Whitepaper: A Case for SAGA as Access Layer for Production Distributed Computing Infrastructures

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December 20, 2010

Aim and Audience of this White Paper

The aim of this document is to inform providers, design architects and users of production Distributed Computing infrastructures (DCI) of the role and relevance of the SAGA API for their DCI. In particular, we focus on how SAGA can increase the number of users and application usage modes by providing SAGA as an access layer to DCI.

1   Introduction

SAGA is an acronym for "Simple API for Grid Applications". As the name suggests, a simple API which facilitates the development and execution of distributed applications on most types of distributed infrastructure. Modern distributed computing environments are very complex infrastructures, and allowing applications to make use of these complex systems is not trivial. By defining a simple API, one requires those complexities to be dealt with at levels other than application code and development. Simplicity of the interface is the primary design principle and objective of SAGA. Functional goals of SAGA are:

1. Provide a stable programming interface to distributed application programmers and tool developers

2. Shield developer from heterogeneous and evolving infrastructures and middlewares

3. By providing the building blocks to distributed and remote operations enable the expression of high-level abstractions and support of distributed application requirements

The fact that SAGA is an OGF standard ensures the community-wide adoption and stability of the API.

2 The SAGA Landscape

2.1 SAGA API Specification

The SAGA API specification is object oriented, and language independent (the API is defined in IDL). The API is structured into various packages (e.g. jobs, replicas, streams, etc.). Those packages have limited dependencies amongst each other - not all SAGA implementations implement all packages. All API packages share certain properties: how are synchronous methods expressed, how are notifications realized, how are security tokens expressed, what types of exceptions are defined, etc. Those properties are specified in the SAGA-Core, the API's look and feel.

That design of the SAGA API allows to specify additional API packages, which adhere to the same look-and-feel. In fact, several such API packages have already been defined (e.g., Service Discovery, Remote Procedure Calls etc.), and are standardized as well, or are in the process of being standardized.

2.2 SAGA: A Community Specification

The SAGA API specification has been developed and guided by the broader distributed computing community at the OGF[1]. An analysis of the requirements led to abstractions that were mapped into different SAGA API packages, while ensuring that (a) the overall usability (e.g. the API look-and-feel) was consistent over the whole scope of the API, (b) the API functionality maps relatively well onto existing middleware features, and (c) the API is simple to use. The API is simple, even if the semantic translation and across layers and maintaining implementation fidelity for middleware specific features is not trivial.

The SAGA standardization effort is closely syncronized with other specification and community efforts, within and outside of OGF. In particular, OGF groups ensure that SAGA semantics map well to lover level specifications, such as JSDL, BES, GridFTP, etc. But also, and possibly more importantly, it is now widely and independenly acknowledged that a uniform, simple and stable access layer is neccessary (but not sufficient) to improve end user experience on distributed computing infrastructures, and that SAGA can indeed play that role for a specific set of use cases. As such, SAGA is now integral part of the GIN (Grid Interoperation Now) community effort, and also plays an active role in current efforts like OGF's PGI group and US's XD proposals.

2.3 SAGA Components

As discussed, the SAGA API specification is language independent. The SAGA distributions contain various language *bindings* for that API. The SAGA-Core distributions deliver those bindings as class files for Java, as modules for Python, and as shared and/or static libraries for C++.

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[1] http://www.ogf.org/

SAGA as an API would be rather useless if it would not also offer bindings to the various middlewares. Those bindings are, for all major SAGA implementations, provided as *adaptors*. Some simple adaptors are usually packaged with the SAGA-Core distributions, but otherwise are packaged and distriubuted separately (details see in section 2.5).

While SAGA is foremost an API, the SAGA distributions support end users in a variety of ways. In particular, the SAGA distributions also include command line tools implemented via the SAGA API, and higher level libraries for common distributed programming patterns, also basing on the SAGA API. Further, the SAGA distributions provides comprehensive support to compile, link and run SAGA applications (configure scripts, make support, runtime wrappers, developer tutorials , etc).

Command line tools are, in our experience, amongst the first components of any distributed middleware to be exploited by end users. SAGA-C++ provides a set of command line tools which basically cover the complete semantic set of SAGA API calls, such as job submission and management, file management, replica management, etc.

Several SAGA based projects are actively developing and using higher level programming abstractions, such as pilotjobs, bigjobs, mapreduce, or workflows. Such components are routinely installed and used by a number of user communities, and represent significant added avlue, although they are not part of the SAGA core code base. It should be noted that the SAGA Python bindings, which are usually installed by default, are very frequently used to provide tooling and higher level programming abstractions.

2.4 SAGA Core: Implementations and Deployment

2.4.1 SAGA Implementations

The language independent SAGA API specification has been mapped to multiple programming languages, in particular to C++, Java and Python. Multiple implementations exists, the most notable ones are SAGA-C++, JSAGA and JavaSAGA.

SAGA-C++ is, as the name suggests, a C++ implementation of the SAGA API, mainained by CCT/LSU, and a growing international community. The SAGA-C++ development is in close lockstep with the API specificatin efforts, and the most widely used SAGA implementation to date.

JSAGA (from IN2P3 in France) and JavaSAGA (from the Vrije Universiteit, Amsterdam) are API compatible Java implementations (they use the same set of abstract class definitions). JSAGA caters to an active, but small user community in France, and supports a realitvely large set of adaptors for the job and file API packages. JavaSAGA is mostly a academic research vehicle, which bases its middleware bindings mostly on JavaGAT (its predecessor), and sees some uptake in the Netherlands and the German D-Grid project.

All three implementations provide python bindings - the Java implementations realize those via Jython, the C++-implementation via Boost-Python. The two Python bindings are at the moment being unified, and have already been shown to be interoperable. The Python bindings are implemented as a wrappers around the C++ and Java implementations, and are thus able to utilize their complete set of middleware adaptors.

This white paper focuses, from here on, on the SAGA-C++ implementation.

2.4.2 Important SAGA Deployments

The different SAGA implementations, and in particular SAGA-C++, have by now been in use in different user communities for a number of years, and thus have matured enough to enter the field of production cyber infrastructures. At the same time, the number of supported backends has grown to a level that basically all current production infrastructures are supported (e.g. for jobs we support ARC, gLite, Globus, Condor, PBS, Torque, DRMAA, EC2, Eucalyptus, BES, Naregi, Unicore, SMOA, Genesis-II, fork, and ssh)[2].

SAGA has so far been successfully and routinely used on the TeraGrid, LONI, FutureGrid, DEISA, NAREGI/RENEKI and a number of smaller, more localized DCI. It has also been used by a range of e-Science projects such as EGEE, DGrid, VPH etc.

SAGA-C++ has one major external dependency, which is Boost[3], a set of C++ headers and lbraries widely used in the C++ community. While Boost itself is a fairly complex code base, it is routinely packaged by the various Unix distributions, and thus usually available out of the box. Further, SAGA-C++ is able to compile against a wide range of Boost releases, including those which are the default versions for the currently used Linux distributions. Postgresql client libraries are not strictly required, but recommended for some of the core SAGA functionality.

While SAGA is relatively easy to deploy in applications space (i.e. user space), its overall goal of improving the end user experience of distributed systems benefits greatly from system level installations. It is straight forward to install SAGA in user space (`configure; make; make install`), but in our experience, the correct environment setup to use a SAGA installation in user space is still a stumbling stone for many end users (`LD_LIBRARY_PATH` etc). We thus prefer SAGA to be available in system space, which lowers the entry barrier significantly.

We are currently working to provide binary releases, in the form of Debian and Ubuntu packages, and RPMs. Also, we are currently integrating SAGA into NMI and ETICS build and testing environments, which we hope will lower the effort for system level installations significantly.

2.5 SAGA Adaptors Implementations

Interestingly, all three SAGA implementations discussed above are adaptor based: a relatively small library provides the SAGA API, and a set of adaptors translate the SAGA API calls into the respective middleware operations. It is those adaptors which encapsulate most of the complexity which was formerly present in the applications layer. While SAGA adaptors are relatively easy to implement (or at least as a prototype), they require significant maintainance effort to keep up with the middleware intricacies and evolution.

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[2]http://cyder.cct.lsu.edu/saga-interop/mandelbrot/demo/today/last/
[3]http://www.boost.org/

SAGA-C++ supports the implementation of adaptors with a tool, which generates a complete, but semantically empty adaptor stub. The adaptor developer has then to fill that stub with the respective native middleware calls. SAGA-C++ further provides tools and support for adaptor compilation, documentation and packaging.

The SAGA web page[4] has an (incomplete) list of adaptors currently supported by SAGA-C++.

3   SAGA Usage and Active Projects

3.1   Standards promote Interoperability

ExTENCI

ExTENCI[5] is an NSF funded 2 year project to promote interoperability between the TeraGrid (and/or its successor – XD) with the OSG (and its successor). The role of SAGA is provide a common job-submission mechanism across TeraGrid and OSG, for both command-line access as well as for Cactus based application via Gateway. The different application scenarios that are/will be supported are:

- Ensemble of Cactus Simulations (NumRel, EnKF (Petroleum Eng))

- Multiphysics Code (GR-MHD, CFD-MD)

- Spawning Simulations (Realtime outsourcing from BlueWaters/Ranger to specialised architectures or less powerful resources)

VPH - Efficient Free Energy Calculation Methods using HPC Interoperation

The Virtual Physiological Human (VPH) project is concerned about providing computer models for personalized patient specific healthcare and also trying to create tools for modelling and simulation of human physiology. There are multiple use cases: The first consists of simulations of so-called ensembles which are non-interactive and thus their computation can be considered embarrassingly parallel. The second step consists of loose coupling of the simulated ensembles, which requires limited interaction between the jobs.

This is a computationally intensive problem and could utilize as many HPC resources as could be possibly made available or acquired. Current efforts are aimed at using the high-end TG and DEISA (soon to be PRACE) machines collectively to finish a work-load. The underlying kernel is the same (NAMD) but the execution management is needs to be intereoperable; this is provided by SAGA.

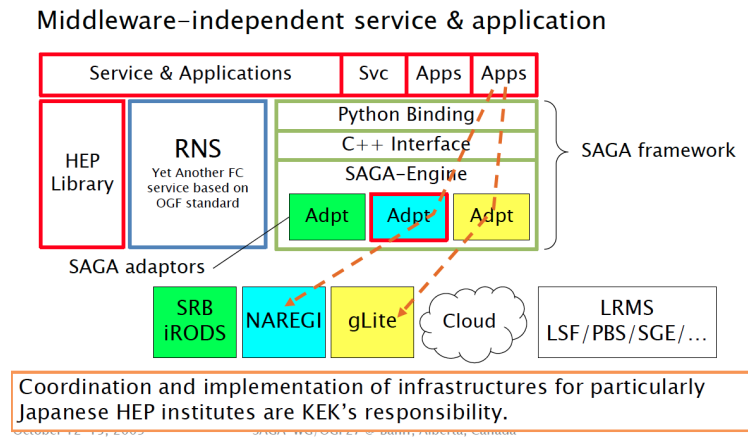
[4]http://saga.cct.lsu.edu/software/cpp
[5]https://sites.google.com/site/extenci/

Figure 1:

gLite / Ganga

GANGA is a very commonly used tool to submit jobs to EGI/EGEE. GANGA does not provide explicit support for submission to globus-based systems. There exist multiple application (eg LatticeQCD) that would benefit from both HPC-HTC job submission capabilities. Therefore Ganga uses SAGA and its globus adaptor to extend the capabilities of GANGA. See `http://svnweb.cern.ch/world/wsvn/ganga/trunk/ganga/python/GangaSAGA/Lib/SAGA/#path_trunk_ganga_python_GangaSAGA_Lib_SAGA`

RENKEI/NAREGI

The RENKEI e-Science project is using SAGA in two distinct ways: as shown in Fig. 1, one mode is as an access layer to multiple middleware distributions, including but not limited to globus and Naregi. The second is to provide Python scripting capabilities for simple workflows executing over multiple resources – job submission, task management (coordinated execution) and data/file management. See details at the following: `http://saga.cct.lsu.edu/projects/tools-and-infrastructure/kek-1`

3.2 Applications Scenarios

FEDEX: A SAGA-based Runtime Framework for Dynamic Execution of Multi-Physics Simulations

SAGA provides a runtime framework for dynamic execution (FeDEX) which can be used to support the execution of coupled multi-physics simulations. This is being used by several projects including the $2M NSF-funded Cybertools Project (`http://www.cybertools.org`) and the EU FP7 Mapper Project (`http://www.mapper-project.eu/`).
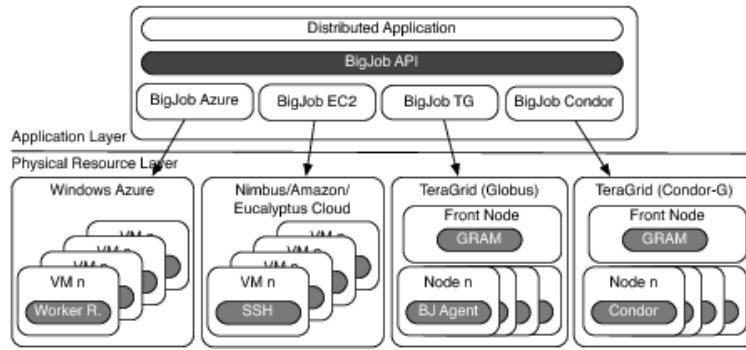
Figure 2:

NeuGrid / UWE

Use SAGA based Glueing Service and DAG-execution for Medical Imaging and workflow on the EGI/EGEE. See following: `http://www.futuremedicine.com/doi/full/10.2217/fnl.09.53` & `http://www.neugrid.eu/download/deliverables/D6.2_final.pdf`

3.3 Tooling

"One persons application is another persons application". So what distinguishes a tool from an application? In our viewpoint, a couple of items: The end-user is also the developer of an application; typically these are different for a tool. Additionally, typically there is a single user of an application, whereas by definition there are multiple users of a tool. Both these attributes hold for the tools discussed below.

EGI- Service Discovery

The SAGA Information System Navigator API provides a uniform interface to access additional details published by the information system. For details see `http://hepunx.rl.ac.uk/egee/sa3-uk/sd/` and `http://rgma03.pp.rl.ac.uk/InfoBrowser/`

SAGA-based Pilot Jobs (BigJobs)

Pilot-Jobs provide a very common usage model for distributed computing infrastructure. There exist many/multiple pilot-job implementations for different DCI, often with there own semantics but definitely with their own access/usage APIs. SAGA provides a common API to access *different* Pilot-Jobs; this API is called the BigJob API. A BigJob provides a concrete implementation of the API along with specific adaptor so as to be usable for a given backend. See Fig 2 for an example of this well-defined API and its usage on four different infrastructure types.

The BigJob API provides an interesting example of a "higher-level abstraction" that build-upon the *primary* distributed computing functionality that SAGA provides. Another

example of such a higher-level abstraction is a DAG executor (called diggedag) that uses the same job-model as SAGA along with other consistent semantics.

Computational Biology Gateways

Gateways have emerged as a successful resource access and job submission environment. In particular, where a community of users have similar usage requirements and patterns, Gateways are particular effective. SAGA has been used to build and design Gateways in such a way that they are agnostic to the details of the underlying DCI. For two examples see, DARE-RFOLD (`http://cyd01.cct.lsu.edu/`) and GridChem (`http://www.gridchem.org`). SAGA provides a critical risk mitigation strategy via the the standards based approach that it supports.

4   Analysis of Use Cases

Distributed Computing is more than just submitting isolated jobs. It is also about federating resources dynamically; about coordinated execution of heteregeneous and dynamic workloads; it is about distributed data management etc. So while SAGA is used for multiple reasons. Three primary usage modes of SAGA are the following: (i) Simplifying access layer, (ii) building block for tools and distributed execution execution, and (iii) a distributed scripting and programming capability.

4.1   SAGA as a Standardized Programmatic and Access Layer: Advantage to DCI Providers

Providing Distributed Scipting and Programming Capbility

The Structural Biology Grid (`http://SBGrid.org`) currently implements sophisticated analysis and user-defined pipelines. However, these are inherently localized and confined to specific infrastructure. Replacing "local python" calls with "distributed (SAGA) python" calls would enable the seamless utilization of DCI. This provides a simple mode of extensibililty of infrastructure, without any major refactoring of code. Further, as the API specification and implementation is *standardized*, and thus stable, it allows for a 'write once, run anywhere' approach, which is in general not available otherwise (or at least not without *significantly* increase of application complexity). The advantages of this to the end-user is obvious; the lowered barrier-to-entry for novel users and communities will increase the ease and uptake of DCI thus benefitting DCI providers/organizations. As part of the ExTENCI project, SAGA will make major advances towards becoming a broadly usable programmatic access layer to Condor/OSG.

4.2   Application Development Advantages

Application Prototyping and Tooling

The SAGA Python bindings have been proven to be immensely helpful for application prototyping. But also, they are very helpful when interactively testing remote operations (in the interactive Python interpreter / Python shell). Finally, it is very easy to implement small command line tools in Python, which are able to mimic and test smaller portions of the overall application. For example, it is straight forward to implement a specific job control component of an application in a stand alone Python script, and to later include the same functionality in the application proper, with the confidence that the semantics of the remote operations will be well preserved.

Application Development

4.3   SAGA usage modes

Although SAGA is foremost an API, the SAGA distributions support end users in a variety of ways. In particular, the SAGA distributions also include command line tools implemented via the SAGA API, and higher level libraries for common distributed programming patterns, also basing on the SAGA API.

5   Relevance to EGI/UMD

EGI (and EMI) encompass, at the moment, the three major European middlewares: Unicore, ARC and gLite. Additionally to the respective native service interfaces and client access layers, EMI is in the process of defining a unified service interface for these systems. EGI users have thus be able to handle the three existing interfaces, and have to be able to cope with the evolution of the new EMI interface, *or* have to limit their selection of available resources (by selecting resources which support their preferred access layer), *or* they can be shielded from the middleware heterogeneity and evolution by an intermediate layer (tooling and/or API).

SAGA is one way to provide that additional, shielding abstraction layer, and should thus, in our humble and biased opinion, considered as a candidate for inclusion into UMD. Additionally we argue that SAGA is *easier* to use than the native APIs, as it provides higher levels of abstractions. Further, SAGA has shown well to work with other infrastructures, in particular with Globus, which IGE will additionally provide to UMD (In fact first few success stories of IGE are built around applications that use SAGA.). Those points hold for both programmatic access via the SAGA API, as for the scripting (Python) and tooling (command line) components provided by the SAGA distribution.

Support of SAGA for the UMD/EGI user base also provides the additional benefit to the end user that applications codes and runtime environments are compatible, and in fact interoperable, with OSG (Extenci project), TeraGrid/XD, LONI, and other distributed cyberinfrastructures.

The "EGI-InSPIRE UMD Roadmap" (EU deliverable D5.1) lists the capabilities planned to be provided by UMD. SAGA does actually not map into any single of those capabilities, but is rather cross-cutting over most of them: it either provides explicit access, or implicit coverage, for 14 out of 21 capabilities. At the same time, SAGA does not really *provide* any of those capabilities, as it is not a middleware service, but 'just' an API. While 'access' and 'interfaces' are mentioned as general project objectives (see Section VII on page 3), the document actually misses an explicit capability covering the client side access to EGI resources and middleware capabilities. The assumption is likely that this comes separately with each capability, but we would like to remind that the sum of those access components will not neccessarily form a coherent, consistent and simple interface for the end users (it might, of course, depending on the specific capability providers, but the UMD document is at the moment not evaluating that aspect).

On the other hand, the "EGI-InSPIRE Standards Roadmap" (EU deliverable D2.5) lists standardized a Client API as one of the functional capabilities supporting interoperability. SAGA is mentioned explictely as one possible approach for that (page 18, Section 3.2.25).

The "EMI Technical Development Plan" (DNA 1.3.1) includes specific parts of SAGA (service discovery and information system navigation) as components (page 15), and further lists SAGA (in general) as one of its "further objectives" (page 25). The SAGA community is, as we discussed above, actively participating in the GIN and PGI efforts, with the explicit goal to ensure that future PGI and EMI interfaces map well to the abstractions provided at SAGA level.

6 SAGA Future/Roadmap

The evolution of SAGA has two very independent components: the evolution of the SAGA specification as OGF standard, and the evolution of the various SAGA implementations.

The SAGA Core API specification is very close to become a full OGF recommendation (it arrived in literally the last stage of the respective OGF process). As the specification is very modular, it allows for additional functional packages to be specified individually. Several such extension packages have already been specified (advert, messages, service discovery, resource management), and are in various stages of the standardization process - we expect those packages to mature and eventually become published specifications within a year (some of them are already published, others are very close to that). We don't expect any of the published specifications to evolve anytime soon – so far there seems to be no need of new versions of the API, despite the increasing set of implementations, users, and use cases.

On the implementation side of things we expect a limited amount of evolution on the actual API level (the standard is stable after all). Most of the current development efforts are spent on adaptor level, and in fact the quality and usability of SAGA stands and falls with the quality of the middleware bindings, i.e. of the adaptors. We thus expect that those will continue to demand the majority of our resources. Ideally, adaptor development, and even more adaptor maintainance and support, will eventually be provided by the respective middleware providers, but for the time being that is not the case. At the moment it is very

hard to estimate timeframe and required effort for an eventual support for the future EMI and/or PGI services – that depends on many factors, such as the structure of the upcoming specifications (close to BES or not, close to JSDL or not, etc), on the implementation progress for these services, and on their acceptance in the wider community.

SAGA-C++ has seen significant progress on documentation and end user support (deployment support, ticket management, mailing list activity etc). Those improvements are mostly caused by the increasing SAGA user community, which both requires, but also supports that progress.