



Enhancing Grid Infrastructures with
Virtualization and Cloud Technologies

Final Report on StratusLab Adoption

Deliverable D2.4 (V1.1)
6 June 2012

Abstract

The StratusLab cloud distribution has been adopted by users from a wide range of scientific disciplines: astrophysics, software engineering, machine learning, high-energy physics, meteorology, and bioinformatics. In addition, there has been commercial update of the distribution for a turnkey private cloud solution aimed at SMEs and a large public deployment by Atos within the Helix Nebula initiative. Both partner and non-partner institutes have used the StratusLab distribution to provide cloud services to their users.



StratusLab is co-funded by the
European Community's Seventh
Framework Programme (Capacities)
Grant Agreement INFOS-RI-261552.



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Document History

Version	Date	Comment
0.1	30 Apr. 2012	Skeleton with initial information.
1.0	5 Jun. 2012	Complete version for review.
1.1	6 Jun. 2012	Respond to reviewer’s comments.

Contents

List of Tables	6
1 Executive Summary	7
2 Introduction	9
3 Scientific Adoption	10
3.1 Astrophysics	10
3.2 Machine Learning	11
3.3 NARVAL (DAQ system training)	12
3.4 High Energy Physics	13
3.4.1 CernVM	13
3.4.2 ATLAS and CMS Experiments	13
3.4.3 DIRAC	14
3.5 National Observatory of Athens (Meterology)	15
3.6 Grid Appliance Creation and Testing	16
3.7 Bioinformatics.	17
3.7.1 Bioinformatics Web Services	17
3.7.2 TOSCANI (Bioinformatics).	18
4 Commercial Products	21
4.1 SlipStream	21
4.2 SCOS-2000.	21
4.3 DS-Cloud ReadyPack	22
4.4 Helix Nebula – the Science Cloud	23
5 Cloud Infrastructures	24

6 Lessons Learned	26
7 Conclusions	27
References	30

List of Tables

5.1	StratusLab Deployment Information	25
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1 Executive Summary

Good attendance at StratusLab tutorials and at StratusLab presentations shows strong interest in the cloud technologies developed and packaged into the StratusLab distribution. However moving beyond casual interest into actual adoption provides the best measure of success for the project.

The current adoption comes from a variety of scientific disciplines: astrophysics, software engineering, machine learning, high-energy physics, meteorology, and bioinformatics, demonstrating the broad applicability of the StratusLab cloud distribution. Tests show it is particularly well-adapted for provision of temporary testing or training infrastructure and for short duration analyses. Not surprisingly, it is less adapted for large parallel applications, although it is an effective infrastructure for testing those applications.

Commercial uptake will be critical for the continued support and evolution of the StratusLab distribution. Largely through the efforts of SixSq, the StratusLab software has been included in commercial demonstrators for SlipStream (a commercial testing product), SCOS-2000 deployment (a large control framework for ESA) and DS-Cloud ReadyPack (a turnkey private cloud solution for SMEs). SixSq has also lead the effort for the largest deployment of StratusLab at Atos as part of the Helix Nebula initiative.

StratusLab partners GRNET, CNRS/IBCP, CNRS/LAL, and TCD all have deployed the StratusLab software and offer or intend to offer cloud services. This shows the strong uptake within the project and the desire to continue collaborating on the distribution after the project ends.

Several academic institutes outside the project have deployed StratusLab: Cyfronet, IOIT, RAL, and IFIC. Although modest, this shows some uptake at sites not directly connected with the project. As for the partner institutes, these sites are providing cloud services directly to users via these infrastructures.

Based on the experience of working with users and system administrators over the last two years, some important lessons can be extracted:

- Direct involvement of user communities in the project itself is important for guiding the development of the software.
- Better mechanisms must be devised for interacting effectively with the users and system administrators from outside the project.

- The reference cloud infrastructures were a key to success for the project, but in the future, provisions for a large infrastructure paid through the project should be made.
- More funded support should be provided for direct consulting for users and system administrators.
- Despite the quality of the StratusLab software, the short duration of the project brings worries of continued development and support. More effort to create a community within the project would have helped here.

These lessons provide points on which future, similar projects and the planned open-source consortium for StratusLab should concentrate effort.

Based on the current adoption, it appears that the niche for StratusLab deployments are small to medium-sized private cloud infrastructures. Interestingly, both system administrators and users are most interested in StratusLab as a “pure” cloud solution, despite the project’s convincing demonstration that cloud infrastructures can host grid services.

2 Introduction

Good attendance at StratusLab tutorials and at StratusLab presentations shows strong interest in the cloud technologies developed and packaged into the StratusLab distribution. However moving beyond casual interest into actual adoption provides the best measure of success for the project.

This document provides an overview of the current adoption of StratusLab by both end users and system administrators. The three following chapters describe the scientific use, commercial use, and infrastructure deployments. The document ends with some “lessons learned” concerning the interactions between the project and the users and system administrators and some conclusions concerning the current adoption of the StratusLab cloud distribution.

3 Scientific Adoption

The potential benefits of cloud technologies appeal to scientists and engineers, especially the abilities to provision resources dynamically and to provide services to others. This section contains a number of concrete examples of scientific use and adoption of the StratusLab cloud technologies. These examples span a number of different disciplines and take advantage of different aspects of the cloud. They provide a solid validation of the StratusLab platform, directions for future improvements, and mechanisms for “marketing” the accomplishments of the project.

Each section describes the application, what aspects of the cloud have been used, and the future plans for the application. The content in each section and in most cases the text, have been provided by the named contact person for each section.

3.1 Astrophysics

(Contact: Cecile Cavet)

The François Arago Centre (FACe)¹ is a project at the Astroparticule et Cosmologie (APC) laboratory². The centre was founded in 2010 with the goal to support space-based experiments facing the challenge of data treatment of steadily increasing and complex data sets. Evaluation of new technologies like cloud, play an important role in meeting this challenge.

A computing engineer from FACe has run benchmarks and standard analysis code to determine the advantages and disadvantages of the cloud within astrophysics. The benchmarks covered I/O bandwidth, CPU efficiency, etc. The numerical code RAMSES³ (MPI parallelization and adaptive mesh refinement) was run on virtual clusters to test the overall performance from an application point-of-view.

This evaluation used computing, storage, and image management services of the StratusLab cloud. For computing, single virtual machines with specific resources (maximum of 8 VCPUs and 4.1 GB of RAM) and virtual clusters (maximum of 4 virtual machines, 2 VCPUs each, 1.1 GB of RAM each) were used. Virtual disks (2 GB of size) were allocated with the Persistent Disk service. The

¹<http://www.apc.univ-paris7.fr/FACe/en/home>

²<http://www.apc.univ-paris7.fr/>

³<http://web.me.com/romain.teyssier/Site/RAMSES.html>

Marketplace and other image management tools were used to take advantage of existing images and to create new customized images.

The evaluation is still in progress, but there is already some initial successes. An image of Scientific Linux 6.2 including Cloud contextualization has been created using VirtualBox. This image has been registered in the Marketplace and successfully launched via the StratusLab command. This image uses NFS to allow for a shared storage space between nodes in a virtual cluster; this configuration has been verified. The final results for the benchmarks are not yet available, but the virtual cluster in the cloud produces the usual, correct values for RAMSES.

One problem when using the StratusLab reference infrastructure was the transmission of operational information and problems to the user. This is not done systematically and can lead to wasted time trying to find a problem with an appliance or application when the problem is with the cloud infrastructure. Also, it would be good to publish the available resources so the users can determine how many resources are actually free.

Based on the initial evaluation and promises of cloud technologies, there is huge interest in continuing with these technologies. In particular for this application, it allows for debugging of the parallel code and direct testing on virtual clusters. There will probably be limitations when running numerical simulations for production phase (huge quantity of CPU needed and higher risk of data loss on the cloud) but other platforms, like supercomputers, can be used for this step.

3.2 Machine Learning

(Contact: Matthias Brendel)

Our research in the Machine Learning and Applied Statistics Group is connected with the parameter tuning of machine learning algorithms. For the purpose of our research a lot of runs have to be executed with a certain target algorithm (in our case Multiboost [1]) with different parameters and different datasets. One such run and its result is an input for the tuning algorithm itself. To make the process easier, we decided to go with an off-line approach, i.e. a large amount of runs were precomputed.

One such run with a fixed parameter-setting and data set can take a few minutes to many hours on one core. Multiboost itself was a single-core executable in our experiments. The scheduling of all the runs is on the one hand simple, since the algorithm simply has to be run on all parameter values and all datasets. On the other hand, the runs take different times. Therefore, a simple bash script was used to monitor available cores, to monitor the workloads and to start the runs. This script only needs a server with Linux running and a considerable number of free cores. All the runs had to be repeated 5 times, because a 5-fold cross-validation was used. All the 5-folds had to be executed for a set of repositories containing a large number of datasets.

Consequently, I was using the StratusLab cloud in a very simple way, by allocating the maximum number of CPU cores per virtual machine (24 on the LAL

cloud infrastructure), uploading to each of them the executable, the repository (set of datasets), the scripts needed and then starting the script. When runs were finished the results were simply downloaded from the server and processed by our parameter tuning algorithm offline. I was using different virtual machines for different folds and then reusing finished machines for the next repository. Basically only the `stratus-describe-instance`, `stratus-run-instance` and `stratus-kill-instance` commands were used. A single Ubuntu VM appliance was created and used to create five machine instances. Only `zip` and `unzip` was installed in addition. All of the high level organization was made by hand, since all the runs for one fold and one repository, so the runs on one virtual machine were taking one or a few days, and the scripts had to be modified from case to case.

The datasets are coming from different repositories (e.g. UCI Machine Learning Repository) and were of different kinds. Some are toy-problems, some are more serious samples of medical imaging, character recognition and other problems. Our research was a general case study with no specific application domain singled out, at least concerning the application of the machine learning algorithm itself. The use of the StratusLab cloud helped our work practically by providing us 24-core machines in a flexible way. Our application could make use of machines with fewer cores and we could tolerate the case when the same physical machine is used for other purposes and we share the physical machine's capacity.

Our only significant problem was the failure of one VM, where we could first recover our results, and later the machine itself was taken out from the cloud which meant for us only less VM's available. Porting of the application needed no big effort, since it was designed to run on a multi/core Linux server anyway. We did not need to use shared disks and any complicated scheduling or signaling process, since we could naturally and easily cut the data itself into pieces for the different VM's. Even the folds consisted of different data to be uploaded separately. During the planning we were thinking of an online algorithm, where the runs would be generated on the fly by the parameter tuning algorithm. This needed however some additional scheduling, and the signaling back would be a difficult issue. I do not know what mechanism is implemented in StratusLab, if any. I would definitely use StratusLab cloud and probably use more complex solutions like such an on/line algorithm if I continued my research.

3.3 NARVAL (DAQ system training)

(Contact: Eric Legay)

NARVAL is a highly-distributed and modular framework for the acquisition of experimental data. It is used by a number of nuclear physics institutes including IPN, INFN, GSI, and GANIL. NARVAL's implementation allows easy integration of experiment-specific code and optimization of the overall application.

From the 15-21 October 2011 there was the first "Narval School" organized by the Nuclear Physics Institute (IPN) in Orsay, France. By using the StratusLab services and infrastructure, the organizers were able to provide a highly-flexible,

customized environment for each student, while minimizing the effort to do so. This takes advantage of the rapid provisioning aspects of the cloud to create this dynamic training infrastructure.

The organizers trained a total of 20 students from a variety of different institutes and backgrounds (physicists, software engineers, and electronic engineers) on the NARVAL system. Following on from this success, the developers also used the StratusLab infrastructure for an “optimization school” to improve the NARVAL system itself.

The intention is to keep using the StratusLab cloud infrastructure for future training events and for optimization and testing of the NARVAL platform itself.

3.4 High Energy Physics

3.4.1 CernVM

CernVM⁴ is an initiative from CERN to provide virtual machine images adapted to the needs of the high-energy physics community. In particular, these images contain the software of the four Large Hadron Collider (LHC) experiments. The project and CernVM developers have worked together to allow these images to be used directly on a StratusLab cloud infrastructure. Differences in the contextualization procedure have been resolved (on both sides) to allow current and future versions of these images to be run on StratusLab infrastructures. Having the CernVM images available is an important prerequisite for adoption of StratusLab within this community and for the work described in the following sections.

3.4.2 ATLAS and CMS Experiments

(Contact: Maria Girone)

High-energy physicists, in particular those from the experiments using the Large Hadron Collider (LHC) in Geneva, use a large amount of computing resources to analyze their real and simulated data. These analyses treat a series of “events” that are independent from each other, making them amenable to high throughput computing techniques and infrastructures, like grids and clouds. The size of the datasets (tens of petabytes per year) require the use of resources distributed at the many participating institutes from around the world.

ATLAS and CMS, the two largest LHC experiments, have been using the StratusLab reference cloud infrastructures to test the project’s cloud distribution and services. They have a wide range of use cases to evaluate on cloud infrastructures: large-scale production of simulated data, analysis of real and simulated data, integration of cloud resources in their experiment-specific computing platforms, and automation of their development/testing processes.

The StratusLab cloud distribution will also be used within the Helix Nebula project for the Atos cloud infrastructure. Consequently, these initial tests with StratusLab will allow them to more quickly deploy on the Atos infrastructure and

⁴<http://cernvm.cern.ch>

to more thoroughly test the application and service scalability on Atos' larger infrastructure.

Concretely, people from both ATLAS and CMS have obtained accounts on the reference infrastructure and verified that they can run their software in virtual machines deployed on those infrastructures. This was rather trivial to do because of StratusLab's support of the CernVM virtual machine images. These images (see below) provide the standard operating system environment and facilities to use easily the experiments' analysis software (comprising several GB of code). These tests showed that there are no technical limitations for the use of StratusLab cloud services for their use cases.

Building on this, a more complete battery of tests will be run in June 2012. These tests will concentrate on performance and ease of integration with existing services. They will define a set of metrics to be able to compare the performance of their data analysis on cloud, grid, and traditional computing resources. They will also see how easily they can integrate resources in their computing fabric by deploying Condor worker nodes in the cloud. They also plan to look at using SlipStream as a means for automating and controlling the deployment of virtual machines for these tests.

Future use of cloud resources depends on the outcome of the tests in June and the follow-on tests on the Helix Nebula infrastructure at Atos. Nonetheless, the initial tests have shown no technical barriers to the adoption of cloud technologies by the experiments and indeed point to potential benefits in the simplification of the experiments' computing platforms and federation strategies.

3.4.3 DIRAC

(Contact: Andrei Tsaregorodtsev)

DIRAC⁵ (Distributed Infrastructure with Remote Agent Control) provides a platform for federating computing resources for use by scientific communities. Users submit jobs to DIRAC, which are then matched to computing resources managed by the system. LHCb, one of the four LHC experiments, uses DIRAC as the backbone of their computing infrastructure.

The developers of DIRAC are interested in investigating how the DIRAC system can use cloud resources and how the DIRAC services themselves can be integrated with a cloud. The technically easiest use of cloud resources is to have DIRAC workers running in the cloud. These workers then register into the DIRAC system and are used like any other DIRAC resource—clusters, grid worker nodes, individual machine, etc. Starting and using virtual machines inside of a StratusLab cloud has been demonstrated by the DIRAC development team.

Carrying this further, they would like to demonstrate a real LHCb workload on the StratusLab resources. With the availability of the CernVM images, it should be trivial to demonstrate this with the LHCb workload. Currently however, there is a problem running Gaudi (a major component of the LHCb analysis software) from

⁵<http://diracgrid.org>

the CernVM image. The developers are trying to determine if this is a problem with the image itself or running the image in a StratusLab environment.

More ambitious plans are to demonstrate active control of the cloud resources, where the DIRAC system scales-up and down—the number of cloud-based workers depending on the workload in the system. Further, running the DIRAC management services directly in the cloud would allow the full system to become a cloud-based platform. This would make specialized deployments (e.g. for other experiments or short-lived analyses) easy. It would also allow those management services to take advantage of the cloud elasticity to allow the whole system to better scale with the workload.

3.5 National Observatory of Athens (Meterology)

(Contact: Vangelis Floros)

MM5⁶ (short for Fifth-Generation Penn State/NCAR Mesoscale Model) is a regional mesoscale model used for creating weather forecasts and climate projections. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modeling system. The MM5 modeling system software is mostly written in Fortran and has been parallelized using MPI. The software has been developed at Penn State and NCAR as a community mesoscale model with contributions from users worldwide. MM5 has been used in many production environments for weather prediction. For example the National Observatory of Athens (NOA) has been using MM5 for many years to generate daily weather forecasts for the Greek region⁷.

In collaboration with NOA we ported a specific MM5 modeling system workflow on the StratusLab IaaS cloud. The workflow allows the parallel execution of the model for deterministic weather prediction, for any user defined geographic region as long as the appropriate initial and boundary conditions are given at run time. A virtual machine appliance based on CentOS 5.5 has been created in order to run MM5 and is available from the Appliance Marketplace⁸. The appliance contains the necessary precompiled binaries and libraries for the model and its supporting tools, along with the required OpenMPI packages that allow the parallel execution of the code. The appliance also provides an experimental REST service (AppRun) that permits the remote configuration, execution, monitoring and control of the model.

The virtualized cluster is created using the *stratus-run-cluster* command passing as parameters the NFS shared folder (/home) and using a command line switch in order to generate the necessary *machinefile* with the hostnames of all the nodes participating in the cluster.

As mentioned, the execution of the model relies on a number of initial and boundary conditions provided as input files. The initial conditions are pulled at

⁶<http://www.mmm.ucar.edu/mm5/>

⁷<http://cirrus.meteo.noa.gr/forecast/bolam/index.htm>

⁸<http://marketplace.stratuslab.eu/metadata/K8mbTAE2HLrXtHQyPSTwala.kAC>

startup from the NOMADS (National Operational Model Archive & Distribution System)⁹ servers in US in GRIB2 format using HTTP. The boundary conditions (i.e. terrain and sea level temperature information) are user provided and are stored on a WebDAV service. The final results (numerous files of around 100 MB total) are also staged to the WebDAV service after the completion of the model workflow. Overall, the application has modest storage requirements and usually a few GBs available from the VMs boot device are sufficient. Nevertheless, the availability of an Object Storage service from StratusLab would be useful in order to avoid using third party WebDAV services and to facilitate data reuse among different users and VM instances.

Performance-wise, comparing to the same production code running in NOA's private cluster, the cloud version exhibits poorer performance characteristics. Virtually, it takes twice as much time to run the model on the StratusLab cloud than on the local cluster (1h20' in the former 40' in the latter). Although not confirmed, this most probably has to do with the optimization of the model binary itself rather with the performance losses due to the virtualization layer overhead. By adding support for virtio_net paravirtualized drivers there is also a slight improvement in the overall performance figures (5-10%).

Based on this results it is safe to say that the above porting of MM5 to the cloud is not a strong candidate to replace the production code running in the "traditional" physical cluster at NOA. Nevertheless it provides a very useful tool for parametric runs, training and experimentation with the model and the underlying workflow. Users can experiment easily with various boundary conditions, temperature levels, sea conditions and other characteristics in order to validate different configuration before applying them in the production environment. A tutorial for running MM5 on the cloud is available on YouTube¹⁰ and has been demonstrated in the European Geoscience Union General Assembly 2012¹¹.

3.6 Grid Appliance Creation and Testing

(Contact: Adrian Colesa)

The IGE (Initiative for Globus in Europe) project¹² used StratusLab to publish and run appliances having Globus (Globus Toolkit 5) components installed on them. Globus is a Grid middleware promoted and sustained by IGE in Europe. The purpose was to provide the Globus users with an easy and flexible way to test Globus in different configurations, regardless of the number of machines, the operating systems used on those machines and settings of the Globus services. We created different types of Globus appliances. The difference between the different types of Globus appliances is related to the level of configuration of the installed Globus components (GridFTP, gsissh and GRAM5).

⁹<http://nomads.ncdc.noaa.gov/>

¹⁰<http://www.youtube.com/watch?v=yD3kordYRHk>

¹¹http://meetingorganizer.copernicus.org/EGU2012/oral_programme/9105

¹²<http://www.ige-project.eu/>

The prepared IGE's Globus appliances were published on the standard StratusLab Marketplace¹³. They were named such that to identify IGE as their originator, the Globus version and OS installed on them. We have for instance: "IGEv2.0-GT5-centos v6.0 i686", "IGEv2.0-GT5-ubuntu v10.04 x86_64", "IGEv1.0-GT5-fedora v15 i686". The "type" field in their description also differentiates between different types of Globus appliances. Such that, we have for example: "IGEv2.0-GT5-packages-configured", "IGEv1.0-GT5-src-compiled" etc.

IGE not only provided Globus appliances in the StratusLab's Marketplace, but also ran the Globus appliances on the StratusLab cloud infrastructure for the certification of the IGE software. The use of Globus appliances on StratusLab cloud offers the IGE certifiers the possibility to create new clean Globus installed virtual machines in each certification cycle and also to use different types of OS and platforms.

Generally, the use of the StratusLab features (Marketplace and cloud) was very successful. The collaboration with the StratusLab support staff was also successful; they were helpful and generally very prompt. The collaboration with StratusLab was positive and generated good results.

However, some features we perceived as limited (or limiting) and candidates for future improvements:

1. The possibility to create a more flexible and pleasing description of an image published on the StratusLab Marketplace (e.g. in HTML format),
2. The way an image and its main characteristics could be advertised and searched for on the marketplace in order to make easier for the users to identify the type of appliance they could be interested in,
3. The addition of a web interface to manage easily the VMs from different places.
4. The lack of detailed log info regarding VM instantiation failures. The command `stratus-describe-instance` gives actually no information regarding the reasons of the failure and thus the StratusLab support had to be contacted to solve the problems.

We consider the cloud a very useful technology for our purposes. We intend to use it in the future and even extend the Globus appliances collection with other types of appliances and use them during demos and hands-on sessions we prepare for different events.

3.7 Bioinformatics

3.7.1 Bioinformatics Web Services

(Contact: Christophe Blanchet)

¹³<http://marketplace.stratuslab.eu/metadata>

Biologists and bioinformaticians are regularly combining multiple software packages to study their data via analysis pipelines. These software packages access reference databases via POSIX for their analyses. Two bioinformatics appliances have been created (and continuously improved) that can be deployed on demand for scientists and engineers to perform their analyses.

The ‘biodata’ appliance contains configurations for the SwissProt and PROSITE databases. Bioinformaticians can use the appliance to set up their own cloud biological databases repository. They can add the databases they want with the help of the BioMaj system. This appliance can mount a persistent disk to allow the biological database sharing to benefit from a large storage area.

The ‘biocompute’ appliance is configured with different bioinformatics tools like BLAST, ClustalW2, Clustal-Omega, FastA, etc. The comprehensive list is available on the cloud web interface. This list can be used to apply a filter on and select the bioinformatics appliances at the ‘launch instance’ step. Scientists can use this appliance through SSH or through a web portal.

We have used cloud features such as the contextualization to mount automatically the biological databases repository during the start-up of machine instances. Biocompute instances can mount the biological database repository of the local cloud (if available) through contextualization options provided by the user¹⁴. We have also instrumented the appliances to use the ‘persistent disk’ cloud feature for storage.

We have developed a specialized Cloud Web Interface for Bioinformatics for the StratusLab framework. The main goals are to make it easy to use by non-computing and non-cloud-specialist scientists like biologists and bioinformaticians, and powerful enough to perform the main tasks of the VM lifecycle on a StratusLab infrastructure. The available features allow the creation and termination of the virtual machines, allow the management of the persistent disks, and provide assistance for bioinformatics appliance selection and instance contextualization. A screenshot of the interface can be seen in Figure 3.1.

The adoption of clouds for bioinformatics applications will be strongly correlated to the capability of cloud infrastructures to provide ease-of-use of common bioinformatics tools and access to reference biological databases. In that way, clouds for bioinformatics have to be connected with public bioinformatics infrastructures and StratusLab is collaborating with the French Bioinformatics Network RENABI¹⁵ to help fulfill the requirements of the Bioinformatics community.

3.7.2 TOSCANI (Bioinformatics)

(Contact: Michael Nilges)

TOSCANI (TOwards StruCtural AssignmeNt Improvement) is a project to improve the determination of protein structures based on Nuclear Magnetic Reso-

¹⁴For example on the IBCP’s cloud, setting the BIO_DB_SERVER parameter to the value ‘idb-databases.ibcp.fr’ will mount our local bio repository.

¹⁵www.renabi.fr

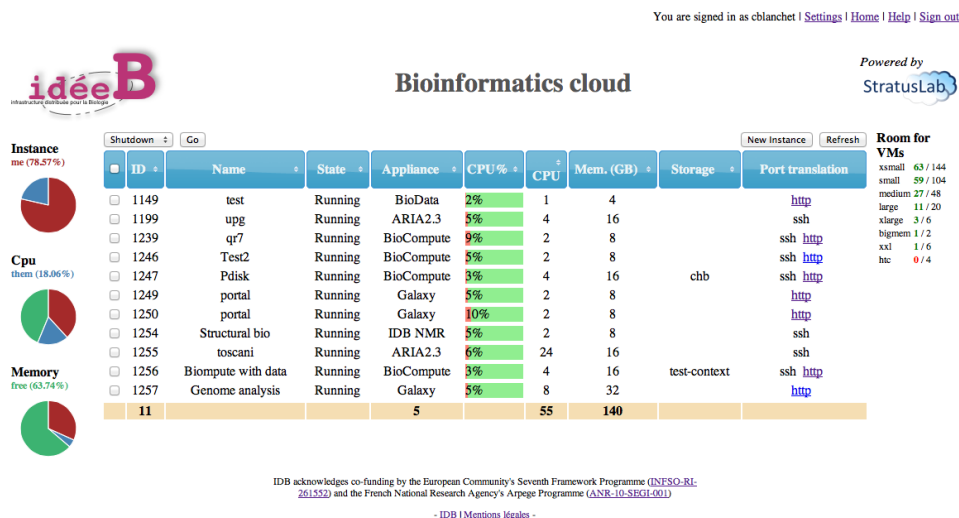


Figure 3.1: Bioinformatics Cloud Web Interface

nance (NMR) information. This relates the bioinformatics, molecular biology, and structural biology scientific domains.

The program ARIA [2] was used to calculate the structures. ARIA uses a computational model where the master schedules the structural computation on a number of worker nodes. One appliance was built with ARIA pre-installed, according to its requirements and the constraints of the StratusLab services. The main requirements are the management of the input and output data (at the scale of GB) and the deployment of a complete infrastructure, including one master and up to 100 compute nodes for usual experiments. Shared storage, between the ARIA master and CNSsolve compute nodes, is required; additionally, the data produced need to be kept for further analysis. The persistent disk utility corresponds well to this requirement.

ARIA version 2.3 has been installed and configured, and the appliance has been registered in the Marketplace. The appliance has been evaluated with real data and the experiments concluded with good performance of the CNSsolve part. This first version has been improved according by adding more computing (BLAS, LAPACK) add-ons. Users can connect to the ARIA VM with SSH, upload their data and directly run the tool from the current directory. Only one instance, containing both the ARIA master and the CNSsolve tools, needs to be run by the user. The computing resources are tuned via the instance used to launch the machine, up to the maximum allowed by the High Throughput Computing (HTC) instance on the CNRS IBCP infrastructure with 24 CPUs and 16 GB RAM, and the 'HTC+' instance with 48 CPUs and 120 GB RAM. New versions of the appliance are planned that will allow for one instance of the ARIA master and many instances of the CNSsolve nodes.

A second version of the appliance (2.0) following the IaaS model has been

developed and released. With the usual cloud interfaces, scientists can launch a bunch of virtual machines that will be used for a CPU-intensive computation. They connect to the virtual machine that will be used as the ARIA master and run the script 'aria-clouder' we have developed and placed in the ARIA2.3 appliance. This tool finishes the configuration of the virtual cluster, setting up the system services and the ARIA configuration file to adapt to the virtual infrastructure. Scientists have then simply to run the ARIA tool as usual and can obtain their results once the calculations are finished. This appliances is also compatible with all the instance types available on the IBCP's cloud (large, bigmem, HTC), and with the StratusLab reference infrastructures in GRNET and LAL.

The TOSCANI use-case takes advantage of the image creation and management services as well as the data management facilities. Another requirement is the ability to run a bunch of virtual machines linked together as a cluster devoted to the computation, using the public/private IP address distinction. Other useful cloud feature is for example the persistent disk service that allow users to share a large storage area among their different instances, and to store their data longer time than the life-cycle of the machines used for computation.

Significant increase in the number of calculated protein conformations improves the statistics on the NMR conformations and can help to overcome the inherent ambiguities in the calculation, at the price of larger computing resource requirements. The large computing power required for this is concentrated in the simulated annealing procedure with the CNS software. Because of these large computational needs, an NMR laboratory not specially involved in bioinformatics developments will not invest in building a cluster of about 100 nodes to be able to run NMR structure calculations for example with ARIA. Thus the elasticity of the cloud could be an advantage by waking the CNS VMs only during the simulation periods and putting them in sleep mode the rest of the time. Moreover, there is a commercial and academic interest in providing such tools to structural biologists on a 'pay as you go' basis.

4 Commercial Products

The long-term sustainability and relevance of the StratusLab cloud distribution depends on update in both the scientific and commercial sectors. SixSq has done an extraordinary job in promoting StratusLab in the commercial sector. Based on the outcomes of these initiatives, StratusLab has a clear niche as an efficient, easy-to-install private cloud solution for small to medium-sized infrastructures. However, the work with Atos also shows StratusLab's potential on large infrastructures as well.

4.1 SlipStream

SlipStream is a software engineering PaaS (provided as both a product and service) that facilitates automated, on-demand, creation of multi-machine runtime environments. SlipStream uses the dynamic provisioning of public and private cloud solutions to automate these complex deployments.

SlipStream has been adapted (through a plug-in) to allow it to take advantage of StratusLab cloud infrastructures. The service uses most of the features of the StratusLab distribution, including bulk deployment, image creation, the Marketplace, REST APIs for services (except OpenNebula), and the simple image contextualization methods.

When using StratusLab, SlipStream's image factory produces images from user specifications and registers those images in the StratusLab Marketplace. These machines can then be deployed alone or a part of a multi-machine service. SlipStream handles any necessary configuration and coordination between machines. This allows, for example, deployments of complete clusters or complex multi-machine systems, in a completely automatic and reproducible way.

Using SlipStream in conjunction with StratusLab provides additional commercial opportunities. Many companies are interested in using SlipStream but are wary of allowing their code or data to be used on a public cloud. Using StratusLab as a private cloud distribution, allows these companies to take advantage of SlipStream without the data and code protection worries.

4.2 SCOS-2000

SCOS-2000 is the main ground control software system of the European Space Agency Operation Center (ESA/ESOC). This complex distributed software system

has been developed by a number of companies for ESOC over a number of years and is still being actively developed. Integration, certification and deployment of SCOS-2000 has become a daunting challenge.

To address this, SixSq, in collaboration with Terma GmbH (SCOS-2000 domain expert) demonstrated SlipStream's ability to automatically and autonomously deploy and configure an entire SCOS-2000 system. Because SCOS-2000 includes software with proprietary licenses, it was not possible to perform this proof of concept on a public cloud. StratusLab again provided a private cloud solution for use with SlipStream. This private cloud was deployed on Terma's computing infrastructure in Darmstadt, Germany. With the combined SlipStream/StratusLab system, deploying SCOS-2000 took seven minutes and could be initiated from a single click or command. This is a spectacular improvement over the hours and days for an experienced team to install the system (and even longer for a novice team). This system is now being reviewed by ESOC for building a larger proof of concept at ESOC itself.

The simplicity of installation and management of the StratusLab distribution allowed SixSq very quickly and cheaply to deploy a private cloud at Terma, on modest hardware. Since SlipStream was adapted to work with StratusLab earlier in the project, the interfacing was transparent for the users.

This work required unattended image creation and registration with the Marketplace. This requirement provided valuable input and feedback to the project and lead to modifications to permit this.

The fact that SCOS-2000 was not designed for automation was a great challenge. Indeed we had to simulate button clicks to configure some of the applications composing the system. To deploy several instances of a SCOS-2000 system in parallel, in complete isolation from each other, the configuration of the system had to be further tokenized and adapted. But even for such a heavy-weight legacy system, it was possible to "cloudify" the system automate its deployment.

4.3 DS-Cloud ReadyPack

The DS-Cloud ReadyPack is an initiative from IBM (Switzerland), SixSq and Darest¹. The idea is to create a complete, pre-certified private cloud system to small to medium-sized enterprises. This 'cloud-in-a-box' product runs on low-end IBM hardware and integrates a software stack composed of StratusLab and SlipStream.

This product allows SixSq and other partners, such as Darest, to offer cloud based vertical solutions to specific and general markets. The system is certified in a factory environment and interfaced with central StratusLab Marketplace and SlipStream services, such that factory certified VMs and deployment recipes can be pushed to the individual cloud-in-a-box instance, making the offer even more attractive by simplifying the maintenance of the system.

Having a turnkey private cloud solution makes cloud technology attractive for

¹<http://www.darest.com/>

a wide range of companies (banks, pharmaceuticals, insurance, etc.) that cannot consider public cloud solutions because of data handling, confidentiality, and privacy constraints. Having an easy-to-install solution, like StratusLab, further lowers the barriers for their use of cloud technologies.

Having a commercial market for the StratusLab software would guarantee both the interest and resources to continue the development of the StratusLab distribution and to provide support to the entire StratusLab user community. Clearly, success of this product would have a strong, positive impact on the sustainability of the StratusLab cloud distribution.

4.4 Helix Nebula – the Science Cloud

Helix Nebula is an initiative to evaluate the potential of a public/private partnership to provide a scientific cloud for large-scale scientific analyses. Three scientific areas have been chosen as pilot applications—high energy physics, molecular biology, and earth observation—represented by CERN, EMBL, and ESA, respectively. Applications from these areas and the selected commercial cloud providers will be used to evaluate and validate the concept.

Atos, of the commercial partners in the initiative, has chosen to deploy StratusLab as its cloud solution. SixSq is working closely with Atos on this deployment.

This deployment is proving to be an excellent large-scale test case for the StratusLab distribution. The initial experiences have validated the architecture and design of the StratusLab cloud distribution. Detailed feedback both from Atos and the pilot applications has already lead to improvements in the services, particularly in terms of reliability and scalability. Having a large, multinational information technology services like Atos running the StratusLab software, lends credibility to the StratusLab distribution and will help in forging an open, vibrant community around the Stratuslab software.

5 Cloud Infrastructures

The StratusLab project supports scientific and commercial users through its reference cloud infrastructures at GRNET and at LAL. However, the project focuses primarily on development of a complete cloud distribution, so it is important to understand what institutes are installing the software on their own resources. Table 5.1 provides a list of those sites who have deployed the software; it includes both sites who are partners in the project and those that are not.

As can be seen from the table, StratusLab partners GRNET, CNRS/IBCP, CNRS/LAL, and TCD all have deployed the StratusLab software and offer or intend to offer cloud services. This shows the strong uptake within the project and the desire to continue collaborating on the distribution after the project ends.

Several academic institutes outside the project have deployed StratusLab: Cyfronet, IOIT, RAL, and IFIC. Although modest, this shows some uptake at sites not directly connected with the project. As for the partner institutes, these sites are providing cloud services directly to users via these infrastructures.

Importantly, there are also three deployments related to commercial initiatives. The largest of these at Atos, is providing valuable feedback that will improve the scalability and performance of the StratusLab distribution. These deployments also focus on providing cloud services.

It is interesting that all of the current deployments concentrate on providing cloud services to users. GRNET has demonstrated that the StratusLab cloud can support grid services, but apart from this only CNRS/LAL and RAL have shown interest in running grid services (particularly grid worker nodes) in their clouds. There are some tentative contacts with sites within EGI to run grid services over the clouds, but there has been little concrete action along these lines.

EGI.eu, however, does operate its own Marketplace service in parallel with the central Marketplace service operated by TCD. This indicates some limited take up of StratusLab on the EGI infrastructure as a whole and could lead to take up of the core StratusLab distribution at sites.

Table 5.1: StratusLab Deployment Information

Institute	Location	Status	Type	CPU	RAM	Disk	Target
GRNET	Athens, Greece	production	public	256 cores	768 GB	3–20 TB	Academic use for scientific applications
CNRS/LAL	Orsay, France	production	public	216 cores	324 GB	15 TB	European scientists and engineers
Cyfronet	Krakow, Poland	test	public	32 cores	64 GB	1 TB	EGI community users; EGI Federated Cloud Task Force
IDB-IBCP	Lyon, France	production	public	172 cores	536 GB	25 TB	French Bioinformatics community
IFIC	Valencia, Spain	test	private	–	–	–	RENABI
IOIT	Hanoi, Vietnam	test	private	16 cores	36 GB	2 TB	high-energy physics community
LAL-CNRS	Orsay, France	test	private	16 cores	32 GB	300 GB	Scientists simulating tsunami on Vietnam's coast
LAL-CNRS	Orsay, France	production	private	96 cores	144 GB	15 TB	LAL IT personnel and developers for tests
LAL-CNRS	Orsay, France	pre-production	private	48 cores	72 GB	300 GB	LAL IT engineers for deployment of lab services
STFC/RAL	Oxfordshire, UK	pre-production	private	150 cores	600 GB	3 TB	Evaluation of new version to replace private, production cloud
TCD	Dublin, Ireland	test	private	40 cores	80 GB	1.5 TB	Department developers, WLCG grid, STFC scientific computing
TechData	Gland, Switzerland	pre-production	private	8 cores	48 GB	65 GB	TCD computer science community and EGI Federated Cloud Task Force
Terma	Darmstadt, Germany	pre-production	private	8 cores	144 GB	100 GB	Commercial demonstration of DS-Cloud ReadyPack
Helix Nebula/Atos	Eindhoven, Netherlands	production	public	448 cores	1792 GB	8 TB	Demonstrator for ESA/ESOC. An engineering PaaS with SlipStream. Test user communities in Helix Nebula: CERN, EMBL, and ESA.

6 Lessons Learned

The two years experience that we have had interacting with the targeted user communities and system administrators allow us to reflect on what has worked and what we would do differently.

Involving people from the bioinformatics user community directly in the project has provided valuable feedback on the developed features and a check of the distribution's overall utility. Such constant feedback and their direct contributions to the software would have been difficult to obtain had they not been an integral part of the project itself.

This document has shown that a number of other scientific and commercial user communities have adopted the StratusLab distribution and provided feedback. However, we have not enjoyed the same tight collaboration and constant communication as with the bioinformatics community. This reflects the fact that we have not found the “magic formula” for interacting with people outside of the project, despite the efforts from the dissemination activity, providing a support mailing list, and opening a Google group.

The reference cloud infrastructures that the project has provided have been invaluable for training and initial tests by users. However their rather limited size means that large scale users must deploy their own infrastructure to go beyond the testing phase. In hindsight, providing a large cloud infrastructure funded directly by the project would have been an effective way to motivate users and provide more feedback on the scalability of the solution.

Along these lines when designing the project, more funded effort should have been allocated in the latter stages of the project to provide more support and direct consulting with potential user groups.

The short duration of the project has made it difficult to convince users and system administrators to take the leap in adopting the StratusLab distribution. This is due to legitimate worries about the long term sustainability and support of the software. The project partners intend to continue development and support of the software through an open-source consortium to answer these concerns. Hopefully, this effort will be fruitful and encourage broader adoption of the software in the post-EU project phase.

7 Conclusions

The current adoption shows strong interest from a variety of scientific disciplines: astrophysics, software engineering, machine learning, high-energy physics, meteorology, and bioinformatics. This shows that the StratusLab cloud distribution is broadly applicable to most scientific domains. It is particularly well-adapted for provision of temporary testing or training infrastructure and for short duration analyses. Not surprisingly, it is less adapted for large parallel applications, although it is an effective infrastructure for testing those applications.

Commercial uptake will be critical for the continued support and evolution of the StratusLab distribution. Largely through the efforts of SixSq, the StratusLab software has been included in commercial demonstrators. SixSq has also lead the effort for the largest deployment of StratusLab at Atos as part of the Helix Nebula initiative.

There are at least fourteen StratusLab cloud deployments, half of them at non-partner institutes. This shows moderate interest in using the StratusLab distribution to provide public and private cloud services to various user communities.

Based on the current adoption, it appears that the niche for StratusLab deployments are small to medium-sized private cloud infrastructures. Interestingly, both system administrators and users are most interested in StratusLab as a “pure” cloud solution, despite the project’s convincing demonstration that cloud infrastructures can host grid services.

Acknowledgements

The authors would like to thank all of the users and system administrators that provided feedback and content for this report.

Glossary

Appliance	Virtual machine containing preconfigured software or services
DCI	Distributed Computing Infrastructure
EGI	European Grid Infrastructure
IaaS	Infrastructure as a Service
NFS	Network File System
Public Cloud	Cloud infrastructure accessible to people outside of the provider's organization
Private Cloud	Cloud infrastructure accessible only to the provider's users
VM	Virtual Machine
Worker Node	Grid node on which jobs are executed

References

- [1] D. Benbouzid, R. Busa-Fekete, N. Casagrande, F.-D. Collin, and B. Kgl. Multiboost: a multi-purpose boosting package. *Journal of Machine Learning Research*, 13:549–553, 2012.
- [2] W. Rieping, M. Habeck, B. Bardiaux, A. Bernard, T. Malliavin, and M. Nilges. ARIA2: automated NOE assignment and data integration in NMR structure calculation. *Bioinformatics*, 23:381–382, 2007.