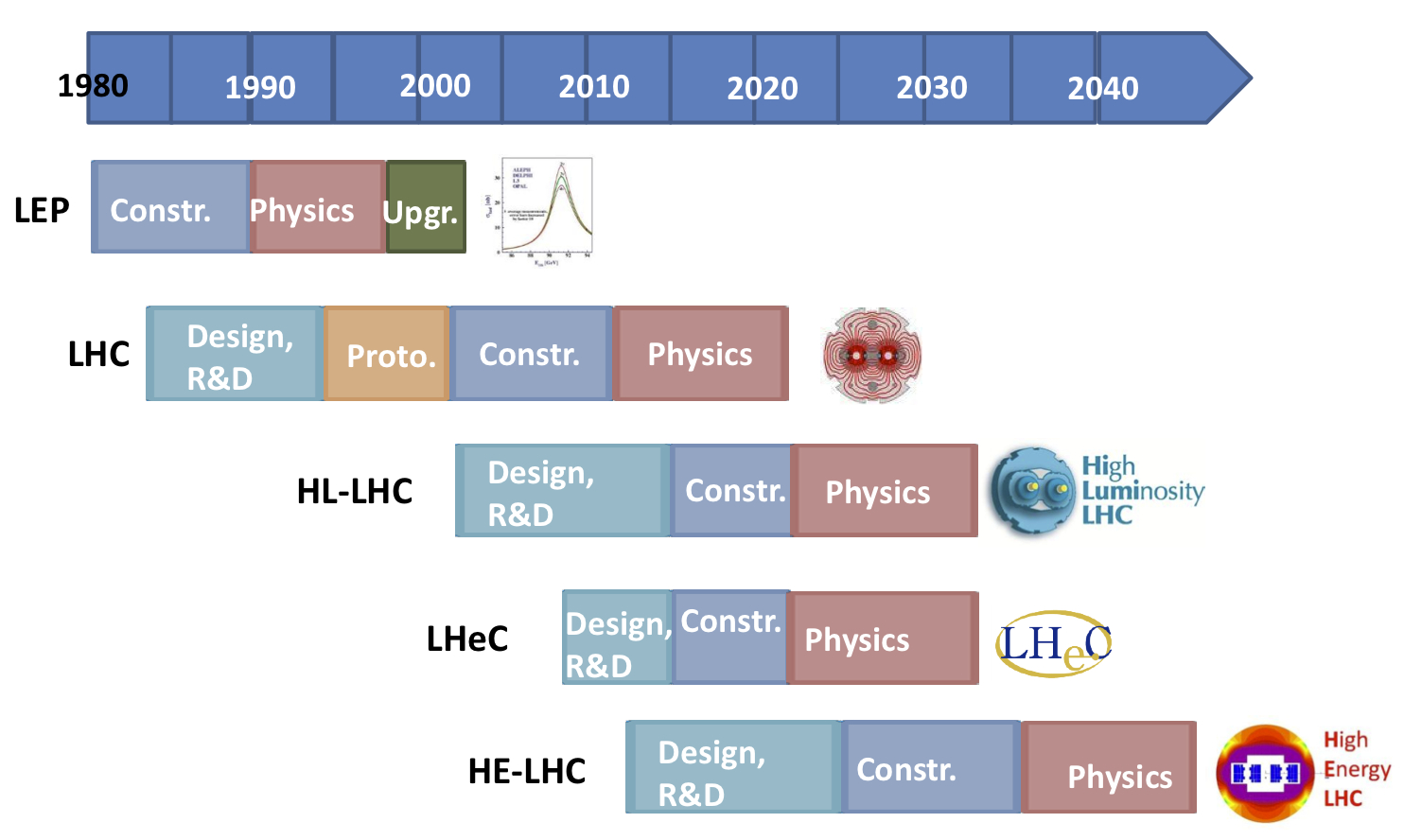


Figure 1 - Timeline for LHC Collider and Possible Variants

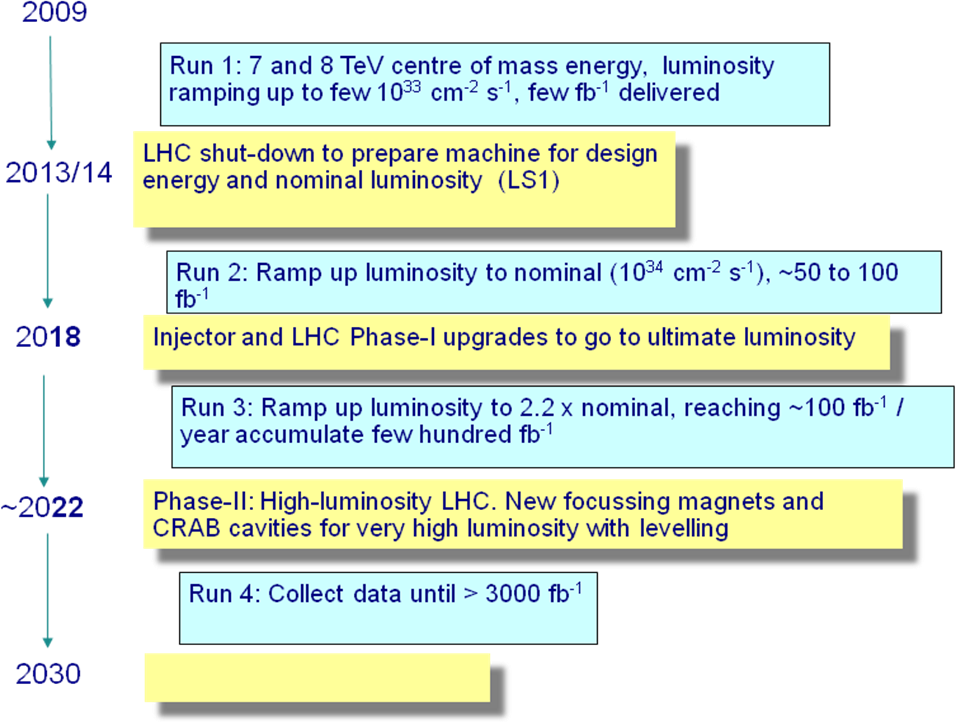


Figure 2 - Timeline of LHC Data Taking (blue) and shutdowns (yellow)

### Progress on Implementing Sustainable Support

The basic model within HEP for sustainability is that of collaborative development. In such a scenario, each tool, package or service is supported by a collaboration involving a number of sites and / or experiments. Whilst this does not provide absolute protection against global reductions in resources, it does limit the exposure and has served the community well for many decades.

Building on work done in previous years, and in particular on that of the WLCG TEGs during PY2 – which in many cases involved members of EGI and other grids such as OSG – a specific plan has been drawn up for each of the packages supported through EGI-InSPIRE SA3. These packages are described in more detail below: in this section we focus on the concrete steps towards long-term (i.e. for the remainder of the useful lifetime of the LHC – some 10-20 years) sustainability.

Basically, all developments have been completed and fully documented, the systems put into production and long-term support agreed with appropriate non-EGI-InSPIRE parties. This support is guaranteed as long as the packages continue to be of strategic necessity to the communities and/or through the lifetime of the LHC research programme. **The on-going monitoring of the effectiveness of this implementation is undertaken by WLCG not only for the key LHC experiments but also for approved affiliated projects.**

Progress on the implementation of this plan has been regularly updated through EGI-InSPIRE documents, notably the Software Roadmap and Sustainability plan for PY3 – MS620.

|  |  |
| --- | --- |
| Tool / Package | Implementation of Sustainable Support |
| Persistency Framework | POOL component maintained by experiments; COOL and CORAL by CERN-IT and experiments. In the medium to long term it is expected that the full responsibility will be taken over by the experiments. |
| Data Analysis Tools | Proof-of-concept and prototype developed partially using EGI-InSPIRE resources. Production system – if approved – to be resourced by key sites (e.g. CERN, FNAL, ...) plus experiments. The development of this system is in any case outside the scope of EGI-InSPIRE SA3, although the work of SA3 made it possible. |
| Data Management Tools | Released to production early in PY3. Long-term support taken over by PH department at CERN (outside SA3 scope). |
| Ganga | CERN’s involvement in Ganga-core will cease some months after EGI-InSPIRE SA3 terminates and will be picked up by the remainder of the Ganga project (various universities and experiments). |
| Experiment Dashboard | All key functionality has been delivered to production before or during PY3. Long-term support guaranteed through CERN-Russia and CERN-India agreements, in conjunction with other monitoring efforts within CERN-IT. |

Table 2 - Implementation of Sustainable Support by Package

## Persistency Framework

Persistency and detector conditions cover two essential areas for HEP data processing and analysis, namely the handling of the event data and detector conditions data of the LHC experiments. Event data, that record the signals left in the detectors by the particles generated in the LHC beam collisions, are generally stored in files, while conditions data, that record the experimental conditions (like voltages and temperatures) at the time the event data were collected, are commonly stored using relational database systems. In three of the LHC experiments (ATLAS, CMS and LHCb), some or all of these types of data are stored and accessed inside data processing jobs using one or more of the three software packages developed by the Persistency Framework [PERS-FRAME] project: CORAL, COOL and POOL.

The Persistency Framework software has been developed over several years (since 2003 for POOL, 2004 for CORAL and COOL) through the well established collaboration of developers from the LHC experiments with a team in the CERN IT department (now partly funded by the EGI-InSPIRE project), which has also managed the overall project coordination. Within the common project, the personnel pledged by ATLAS, CMS and LHCb, coming from a large number of institutes in several countries, have contributed to the development and continue to support the components used by their experiment. The common project, in particular the effort from the IT Department (and from EGI-InSPIRE through it) only deals with components that concern (or, initially, that show the potential to concern) more than one experiment: in the past, individual experiments have already taken up the sole responsibility of components that have been proven to be relevant to that single experiment. This is in line with the more general focus on common solutions as a strategy for the sustainability of the HEP community. The usage of the three packages is periodically reviewed with the relevant stakeholders in the IT Department and the experiments. In particular, the sustainability of the support model for POOL, CORAL and COOL, taking into account the upcoming termination of funding from EGI-InSPIRE, was been discussed within the context of the WLCG Technical Evaluation Groups in PQ4 2011.

Regarding POOL, these discussions have already successfully converged on an agreed sustainable support model. LHCb has already stopped using POOL, after replacing it by a new software layer, inspired from POOL but maintained internally, which is also able to read existing data stored in POOL format; as a consequence, LHCb no longer needs support from POOL through EGI and its software has no pending dependencies. ATLAS will continue to use POOL for as long as the 2012 production version of the ATLAS software is actively used, but it will no longer use it or need POOL support in the longer term (LS1 / Run2).

CORAL and COOL, the proposed support model for the future is based on core support from CERN IT department complemented by a smaller amount of effort from the VOs that depend on the software. While the software is by now mature in its development cycle, a large development and support effort (approximately 3 FTEs) is still required for user support, service operation and maintenance tasks. Software releases are prepared as requested by one or more of the LHC experiments, leading to one release per month on average: this is generally motivated either by functionality enhancements or bug fixes in the Persistency Framework packages, or by upgrades in the versions of the “external” dependencies (ROOT, Boost, Python, Oracle...).

Thus in concrete terms, 2 FTEs would be provided by CERN IT with the third FTE being provided by the experiments / institutes.

## Data Management

### ATLAS Distributed Data Management

ATLAS, one of the LHC experiments, fully relies on the use of Grid computing for offline processing and analysis. This processing is done worldwide using the well-known tier model across heterogeneous interoperable Grids and the ATLAS Distributed Data Management (DDM) project is responsible for the replication, access and bookkeeping of ATLAS data across more than 100 distributed Grid sites.

The work during PY1 and PY2 has focused on the consolidation of the current production system in different fronts. SA3 funded effort has improved and extended a variety of the DDM components and monitoring, focusing on a future sustainable operation. As well, the data placement agents that use the underlying EGI middleware (mainly FTS, LFC and SRM) have been adapted to the latest requirements in the Computing Model and to the changes in the ATLAS Distributed Computing infrastructure. The current ATLAS DDM software is now in a mature state and is managed by the experiment and the CERN PH department, being the present work focused on maintenance and support operations.

### CMS Data Management

Building on the previous experience acquired by the ATLAS experiment, the CMS Popularity Service has been developed to monitor the experiment’s data access patterns (i.e. frequency of data access, access protocols, data tiers, users, sites, CPU usage). The understanding of this framework provides a crucial step ahead towards the automation of data cleaning and data placement.

In addition, a fully automated popularity-based site-cleaning agent has been deployed (re-using directly the ATLAS code) in order to scan the Tier2 sites that are reaching their space quotas and suggest obsolete, unused data that can be safely deleted without disrupting analysis activity.

CMS is currently exploring how to extend the Popularity system with the usage patterns of the data accessed through the XRootD protocol. The services are considered in maintenance, although future development may arise based on the evolution of the Common Analysis Framework (see section 3.4). The funding for this effort was partly through the EGI-InSPIRE project, and is now mainly absorbed by the CERN-IT department.

### LHCb DIRAC

The DIRAC framework provides a complete solution for using the distributed computing resources of the LHCb experiment. DIRAC is a framework for data processing and analysis, including workload management, data management, monitoring and accounting. The support of the LHCb DIRAC Data Management system (DMS) has focused on the consolidation of a data consistency service between file catalogues and SEs, especially in the operational aspects. The visualization of the storage accounting has been developed and put in production and is extensively used by the members of the collaboration. During PQ7 the development of a popularity service started to provide metrics to assess the dataset popularity and provide a ranking of the most popular datasets. The final goal is to use the information about data popularity to implement a dynamic data placement model, where the number of replicas of a given dataset is related to its popularity.

The funding for this effort was partly through the EGI-InSPIRE project, and is now mainly absorbed by the LHCb collaboration.

## Analysis and Tools

For the past two years of LHC data taking, the distributed analysis frameworks of the CMS and ATLAS experiments have successfully enabled the experiments’ physicists to perform large-scale data analysis on the WLCG sites. The experiments have enjoyed significant effort for development activities supported by external projects, such as EGI-InSPIRE SA3, the laboratories, and country contributions. Constrained budgets and completing external projects are reducing the effort available for development and sustainable operations. CMS and ATLAS need to evaluate ways to reduce the needs while maintaining a strong program. A common infrastructure to support analysis is a step in the direction of reducing development and maintenance effort and thereby improving the overall sustainability of the systems.

The Common Analysis Framework is an initiative from ATLAS, CMS and the Experiment Support group in CERN IT (IT-ES) that started in March 2012. The eventual goal of the project is for the experiments to use a common framework based on elements from PanDA and the glideinWMS. PanDA is the ATLAS Production and Distributed Analysis system which includes a workload management component and has been in use since 2005; it has managed the production and analysis activities for more than five years, reaching peaks of up to 100k-150k concurrently running jobs globally and up to 1 million jobs per day. CMS production and analysis is managed by the WMSystem, which includes CRAB for distributed analysis. The WMSystem executes jobs on both the gLite WMS and the glideinWMS. CMS currently uses the glideinWMS to manage the global MC production activities and parts of distributed analysis.

The present feasibility study is the beginning of the work toward a common framework. The feasibility study has the following goals:

1. Review the architecture and functionality of the current analysis frameworks
2. Determine which elements could be provided in common
3. Identify how to interface to existing external services
4. Develop an architecture identifying which experiment specific services could be replaced with common elements.

Whilst this work extends beyond the lifetime of EGI-InSPIRE SA3, it is clearly strongly aligned with the latter’s goals and has been an important additional result in the area of reduced long-term support costs and sustainability in general.

## Monitoring and Dashboards

The LHC experiments all share a common computing model, albeit with minor variations, that is largely that exposed by the presumed late but definitely great Jim Gray in his final paper based on the NASA terminology[[1]](#footnote-2). This model is based on a hierarchy of centres and maps well to activities involving a large international centre, a number of national centres and then more regional centres and universities. The activities performed by the experiments consist of a series of well-defined tasks that can be characterised by data transfers, production jobs, further transfers, analysis jobs and so forth. The expected levels of activities are well understood by both the VOs and sites and this lend themselves well to a common monitoring framework. Sites and managers can understand from well-defined views whether the activities are normal or not.

The specific support provided by SA3 in this area has led to a re-implementation of the core dashboard framework: a single common schema and single common set of applications. This will significantly reduce the support load in coming years.

All of the key use cases are now covered. Clearly, ongoing work will be needed to fix bugs and provide enhancements – in particular those that arise from changes in the infrastructure and/or computing models – but a large fraction of the work has already been achieved.

Development and support effort for the dashboards will continue to be provided by the key stakeholders that include CERN, the experiments and a number of institutes. Additional effort can be expected from other communities or projects that wish to use the framework.

The relevance of the dashboards to the overall process of the Higgs announcement can be seen by the following plot – used in the ATLAS presentation to underline the contribution of grid computing to the scientific result. This is the direct result of SA3-funded effort in this area – the slide was entitled: *“It would have been impossible to release physics results so quickly without the outstanding performance of the Grid (including the CERN Tier-0)”.*

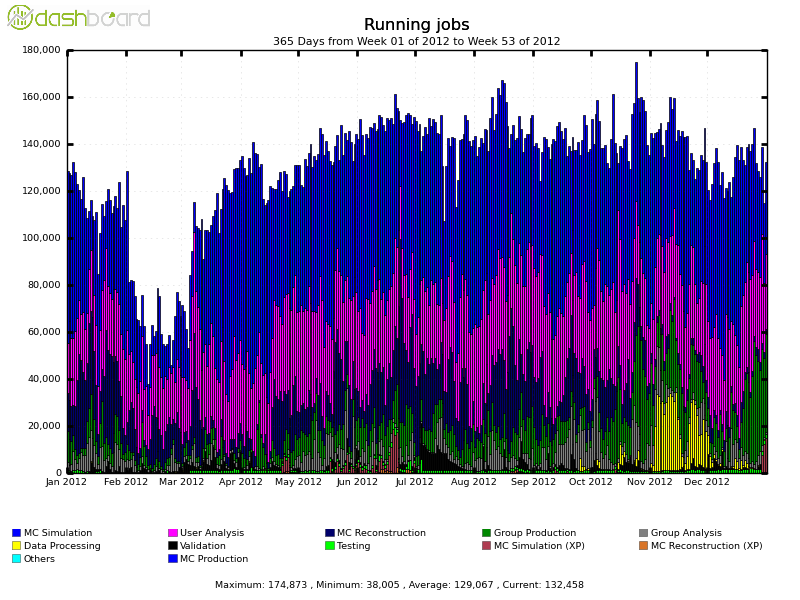


Figure 3 - Number of concurrent ATLAS jobs Jan-Dec 2012

## Ganga

Ganga – which was initially an acronym (Gaudi and Grid Alliance) – is an example of collaborative development and support *par excellence*. The project itself is led by Imperial College, London with contributions from additional universities and institutes in the UK, Scandinavia and Germany to experiment-specific components (ATLAS, LHCb). CERN and EGI-InSPIRE have contributed mainly to the core component “Ganga-core” for which CERN currently has responsibility. Ganga has also found usage far beyond the original HEP VOs and additional funding has come from Earth Science and Life Science projects. It will be supported by these communities for as long as it is required – indeed, it may well get a new lease of life in cloud environments through its “write once, run anywhere” philosophy.

## WLCG Sustainability Model and Plans

Whilst the rest of this section deals with the sustainability of the support that has been provided through SA3, the overall context (for HEP) is that of the WLCG project. As explained during the above-mentioned EGI sustainability workshop, the WLCG collaboration *is* the WLCG sustainability plan. It is based on the following elements:

* Funding agencies providing resources to WLCG have signed a Memorandum of Understanding (MoU) with CERN
* The agreement that the signature of this MoU entails renews automatically and is expected to last the lifetime of the LHC (>20 years)
* The MoU defines the [Minimal Computing Resource and Service Levels to qualify for membership of the WLCG Collaboration](https://espace.cern.ch/WLCG-document-repository/MoU/admin/MoU_basics/Annex3_min_membership.doc) – the actual resource needs, the corresponding pledges and their delivery are all monitored through official CERN and WLCG committees (both hardware resources as well as service delivery)
* The list of funding agencies and their representatives can be found via <https://espace.cern.ch/WLCG-document-repository/MoU/admin/MoU_basics/Annex4_Funding-Agencies_Representatives_12APR12.pdf>
* Further information can be found on the WLCG MoU page: <http://wlcg.web.cern.ch/collaboration/mou>

These structures are analogous to those employed by the large scientific collaborations (ALICE, ATLAS, CMS and LHCb) that WLCG serves and have been used successfully by HEP organizations around the world for some 50 years.

## Conclusions for HEP

One of the key goals of SA3 – namely to provide continued support for the Heavy User Communities of the Grid – has clearly been successfully achieved, at least in the context of its support for HEP. This can be demonstrated not only through key scientific results that have been made available through this powerful distributed computing infrastructure but also be the measurable improvements in service quality that have been seen throughout the first run of the LHC (late March 2010 – early March 2013) that overlapped almost completely with the SA3 work-package (1st May 2010 – 30th April 2013).

By the end of SA3, all of the tools supported for the HEP community will have demonstrated themselves under full production load for several years (the exception is the on-going work on a common analysis framework). A part of the reduction in effort that comes from the end of this work package will be absorbed by further commonalities across the VOs and increased maturity of the products. On-going studies into new technologies and eventual migration to those selected will nonetheless require additional effort. However, this was outside the scope of SA3 and will have to be funded from other sources.

The LHC programme will continue for many years to come: lower support costs are a key priority for the WLCG project and the work carried out in SA3 has had a strong impactimpact on this issue.

# Earth Sciences

## Introduction

The fundamental topics in Earth Sciences are the understanding of the Sun-Earth system through observations and models, and fulfilling societal needs on environmental topics.

Key areas in the Earth Sciences discipline include natural resources identification and exploration, reaction to natural and human-induced changes, long term climatology – observations and modelling, cross scientific domains (physics, chemistry, fluid mechanics, etc) and Civil Protection which involves risk assessment, disaster forewarning, impact studies and mitigation of natural hazards.

Furthermore there are international societies and programs such as the United Nations Environment Program, International Union of Geology and geosciences, Global Monitoring for Environment and Security programme, Intergovernmental Panel on Climate Change, and the European Geosciences Union.

### Distributed Computer Infrastructure (DCI)

There are currently 10 Earth Science related Virtual Organisations defined in EGI, the most recent being verce.eu for seismology research. Besides such VOs that focus on a specific discipline inside Earth Sciences, a general Earth Science Research (esr) VO is also maintained, to allow new or yet unorganised users an easy entry point to carry out their research on the Grid. Resources come from ES related sites directly at NGIs and from EGI. The partners of the VRC[[2]](#footnote-3) are engaged in different projects or have institutional funding; with large variety of funding and person-power conditions.

Community tools consist of web presence, collaboration tools and portals. These are committed by core VRC members for at least the next few years.

For publications, see actual papers from climate, hydrology, and satellite data exploitation.

### Support

Organisationally, collaboration has been achieved with (former) GENESI-DR, ESGF and VERCE. The participating institutions continue to provide support to the community, currently partly funded through EGI-Inspire, the French NGI and institutional funds. For generic VOs and services it depends on the evolution of the usage model. The intention is to collaborate with new projects that are interested in the Grid experience and generic services.

As the developed software is rather focused and consists of atomic applications developed for specific use-cases of the Earth Science community, we fear that the prospective gains for other communities are rather limited. Nevertheless, the inquiries and technical developments may be of assistance, or even serve as groundwork for other communities. Although the specific technical conditions for the application areas, such as the data handling the tools deal with, discern seriously throughout the different communities, common requirements, issues, and principles could be identified. The underlying basics are however not part of this task, that is more practice-oriented. As the tools are self-contained, we foresee that they can survive as open source projects.

The investigation on authentication schemes, or put more generally, bridging infrastructure security functions, are of general interest. The development is aligned and communicated to both the ESGF as well as EGI. Members of the task have participated in identity management workshops and plan to continue to engage in further developments. We hope that this issue will be solved in a larger scale than the ES task of SA3, such as in the infrastructure projects, as they can be helpful in numerous situations.

## GENESI-DR

For EGI users, the GENESI-DR infrastructure provides a standardized data discovery interface based on OpenSearch and metadata standards for a federation of data repositories. While, in the context of the European project behind it (GENESI-DEC), it focuses on a central portal as an interactive entrance point, its usage within EGI (and possibly other DCIs) requires versatile clients such as a non-interactive, bulk oriented command line tool. The work on providing such a client that facilitates the usage in Grid jobs is on-going. A data transfer component was included that downloads the bulk of resources found through the discovery process. This is required as the discovered data sets are not accessible through a unified channel, but depending on the data set instead through different access protocols such as HTTP, GridFTP or others. The command-line tool also provides an ncurses text-based user interface for command-line usage, e.g. for the typical terminal SSH connections to gLite User Interface nodes, and configuration through dot files.. Documentation is available on the webpage, as well as a few standard user scenarios and examples to help users getting started with the utility. For the future, it is planned implement more protocols for data transfer and to carry out broader testing and improve the general reliability of the tool.

Additionally, a flexible web GUI was designed, which indirectly accesses GENESI-DR, among other sources. It uses the OpenSearch interface provided by a running GI-cat instance. The GI-cat web service is developed by ESSI-Lab (http://essi-lab.eu/gi-cat) and uses a mediation approach to execute both remote searches, as well as remote catalogue crawling federating the results and for the remote sources building up a local database for search queries. As it evaluates and transforms the meta data of its sources to a common internal scheme, it can, at the same time, offer different catalogue interfaces, allowing access to existing clients through different protocols (such as OGC CS/W, OpenSearch, GeoRSS and OAI-PMH). GI-cat acts as a broker for catalogue services and can thus serve and search various existing ES data catalogues (e.g. GENESI-DEC, SeaDatanet and EuroGEOSS broker). The web interface accepts search parameters such as a keyword, lower and upper time limits, a geographical bounding box (see figure 1), and more. The interface leverages the OpenLayers capabilities for defining the geographical bounding box. The list of results is subsequently being used to generate search queries for the respective datasets such as AIRS, MODIS, GOMOS or GOME (mainly depends on the catalogues that are managed by GI-cat). Most of these datasets provide OpenSearch interfaces as well. The user defined search parameters from the first steps are then delegated to these second layer interfaces. The found data are presented to the user, who is able to select the required files.

## ESG

The Earth System Grid Federation (ESGF/ESG) is a distributed infrastructure developed to support CMIP5 (The Coupled Model Intercomparison Project, Phase 5), an internationally co-ordinated set of climate model experiments involving climate model centres from all over the world. Data access within ESGF is provided with two main services: OpeNDAP and GridFTP. A site that hosts these services is called a “Data node”. The team that works on ESG interoperability uses a scenario based on an application from IPSL that processes CMIP5 data (climate model data stored on the ESG). An important activity was the implementation of a multi-threaded climate data transfer program to download the data from the ESG data nodes. This smart data transfer tool, named ‘*synchro-data*’[[3]](#footnote-4), facilitates the command line, bulk oriented access to ESG CMIP5 data. The tool can download files from the CMIP5 archive in an easy way, through a list of variables, experiments and ensemble members. The user defines one or many templates that describe the desired data, each of them listing variables, frequencies, experiments and ensemble members. The user separately defines a list of climate models to take into account. Using these templates, the tool explores the ESGF Grid and downloads all the corresponding available files. The program may be run regularly to download the possible new files. This tool provides advanced features including fine grained priorities for transfers, support for CMIP5 "ensembles", an installer, an error watchdog, multi-threaded downloading, incremental downloads through keeping a history, caching to limit the stress on ESGF metadata server, additional actions (delete, cancel, retry), and a statistics module to report about remaining download volume, disk space requirements, etc.

The testing scenario receives further development. It is based on an application from IPSL which uses climate model data stored in the ESG belonging to the fifth phase of the Climate Model Intercomparison Project (CMIP5). The scenario involves software development on three different components: the above mentioned CMIP5 data transfer tool, a credential testbed, and the application itself. The credential testbed is used for prototyping solutions to the challenge of different authentication schemes on EGI and ESG. Separate credentials are required for EGI and ESG, which imposes problems on non-interactive usage in Grid jobs. For the interoperability, a prototype adaption of MyProxy was developed that allows access to previously stored ESG certificates based on EGI certificate authentication. The testbed is planned to be used for running the prototype application in a larger scale, to demonstrate the technical feasibility of the approach. A follow-up research application that will re-use the developments is planned.

The EGI Earth Science community is part of the FP7 project Virtual Earthquake and seismology Research Community e-science environment in Europe (VERCE), which aims at integrating a service-oriented architecture with an efficient communication layer between the Data and the Grid infrastructures, and HPC. A second novel aspect is the coupling between HTC data analysis and HPC data modelling applications through workflow and data sharing mechanisms. Discussions about effective and goal-oriented exploitation of Grid resources in the projects infrastructure are on-going. An EGI Virtual Organisation for VERCE has been established (verce.eu) and the first applications are being run on the Grid.

# Life Sciences

## Community and sustainability model

The Life Sciences domain covers a broad variety of disciplines, ranging from fundamental research to clinical applications. The emergence of digital medical information acquisition devices and specialized signal processing algorithms used to extract biomarkers have revolutionized clinical research and practice over the past decade. Image biomarkers are used routinely for diagnosis, pathology follow up and therapy planning in some medical areas nowadays. They also provide quantitative indicators that are central to many pre-clinical and clinical studies. Consequently, the design of new algorithms as well as the optimization or fine-tuning of image biomarker extraction algorithms is an active research area. In addition, multi-scale analysis has become a reality, exploiting data and knowledge acquired at different scales (molecular data, biological samples, electro-physiological signals, radiology, statistical data over populations). A novel clinical study methodology is appearing based on cross-factors analysis, combining patient information (medical and societal), multi-modal images, quantitative image biomarkers, other qualitative clinical scores, and various biology measurements. This new paradigm for clinical research referred to as *translational medicine* is recognized as a key for the progress of medicine in the coming decades. Exploiting new investigation capabilities, healthcare is also increasingly relying on early diagnosis through human body data acquisition, modelling, and data analysis.

The convergence of these factors makes Life Sciences increasingly dependent on computing technologies. Yet, the requirements of such a multidisciplinary scientific domain are extremely broad. The Life Sciences community is scattered in many different groups leading different kinds of experiments. There are no international organizations nor bodies coordinating the overall activities, and standards only slowly emerge. Furthermore, practices are very different between clinics and research. Within the Life Sciences community, distributed computing technologies are often seen as highly technical and only accessible to few experts, mostly coming from the research area. Consequently, the set of Life Sciences-related Virtual Organizations set up within EGI represents a heterogeneous set of research groups with strong expertise in distributed computing.

**Life Sciences Grid Community (LSGC)**

The Life Sciences virtual research community, active on the European Grid Infrastructure (the Life Sciences Grid Community, or LSGC[[4]](#footnote-5)), addresses some of the most demanding IT requirements arising within this domain. The Foundation of the LSGC consists of 5 NGIs (Dutch, French, Italian, Spanish, Swiss) as well as 5 VOs (biomed, lsgrid, medigrid, pneumogrid, vlemed) and 2 main projects (EGI-InSPIRE, Lifewatch ESFRI). Its financial support mainly comes from the human resources dedicated to this domain by NGIs. Life Sciences used to be represented by the HealthGrid association set up in 2003 for promoting the use of grids within this community. However, HealthGrid went bankrupt and was dissolved in 2010.

**EGI’s Virtual Research Community model applied to Life Sciences**

EGI proposed the Virtual Research Community model (VRC) to structure main scientific areas. VRCs are self-organized user communities sharing common scientific goals. In technical terms, VRCs aggregate several VOs making use of the EGI. The LSGC is the closest implementation of a VRC within the Life Sciences domain. It aims at mutualising efforts and resources of multiple stakeholders interested in Life Sciences who are exploiting a grid infrastructure. The LSGC has been active in promoting and maintaining a few services of interest for the Life Sciences user community. But most importantly from its users point of view, the LSGC had a structuring impact on the community by:

* Organising a management board where community requirements and experience are shared;
* Rationalizing grid usage;
* Setting up a technical team able to liaise with EGI bodies (operations, management…) and users;
* Monitoring the infrastructure at VOs level to pro-actively identify and solve (when possible) problems that make infrastructure usage complex for many users;
* Implementing the VRC model and identifying associated limitations.

It should be noted that, unlike what was initially proposed in the EGI proposal, most effort was not invested in community-specific services provision, but to deal with infrastructure stability and usage policy issues. It proved to be difficult to identify and implement specific services of interest for the complete LSGC given its heterogeneous nature and very diverse requirements. Conversely, infrastructure core services stability and ease of used remained major concerns for end users.

**Community sustainability**

The LSGC is a collegial multi-institutions structure that proved to implement an efficient VRC for Life Sciences over time. Its loose structure makes it independent and adaptable to changes in the context of individual contributing institutions. It is backed up by several NGIs, making it a representative and sustainable body over the coming years. For instance, it proved to be resilient against the disappearance of the HealthGrid association. Yet, its operation currently depends on a fragile volunteering investment model. It may undergo periods of weaker activity depending on the good will and availability of few persons.

The LSGC also represents only part of the real Life Sciences activities exploiting the EGI. Although the largest Life Sciences group in EGI, all related sub-communities did not wish to join the LSGC, either because making use of their own infrastructure or for political reason. In some cases, grid computing is considered too complex and costly (compared to cluster computing). In other cases, smaller-scale and more area-dedicated investment is considered more efficient. For instance, Bioinformatics is a large group which has little involvement within EGI although it clearly makes extensive use of distributed computing and NMR is an independent group operated through the WeNMR European project. The LSGC is easing the access to EGI to new comers and smaller groups, but it does not represent a competitive advantage for larger and well-structured groups. As such, it cannot account for all Life Sciences-related activity observed on EGI.

Finally, the LSGC also faced technical problems related to VRC operation. The EMI middleware operated on EGI inherits from Globus and gLite its VO-oriented conception. All services are operated at the level of VOs and authorization is managed per-VO while a VRC is implemented as a group of VOs. There is hardly any VRC aware middleware service. The lack of cross-VO tools often makes VRC administration complex and some functions impossible to implement at a VRC level. Consequently, the Biomed VO played a specific role within the LSGC. By far the largest VO, it also received more attention and was used as a catch-up for many Life Sciences-related activities.

The LSGC therefore implements a collegial and volunteering-based model for a VRC. It only captures a sub-part of the grid-enabled Life Sciences activities. The community structuring work started 3 years ago is supported by several NGIs, which allocate human resources for the LSGC operation. It develops technical solutions for VRC implementation on a VOs-oriented infrastructure.

## Operations sustainability

The LSGC technical team improves Life Sciences user experience by routinely monitoring the infrastructure at VOs-level, identifying problems and tracking defect reports. Experience proves that this activity is never-ending as some issues are periodically spotted out and require specific actions. The Life Sciences technical team has therefore tightened its links with EGI operations to set up better practices and identify causes of failure that are specific to the Life Sciences VRC. This work progressively led to improving operations sustainability through:

* Deploying probes for SEs, WMSs and CEs available to the VRC and monitoring this infrastructure through a dedicated Nagios server[[5]](#footnote-6);
* Developing tools dedicated to community data management (e.g. anticipate resources shortages, storage decommissioning...)[[6]](#footnote-7);
* Contributing to VO Operations Dashboard[[7]](#footnote-8) design (part of the EGI Operations Portal[[8]](#footnote-9)).
* Facilitating infrastructure-related problems reporting;
* Encourage and taking part to the resource allocation policy work group set up by EGI.

It appears that most sites provide resources to the Life Sciences VRC on an opportunistic mode. This mode gives no guarantee whereas the availability of some resources and resources shortage is often not guaranteed by the EMI middleware, leading to more causes of failures for end users. Sustaining operations at the level of the VRC requires renegotiating the commitment of sites providing resources. This activity is on going within the LSGC.

## Tools sustainability

The sustainability of the Life Sciences VRC also depends on the availability of community critical tools and services. As the community and its requirements are heterogeneous, the lack of a specific service usually only has a limited impact on a sub-part of the community alone.

**Hydra**

An important service for Life Sciences is an encryption service to protect sensitive data. The Hydra service seminally developed as a part of gLiteIO is theoretically fulfilling this requirement. Several attempts have been conducted to provision this service at a production level but they failed due to various code incompatibility and packaging problems. The integration of Hydra in EMI is a low priority and there is no foreseeable date for a production encryption service delivery based on Hydra distribution. However, the on-going deployment of EMI CEs and WMS along with the EMI release of Hydra let suppose that a deployment can be envisaged in the middle term. Meanwhile, only non-sensitive data is manipulated through the EGI, or dedicated user-level encryption was set up when deemed necessary on a per-experiment basis.

**GRelC**

GRelC is a service used by some Life Science experiments. It delivers access and management functionality to relational and non-relational databases in a grid environment. GRelC is a cross-project service which funding is secured over the coming years by existing projects (e.g. the Italian LifeWatch Virtual Laboratory) and other demands. GRelC also invests in dissemination, ease of integration in existing systems and applicability to several domains to makes its integration into future proposals possible.

**VRC dashboard**

As explained above, community sustainability is strongly dependent on the tooling available to manage the community at a low cost. A VRC-wide vision of the users’ activity is needed to help the community to mutualise efforts and leverage common tools. Among existing projects, the VO Operations Dashboard[[9]](#footnote-10) (part of the EGI Operations Portal[[10]](#footnote-11)) is a promising tool expected to become the daily tool for VO operation support teams. It covers important operational needs from the LSGC point of view such as visualization and classification of alarms from monitoring sources (Nagios), integration with the GGUS ticketing system to assist in the creation and follow-up of team tickets, cross information with resource status from GOCDB, support shifts organization and takeover reports, as well as possible advanced features like the detection of flapping service or report builder.

Taking the biomed VO as a significant use case, the Life Sciences Grid Community (LSGC) directly interacts with the development team of the VO Operations Dashboard, suggests and discusses features, and provides feed-back as a beta-tester.

In addition, within the coming year, the LSGC plans the development of a portal addressing administration and operation needs uncovered by other tools[[11]](#footnote-12). The project targets communities with comparable characteristics, for instance: no or few dedicated IT support, scattered scientific activities or fragmented user groups, opportunistic usage of the resources. This portal is expected to integrate various VO management services into a single portal:

1. Community users management, covering users life cycle management, identifying users behind robot certificates, interface with external services (VOMS, LFC, Application Database services;
2. VRC-wide accounting, needed to deliver statistics at the VRC level, assessment of future resource needs. The current EGI accounting portal only provides per-VO accounting information
3. Monitoring of computing resources availability to detect possible bottle necks among computing resources, and eventually address this issue at different levels, for instance in job submission policies.

In January 2013, a project named VAPOR (VO administration and operation Portal), which goal is to develop this portal, has been submitted in response to the EGI call for "mini-projects".

# Astronomy & Astrophysics

## Introduction

Astronomy & Astrophysics (A&A) is a worldwide, geographically distributed community that operates large experiments and observing facilities. A&A can now exploit new and increasingly sophisticated instrumentation facilities with enhanced capabilities and capacities. The discipline has developed so that in silico experiments and simulations modelling physical and chemical processes in the Universe which complement traditional ways of conducting A&A. A huge amount of legacy software in terms of applications and libraries was produced in the course of time. High data volumes that are coming from experiments, simulations and observing facilities present challenges for the storage systems. There is a need for facilities to store and share software and data and a need for computing facilities to fulfil the data processing requests which is an extremely demanding job. There is also a need to handle data in a quick and efficient manner to enable the maximisation of the scientific return.

There are currently no user-friendly A&A-specific environments currently in place that are able to globally meet all user’s expectations and to hide the complexity of the underlying DCIs. The A&A community can count now on the Virtual Observatory and on its infrastructure for a full exploitation of large astronomical data collections distributed worldwide.

Typically, funding for A&A research is allocated to international organizations or to national/local institutes by national governments on a regular basis. Funds coming from specific scientific or technological projects are in turn typically funded by national governments, European Commission, international organisations or by profit entities (business, industry, etc). However recent funding cuts imposed by national governments force communities to look for other possible funding channels (e.g. technological transfer).

### Distributed Computer Infrastructure (DCI)

The A&A Grid/DCI community is currently funded through short/medium term national and international projects (e.g. EGI-InSPIRE and former EGEE projects). Funds typically come from Europe and from national governments. Recent project proposals to sustain the A&A Grid/DCI community by means of a general purpose, pan-European A&A SSC (Specialized Support Centre) were unsuccessful. Single institutes and organizations now ensure a survival level of funds to support activities related to Grids/DCIs. NGIs play a key role in providing tools, services, training, dissemination and other important services. Past experience with A&A HUC has shown that setting up a unique large infrastructure does not work and a unique general purpose VRC failed in achieving its objectives.

Grid/DCI activities have to be carried out in the framework of well-focused scientific or technological projects with a dedicated amount of funds allocated to data processing aspects (with corresponding dedicated WPs). Multiple VRCs gathering more restricted and well-focused communities seems now the most promising and viable way to achieve the sustainability goal for the community.

### Support

The most relevant SA3 tool directly provided by A&A is VisIVO. Other activities of A&A in SA3 focus on the provision of requirements, use-cases, test-beds to EGI to create tools and services meeting A&A’s needs.

## Coordination of A&A

This activity, although not officially part of the work plan of task TSA3.5, is closely related to it given that one of the most important objectives of the task is the provision of requirements, use-cases and test-beds to EGI; they concern: a) interactivity between e-Infrastructures based on different technologies (Grid, HCP and Cloud); b) support to access and manage astronomical databases from Grid Infrastructures. To fully achieve this objective, people working in task TSA3.5 (who are also in charge of the coordination of the European A&A community at large in EGI) need to interact with as many European A&A research groups and Institutes as possible.

The coordination of activities within the A&A community concerning the adoption and usage of DCIs by both small-scale and large-scale projects, in particular by the ESFRI projects such as SKA (Square Kilometre Array) and CTA (Cherenkov Telescope Array) has been intensified both in PY2 as well as in PY3. People have been encouraged to contribute to the process of gathering requirements to be fed to EGI; other initiatives aimed at enhancing the use of e-Infrastructures were also carried out. A coordinating workshop[[12]](#footnote-13) was organized at the Astronomical Observatory of Paris on November 7th 2011, where the major astronomical projects and research areas were represented.

During the workshop the current status of the A&A HUC was discussed. The most important topics raised from the discussion highlighted the need of activating multiple astronomical VRCs each of them aggregated around a big project or Institution well representative of one of the major A&A research areas. A unique catch-all VRC, in fact, has proven to not be suitable being it unable to effectively capture and encompass the needs of the whole A&A community and would impose strong limitations for a number of key aspects like the requirements gathering process and the preparation and implementation of a long-term sustainability plan. All participants agreed that the major effort within the A&A HUC should now be focused on the identification of big A&A projects and Institutions for which the adoption of DCIs could be beneficial, so they might be good candidates to lead new astronomical VRCs. The process aimed at the creation of new VRCs is currently in progress with regular checkpoints scheduled to verify its progress.

## VisIVO

During PY2 significant results have been achieved regarding the porting of VisIVO[[13]](#footnote-14) (Visualization Interface for the Virtual Observatory) to the Grid. VisIVO is a visualization and analysis software for astrophysical data; it consists in a suite of software tools aimed at creating customized views of 3D renderings from many types of datasets.

The activity mainly focused on the study and on the porting of the VisIVO MPI (Message Passing Interface) version to a gLite Grid. The relevance of this activity can be easily understood if one considers that, depending on the structure and size of datasets, the Importer and Filters components could take several hours of CPU time to create customized views, and the production of movies could last several days. For this reason the MPI parallelized version of VisIVO plays a fundamental role.

The preliminary study and the porting were mainly focused on the most important modifications of the code necessary to make VisIVO MPI fully compliant with the gLite Grid. The VisIVO MPI version, in fact, works assuming that the shared home directory and each process can directly work on the tables. Some classes of the VisIVO Filter component were modified to allow the execution of selections on a data table and preliminary tests were carried out.

Another important aspect that would enhance performances is the integration of VisIVO with GPUs (Graphics Processing Units) on Grid nodes where they are available. GPUs are emerging as important computing resources in Astronomy; they can be successfully used to effectively carry out data reduction and analysis. The option of using GPU computing resources offered by Grid sites to make visualization processing on VisIVO was therefore considered.

CUDA (Compute Unified Device Architecture) is the computing engine available in NVIDIA GPUs and accessible to software developers through variants of industry standard programming languages. Because VisIVO is developed in C++, the environment of CUDA is used to develop some computing-intensive modules of VisIVO. This activity started at the beginning of PY2 as a preliminary study on how to produce a CUDA-enabled version of VisIVO for gLite. This first study focused on the porting and optimization of the data transfer between the CPU and GPUs on worker nodes where a GPU is available. To provide a service able to take advantage of GPUs on the Grid, A&A acquired a new system (funded by the Astrophysical Observatory of Catania). The heaviest VisIVO Filter, the Multi-Layer Resolution Filter, was also analyzed. This filter makes possible the inspection of a very large user file (hundreds of gigabytes) to create data for the visualization of an entire dataset with different levels of resolution.

The performances of some additional VisIVO visualization filters such as randomizer, cut, select and swap operations on huge user data tables were also considered. Now the first grid-enabled version of VisIVO service has been deployed. It is based on a specific grid-enabled library that allows users to interact with Grid computing and storage resources. The current version of VisIVO is also able to interface with and use the gLite Grid Catalogue. Although VisIVO has been conceived and implemented as a visualization tool for astronomy, it evolved in a generic multi-disciplinary service that can be used by any other community that needs 2D and 3D data visualization.

## Grid and HPC

A working environment where Grid resources and HPC resources can be combined and used together is of utmost importance for many astronomical applications. Some typical A&A applications that could improve their performances in such an environment have been identified: FLY[[14]](#footnote-15) (a cosmological code developed at INAF-OACt) and Gadget[[15]](#footnote-16) + Flash[[16]](#footnote-17), the most common cosmological codes in Astrophysics.

The FLY code (a tree N-Body code) was executed on the gLite Grid. Some problems arise when running with a high number of N-Body particles. To overcome this problem a workflow has been designed; it can be adopted when the code runs in challenging scenarios where data files several tens of gigabytes in size have to be handled.

To test cosmological simulations we are now in the phase of identifying and defining some use-cases; the goal of this activity consists in preparing the environment, the input file and the watchdog procedure to verify the run and the results.

Recently the activities related to Grid and HPC are carried out in close coordination with EGI and with IGI[[17]](#footnote-18) (the Italian NGI) in Italy. A tight coordination with EGI and with NGIs, in fact, is crucial given that collaborations and agreements with PRACE and with other entities that operate and maintain HPC resources (typically supercomputing centres) are very important for this activity. One of the activities recently undertaken within the task TSA3.5 aims at introducing small-size HPC resources in Grid. This is achieved by installing and configuring HPC clusters (based on low latency/high throughput networks, HPC libraries and tools, modules and compilers) and then making the Grid middleware aware of these resources. The plan is to verify such small-size HPC resources and the related middleware aware version vs. the most popular cosmological applications previously mentioned, namely FLY and Gadget + Flash.

This activity, carried out in Italy and targeted at HPC resources, continued also during PY3 in close coordination with all those communities involved in IGI that need HPC and MPI to efficiently run their applications.

## Access to Databases for DCIs

Access to databases from DCIs and interoperability with the VObs (Virtual Observatory) data infrastructure remains one of the hot topics in astronomy. One of the most important related activities deals with the identification of use-cases and test-beds (both applications and complex workflows) that require simultaneous access to astronomical data and to computing resources. The data infrastructure of reference in astronomy is the VObs; end users should be able to access astronomical data through VObs standards[[18]](#footnote-19) and launch computational tasks on DCIs. In this context two key issues concern a SSO (Single Sign On) authentication mechanism able to grant access to computing and data resources by means of a single authentication (users do not need to authenticate themselves multiple times) and tools/services to access astronomical databases federated in the VObs from DCIs.

Another important activity related to the integration of data and computing resources is the work in progress to integrate in Grid the BaSTI[[19]](#footnote-20) (A Bag of Stellar Tracks and Isochrones) Astronomical Database and its feeding FRANEC code. A web portal was developed to make easier the submission of FRANEC code to the Grid. The portal allows the user to define a set of parameters and to simulate stellar evolutions on the Grid, without worrying about the technical details concerning the underlying Grid Infrastructure. The portal is currently based on P-GRADE web portal.Since the portal is designed for the submission of an arbitrary job to the Grid, it was necessary to do some low level “tricks & hacks” to make it able to fully satisfy our needs. The work aimed at implementing a new version of the portal based on the latest version of P-Grade ended during PY2. It is based on Web Services and this enables a low level integration with the Virtual Observatory.

## Sustainability Plan

According to what exposed in previous sections, the A&A activity in EGI-InSPIRE focused on the following aspects: a) creation and deployment of tools and services to make DCIs able to meet the requirements of A&A applications and workflows; b) gathering of A&A requirements, use cases and test-beds so that tools and services being part of future releases of the Grid middlewares take into account the needs of the astronomical applications and workflows. At the same time, in parallel with the participation to EGI-InSPIRE, a significant activity aimed at porting astronomical applications and workflows took place in the framework of other projects. For what concerns these activities the lesson learned from the past experiences is that all of them are hard to carry out if not linked to a specific project and finalized to its needs. The idea of creating VRCs (Virtual Research Communities) transversal to the whole community and to their projects and able to deploy services for the benefit of different research groups and projects do not work and was rejected by the EU Commission. For this reason the creation and deployment of such a catch-all VRC was dropped and the efforts were focused in carrying out DCI-related activities in the context of large astronomical projects.

Obviously this choice has a strong impact on the plans conceived to ensure a long-term sustainability of in-production tools and services. In a short-medium term perspective, the sustainability of tools and services designed and implemented in the framework of past EGEE projects and more recently in EGI-InSPIRE is ensured by increasing the number of their end users; to this end large astronomical projects like the SKA and CTA play a key role. They are flagship reference projects for entire branches of the astrophysical research (radio, astroparticle physics, etc.) able to capture all users belonging to these branches. Tools and services imported (and eventually adapted) in these projects ensure their sustainability over time if they prove to be useful for these communities; considering the lifetime of these big projects (twenty years or more) we can speak in this case of long-term sustainability. Although collaborations with other smaller projects and Universities are always possible and to be anyway encouraged, the long-term sustainability mainly relies on large projects and collaborations. In the framework of these projects funds and, most important, man power could be allocated to continue the development/maintenance of such services.

One of the key concepts worthy to be remarked is that the sustainability closely depends on how big is the community of end users. The wider is this community, the higher is the chance of ensuring a good long-term sustainability plan for tools and services. The projects mentioned above (CTA, SKA and others) are in a good position to ensure such a wide community of end users.

Practically speaking, in the last months some of these big projects were successfully approached and now concrete plans to experiment for them DCIs and their related services and tools are underway. CTA is the most important example in this context, but for SKA and Euclid as well there are good chances to establish a collaboration agreement in the near future.

In the framework of these large projects we are introducing an approach based on the concept of a “well defined” governance model.

A first instance of this model has been conceived and implemented for VisIVO software[[20]](#footnote-21). The governance model in this case led to the identification of the following roles: Users, Contributors, Committers, Maintainers, and Project Lead. Each of these roles imply different responsibilities and a different involvement in the activities related to the development, maintenance and usage of VisIVO.

A set of web tools have been identified and created to ensure an effective participation of the community of users in the decision making process concerning the software; this set of tools is currently made of two mailing lists (“users” and “developers”) and four Issues Tracking (Bug Reports, Support Requests, Feature Requests, Patches).

Our intent is to operate within these projects keeping the EGI ecosystem and its infrastructures as the system of reference for what concerns DCIs, whatever is the underlying technology. As a concrete example of this approach, since January 2013 a VT (Virtual Team) dedicated to CTA is running in EGI; the goal of the VT is to identify and propose concrete technological solutions for the CTA SSO authentication system and the Science Gateways developed for the project.

Another practical example is the creation of a VO and a VRC dedicated to the Euclid project, although this option is still under evaluation.

# Additional Communities

## Dashboards

The Experiment Dashboard system provides monitoring of the WLCG infrastructure from the perspective of the LHC experiments and covers the full range of their computing activities, such as data transfer, job processing, and site commissioning. In contrast to many other monitoring systems, the Experiment Dashboard is not coupled to any particular middleware, workload management, or data management systems. It is shared by several LHC virtual organizations and works transparently across various middleware platforms.

The Experiment Dashboard has proved to be an essential component of the Grid monitoring infrastructure. The LHC experiments rely heavily on the Experiment Dashboard for distributed operations, monitoring user computing activities, and providing user support. The Experiment Dashboard servers are accessed by several thousand distinct users per month. Among the Dashboard applications which are extensively used by the LHC community are Site Status Board, Job monitoring applications, DDM (Distributed Data Management) Dashboard. Experiment Dashboard applications adhere to a set of core development principles: common technology and implementation, loose-coupling to data sources, sharing of monitoring data, and user involvement in the development process. The aims of these principles are to reduce development and maintenance overhead, to allow applications to be easily adapted for use by multiple VOs, to enable reuse of monitoring data, and to ensure that applications meet user requirements. The Experiment Dashboard Framework provides a common foundation for the development of the monitoring applications and facilitates development and maintenance tasks.

The sustainability of the system is ensured by the described development principles and by the collaborative nature of the project. The core development and support team at CERN collaborates with the developers from the LHC experiments. There are also contributions from the institutes participating in the LHC project from Russia, Taiwan, India, and the UK. The LHC experiments also take part in operating the Dashboard services, for example as a part of ATLAS computing shift procedures.

During PY1, substantial progress was made concerning the redesign of the Dashboard applications, achieving complete decoupling of the user interfaces from the data repository through the use of new technologies such as AJAX. New versions of the Site Status Board, ATLAS DDM Dashboard and Site Usability Monitor, as well as of the wide range of the job monitoring applications were deployed in production. Many of the job monitoring applications were developed using a common hBrowse visualization framework, which aided the development process and allowed the integration of common user interfaces with various information sources. The migration of the Dashboard cluster consisting of 50 nodes to virtual machines was accomplished. The functionality of the Dashboard cluster management system was improved. This includes development of the web interface which provides information about status of the nodes belonging to the Dashboard cluster and applications hosted by these nodes. All those changes contributed to the sustainability task through decreasing maintenance and support effort.

In 2012, priority will be given to the common applications shared by multiple VOs. Among them is the Global WLCG transfer monitor that aims to perform common tasks carried out by the LHC virtual organizations in order to monitor their data transfers on the WLCG infrastructure, namely aggregation of the WLCG transfer monitoring statistics and exposing monitoring data via user interfaces and APIs. The first prototype of the system was developed and deployed for validation in 2011. During 2012, the functionality of the system will be extended based on feedback of the user community.

Another important direction of work will be the improvement of the monitoring tools for end users, task monitoring for distributed analysis being one of them. A new version of the task monitoring application based on the hBrowse framework will be released in 2012. All Dashboard data repositories will be migrated to new hardware and ORACLE version 11g; this will improve performance of the Dashboard applications. The functionality of the Site Status Board application will be extended in order to provide better automation of the operations of the distributed infrastructure, which in its turn will address the sustainability task. It is foreseen to be integrated into the SSB framework functionality of the CMS site readiness tool and to enable alarm notification. Apart from the development work described above, the plans for 2012 also include maintenance and support of the Dashboard cluster, services, and software.

## Workflow and Schedulers

### Kepler and GridWay

As described in MS606, Kepler is a software application for the analysis and modelling of scientific data. Kepler allows scientists to create their own executable scientific workflows by simply dragging and dropping components onto a workflow creation area and connecting the components to construct a specific data flow; GridWay [GRIDWAY] is a Metascheduler that automatically performs all the **submission steps** and that also provides the runtime mechanisms needed for dynamically adapting the application execution.

The work of these activities has been focused on building a set of different use cases that can be used as templates by any other scientific community. Up until now, the developed workflows have been using the capabilities of gLite or UNICORE, with the functionalities provided by the standard software of these middlewares. Since some of the applications (and users) were already using Gridway, we decided to also provide support for it from within the Kepler environment. GridWay provides functionalities that have been already developed in the Serpens suite for Kepler. For example, with GridWay, more actions can be delegated into the metascheduler since this software deals with most of the issues regarding job management: send the job, retrieve the results, deal with the information about the status of the infrastructure. By supporting GridWay, we are improving the sustainability plans of Kepler. This development provides enhanced capabilities plus new options for the users. GridWay supports different middlewares, hiding those middlewares from the user or from any piece of software on top of GridWay. Hence, more computing infrastructures (middleware) could be used from within Kepler.

As it has been stated in previous reports, activities have been focused on establishing collaboration with other user groups which have shown interest in our work. Also, the dissemination activities carried out in different locations and meetings show the impact of our work to other communities. We have established contact with the Computer Chemistry users, Astrophysics and are in the process of helping out with the use cases using Kepler (with the Serpens suite). Also the results of the work (Kepler with Serpens suite) have been proposed in terms of the national initiative – PL-GRIDPlus, where the scientists from astronomy and nanotechnology are building their first use cases using this workflow framework. We also plan to approach other user communities.

### SOMA2

SOMA2 is a versatile modelling environment for computational drug discovery and molecular modelling. SOMA2 is operated through a web-browser and it offers an easy access to third-party scientific applications. The SOMA2 environment offers a full scale modelling environment from inputting molecular data to visualization and analysis of the results, including the possibility to combine different applications into automatically processed application workflows. During PQ6 and PQ7, CSC has maintained and operated CSC’s SOMA2 service.

The main outcome of SOMA2 development in the last year has been the integration of the scientific application Autodock 4 into SOMA2 which makes use of the Grid support features. Moreover, in the end of PQ7 SOMA2 version 1.4 Aluminium was released. This release contains most of the EGI-InSPIRE related work so far. In addition, we have continued investigating on how to setup a SOMA2 service which would be provided to other user communities as well, apart from the current CSC users.

Based on the achievements so far, we will provide a grid-enabled application service from national level to other user communities as well. At the moment it seems that CSC is going to set up a separate pilot service for this. We will also operate and support the existing SOMA2 services. In addition, we will advertise the grid enabled SOMA2 service to different user communities.

On a longer timescale, our goal is to expand the selection of scientific applications in the SOMA2 service, and to integrate application services from different grids hosted by different virtual organizations into SOMA2. This should be set as an important milestone because from the end users point of view, this would make using scientific applications on different grids very easy and transparent. We will continue to maintain and operate the SOMA2 service and seek possible scientific applications to be added as part of the service. During all project years, we will support using SOMA2 services. Furthermore, the development of the SOMA2 gateway will continue according to feature roadmap, including possible feature requests from the user community, bug fixes, and other enhancements.

## MPI

The MPI sub-task shall focus on a number of core objectives over its 36 month period (PY1 -PY3).

Many of these objectives are iterative, often requiring updates or fine-tuning. Other objectives, including participation in the EGI Community and Technical forums, shall be repeated at regular intervals. The core sub-task objectives are:

* Improved end-user documentation, addressing MPI application development and job submission in ARC, gLite, and UNICORE,
* Quality controlled MPI site deployment documentation,
* Outreach and dissemination at major EGI events and workshops,
* User community, NGI and site engagement, gathering direct input,
* Participation in selected standardisation bodies.

This sub-task has produced numerous MPI workbenches of increasing complexity with specific high impact on the Computational Chemistry and Fusion communities. These products include parallel implementations of Linear Algebra routines (produced by UNIPG). UNIPG has been working on the parallelization of the CHIMERE application. The detailed analysis has identified the extent to which the application will achieve the highest level of parallelization possible, and thus the greatest efficiency. This model is structured around a task-farming model, in which some worker processes share the work by taking charge of part of the domain (subdomain) under the control of the master that sends and receives the relevant data, and that writes the results. The application can read initial input data based on the output of a previous run for a given timeframe. The model has several advantages:

* By chaining the results of many shorter runs, this allows simulations to run over much longer timeframes, and thus overcomes issues with CPU time-bound usage limitations at most resource centres.
* Can also be used as a form of application check-pointing.
* Allows greater granularity/resolution.

The CHIMERE parallelization model can be reused in many other scientific domains including, among others, the Earth Science and Astronomy & Astrophysics communities. UNIPG has also implemented numerous advanced parallel codes for GPGPU. This code has been successfully implemented on two different GPGPU architectures. In addition, UNIPG shall continue exploration of a parallel implementation of CHIMERE and the GPGPU work in PY3.

Improvements to the MPI documentation[[21]](#footnote-22) were made in PY2. The EGI Wiki now provides the definitive source of information for MPI support. Documentation on the ARC and UNICORE MPI support still require extra attention. The current release of the UMD gLite-MPI 1.2.0 package was released in Project Month 21. The release of the UMD glite-WMS and the glite-MPI products are expected to contain significant middleware changes required to ensure the correct support for many MPI job types. For example, these include:

* User defined allocation of processes/nodes
* Direct Support for OpenMP codes.

Furthermore, end-user support for both MVAPICH (an MPI implementation with advanced Infiniband networking) and support for generic parallel job support is a high-priority in PY3.

This work is under the leadership of CSIC, and is aimed at steering MPI and Parallel jobs technical requirements.

Both UNIPG and TCD are working on exploiting GPGPUs. The UNIPG work is already at an advanced stage: An entire job flow that enables the Local Resource Management System (LRMS) to discriminate the GPGPU resources requests, through Glue Schema parameters, has been defined in order to allocate, in a dynamic fashion, the required resources on a Cloud-like infrastructure. This solution helps overcome some weakness in many job schedulers, which do not currently support GPGPU resources. TCD uses StratusLab – an open-source cloud distribution that allows grid and non-grid resource centres to offer and to exploit an “Infrastructure as a Service” cloud; this is a work-in-progress, and significant results are expected in PQ8. TCD is investigating potential GPGPU Information System support.

As part of User Community engagement effort, the MPI team will regularly survey Virtual Organisations, Users and Site administrators for critical feedback. This will also act as a means to gather information about current deficits and future requirements. The newly founded NA2 driven MPI Virtual Team (MPI-VT) is expected to lead to a concentrated drive to weed out and fix problems observed with some large production-level MPI jobs. This shall create a greater demand on the SA3 MPI support team, led by CSIC and TCD.

The predominant job scheduler “MAUI” needs to be upgraded at affected MPI sites in PY3, due to the fact that a node allocation bug/problem has been discovered in the standard distribution. EMI does not provide support for MAUI, and the software license may impose significant software distribution restrictions. We are currently working around this problem by recommending that sites install a patched version from an unofficial repository. Longer-term support requires that this issue be resolved at the highest level.

The MPI task has not yet fully tackled the issue of sustainability. The MPI community itself has two mature and major open-source framework implantations: MPICH-2 and OpenMPI. These are both well supported and are expected to be maintained and further developed in the medium term (five years). Both are also heavily used by the High Performance Computing community. The two frameworks are also actively developed, and produce several new releases per year. Methods to widely support generic parallel jobs, GPGPU, and cloud integration may be potential research projects for further exploitation on distributed computing infrastructures.

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