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	This is the first public release of the High Performance Computing (HPC) Platform, which will be available for the scientific community.
Abstract:	This document is intended for the users of the HPC Platform. It describes which hardware, software and services are available, their current status, how to access and use them, and where to find more detailed information.
Keywords:	Platform Release, High Performance Computing
Available at:	www.humanbrainproject.eu/ec-deliverables

Important reminder to all users requiring access to high-performance computing resources!

Supercomputers are limited resources shared by several communities. Thus scientists need to apply for compute and storage resources in a competitive process. Applications are evaluated in a scientific and technical peer-review to ensure a fair distribution of resources.

Also users of the High Performance Computing Platform need to apply for compute and storage resources in advance. For more details on how to apply, please see Annex K: Access to supercomputers.





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1. The Aim of this Document

This document presents the High Performance Computing (HPC) Platform v1 and related information.

2. How to Access the High Performance Computing Platform

The High Performance Computing Platform is one of six ITC Platforms that comprise the HBP Scientific Research Infrastructure. All these Platforms can be accessed via the HBP Collaboratory web interface:

https://collab.humanbrainproject.eu/#/collab/19/nav/403

Direct link to the HPC Platform on the Collaboratory:

https://collab.humanbrainproject.eu/#/collab/264/nav/1973

While most software and services of the HPC Platform are directly available to all users of the HBP infrastructure, they must apply for compute and storage resources. More information about this topic can be found in Annex K: Access to supercomputers or in the HPC Platform Guidebook under https://hbp-hpc-platform.fz-juelich.de/?page_id=68.

3. Platform User Instructions

The HPC Platform Guidebook, a collection of all user and developer documentation, can be found in the Collaboratory under *HPC* > *Guidebook*. It can also directly be found under <u>https://hbp-hpc-platform.fz-juelich.de/</u>.

The Platform Documentation constitutes a separate Deliverable (D7.7.6 - High Performance Analytics and Computing Platform v1 - Documentation), which will include direct links to Technical and User Documentation, such as the Platform Guidebook.

D7.7.6 was also scheduled to include a roadmap describing plans for future Platform development, but this topic is covered in this document - see Annex F: Backlog (Remaining bugs and new features to be added).

4. Platform Testing and Quality Strategy

The HPC Platform provides a federated infrastructure with supercomputers at four HPC centres, Cloud storage and high-fidelity visualisation systems. All hardware components are connected with a secure network, either through the PRACE network or via dedicated connections (see Annex A: Platform Architectural Diagram for details). The logical connection of the infrastructure components is realised by an LDAP based account management and a UNICORE installation at all sites.

Most supercomputer users usually login to the system using SSH from the command line. Therefore, most of the software components of the HPC Platform are not integrated into the Collaboratory but instead installed on the supercomputer(s) and/or available for download, depending on the target architecture (HPC and/or local computers). For this reason, and because many of the software components are also funded from other sources, the HPC Platform is using a three-step testing and quality strategy:

1) The HPC Platform team supports users in implementing complex workflows like the ones described in Annex J: User Projects and tests these workflows together with the users (see Annex I: User feedback received in M18-M30 for software and services). The HPC Platform uses this co-design approach to assess the status and quality of Platform services, if the related documentation is well written and sufficient, and if the (user) interfaces provided for the services work correctly. The availability of the





infrastructure and the status of the Platform services are tested by a team consisting of members from WP7.5 "High Performance Platform: operation and integrations" on a regular basis, taking into account feedback from HPC Platform users. This mainly concerns the HPC Core Platform Services that are described in Annex A: Platform Architectural Diagram.

- 2) Software & Services of the outer layer (see Annex A: Platform Architectural Diagram) are first tested by the developers themselves. HPC users who are directly logged in to the supercomputer typically report software bugs and issues to the development teams; the necessary contact details are published in the Guidebook. More details about the testing and quality processes established by the software development teams in the HPC Platform are available in the table in Annex H: Quality and testing strategies for software and services.
- 3) The HPC Platform provides a contact form (<u>https://hbp-hpc-platform.fz-juelich.de/?page_id=152</u>; also available from the Collaboratory) and an email address (<u>hbp-hpc-platform@fz-juelich.de</u>) as a single point of contact for reporting bugs or problems in case the user does not know which component (software, service, operating system, network...) is the actual error source, and for getting in touch with the HPC Platform team in case of more general questions. The HPC Platform Management Team answers all requests received and/or forwards them to relevant experts if necessary. At the beginning of SGA1 an HPC Platform Support Team will be established and take over this role. A central ticket system will also be set up at the same time. A list of frequently asked questions will be collected and published in the Guidebook.

5. Platform User Adoption Strategy

The HPC Platform has mainly two different categories of (academic) users: those that need computing resources themselves, and others who need access to datasets and results produced by the first group and that are stored at the HPC centres. The HPC Platform offers software tools developed by the Platform partners for both types of users. The execution of some of these tools, for example for visualisation and data management, does not necessarily require a supercomputer, but they can be used on standard computers and notebooks. Other software, like parallel programming frameworks, can be used on both types of architectures. The HPC Platform Guidebook describes for every software tool and library on which systems it can be used and where to find more documentation about it (see also Annex A: Platform Architectural Diagram).

The HPC Platform Specification (D7.7.2 "High Performance Computing Platform v1 - specification document", section 2.2) defines eight different user roles:

- Computational Scientific User (CSU) A user with scientific development skills and comfort in launching command line HPC jobs.
- Biological Scientific User (BSU) A user with scientific expertise, but limited technical skills in programming and/or HPC.
- Scientific User (SU) A scientific user, either a CSU or a BSU.
- Scientific Developer (SCIDEV) A user who is developing software to directly realise certain scientific objectives. This user is usually working in close collaboration with scientists, both CSUs and BSUs.
- Developer (DEV) A user who is developing software to realise engineering, operational and/or scientific objectives.
- Portal User (PU) A user who accesses Platform functions through the Web GUI.



- Humar Humar
 - Service User (ServU) A user who accesses Platform functions through a programmatic Service Client API.
 - Infrastructure Personnel (INFRA) An infrastructure system administrator or developer, typically responsible for deploying and monitoring Platform services that are offered directly to customers.

Computational Scientific Users (CSU), Scientific Developers (SCIDEV) and Developers (DEV) mainly belong to the first category of users. Biological Scientific Users (BSU), Portal Users (PU) and Service Users (ServU) fit more into the second category but can also have a need for computing time themselves. The accounting mechanisms established at the HPC centres can deal with the usual number of users expected for the HPC systems.

Standard computers and university clusters usually do not provide the computing and storage resources required to run detailed simulations of larger brain areas. New evolving technologies allow gathering datasets experimentally that are too large to be processed on these small systems either. The HPC Platform provides neuroscientists with the storage and computing resources required for their research. All hardware components (supercomputers, Cloud storage, visualisation systems) are closely integrated into an authentication and authorisation infrastructure and into UNICORE so that users have the same HPC account on all systems and can easily use different HPC systems in the same workflow. In addition, the user's HPC account is linked to the central HBP account, which allows transparent user authentication and authorisation and makes accessing datasets on HPC storage easy also for users less experienced with HPC.

Since many neuroscientific research groups are currently at the border between still being able to use their own systems and having to move to an HPC system, the HPC Platform offers support and services to existing and future users to assist them in making the transition. This type of federated infrastructure with community-specific support is almost unique in the way it is organised. In addition, the HPC Platform partners do a lot of development work in order to provide the community with useful software in the areas of visualisation, data management and (parallel) programming frameworks to support the users in using the supercomputers in the best possible and most efficient way.

User engagement is an important task of the HPC Platform. Some neuroscientific research groups have already discovered how they can benefit from HPC. Others have not realised yet what new opportunities HPC provides for their research. Therefore, the HPC Platform team is reaching out to the community in different ways:

- Organising lectures for HBP Education events that serve as an introduction to HPC because students are most likely to pick up and explore new technologies.
- Proactively contacting HBP scientists, e.g. at the annual Summits.
- Publishing and promoting examples of user projects as success stories to demonstrate the variety of neuroscientific research fields that can benefit from HPC (see Annex J: User Projects).
- Organising workshops to introduce interested, potential new users to the world of HPC.
- Setting up a user database and a mailing list for potentially interested scientists to inform them about news, upcoming events (e.g. introductions to HPC organised by the SP7 Partners) etc.
- Using the HBP Newsletter: Announcement of upcoming calls for proposals in the HBP Newsletter as a service and reminder for all users who would like to apply for project or preparatory access to a supercomputer, information about new releases of teaching material or upcoming workshops, publication of other relevant news.





To make the HPC Platform as beneficial and useful as possible for its users, the HPC Platform team is co-designing the Platform together with its users. Annex J: User Projects contains a (non-exclusive) description of major use cases envisaged for M30 and the beginning of SGA1. To strengthen these collaborations even more, some of the existing, main users will directly be involved in the SP7 work plan for SGA1. Additionally, SP7 (mainly WP7.1 "Technology Evaluation") is in close contact with the vendors of HPC technology to plan the next generation based on the needs of neuroscience.

6. Support and User Feedback

To obtain help in using the platform, please start by checking the online user documentation here: <u>https://hbp-hpc-platform.fz-juelich.de/?page_id=26</u>

If you are interested in the online developer documentation, you can find it here: https://hbp-hpc-platform.fz-juelich.de/?page_id=32

If you need personal assistance, want to provide feedback or contribute to the on-going development of the platform, please contact: <u>HBP-HPC-platform@fz-juelich.de</u>

6.1 User Feedback Received Month 18 - Month 30

The HPC Platform team is in close contact with users that already have computing time allocations. These user projects (see Annex J: User Projects) are co-design efforts between the HPC Platform team and major users. The project groups provide the HPC Platform team with direct feedback on the Core Platform Services (see Annex A: Platform Architectural Diagram) by reporting bugs and missing features on the working level. In return they get support for implementing their workflows.

The collaboration within the user projects revealed that some of the users' requirements that are not yet fully accomplishable are also important for some of the other projects, in particular data transfer mechanisms to upload data to an HPC storage (e.g. for analysis) or to download data stored at an HPC site, and an integration of the planned UNICORE provenance tracking with the other provenance tracking processes established in the HBP Platforms and the Collaboratory. The implementation of these features has already started.

Other important feedback received in the context of the user projects is that some of the users would like to use additional supercomputers hosted by the HPC sites to those that are currently integrated in the HPC Platform, e.g. JURECA at JUELICH-JSC, Piz Daint at ETHZ-CSCS and Pico at CINECA. The main reason for this is that the users' applications better fit to the architecture of these HPC systems. Therefore, these three supercomputers (see Annex D: Summary - Service IT Resource Planning) will become part of the HPC Platform at the beginning of SGA1. The integration in the infrastructure has already started. The existing four supercomputers JUQUEEN, BlueBrain IV, MareNostrum III and FERMI will most likely remain a part of the HPC Platform since they are needed for other neuroscience applications.

The table in Annex I: User feedback received in M18-M30 for software and services summarises the key feedback received on software and services.





Annex A: Platform Architectural Diagram



Figure 1: HPC Platform Architectural Diagram





The High Performance Computing Platform consists of two layers of software and services around the central, federated HPC and storage infrastructure. The four supercomputers JUQUEEN (JUELICH-JSC), BlueBrain IV (owned by EPFL and hosted by ETHZ-CSCS), MareNostrum III (BSC) and FERMI (CINECA) are connected via the secure high-speed PRACE network; a Memorandum of Understanding between HBP and PRACE was signed in January 2015. Three additional supercomputers will be integrated into the Platform at the beginning of SGA1, see Annex D: Summary - Service IT Resource Planning for more details. The high-fidelity visualisation systems at RWTH and EPFL are connected with JUELICH-JSC and ETHZ-CSCS, respectively, through dedicated high-speed connections. All HPC sites and the Cloud storage located at KIT are connected and available via the public Internet. The first layer of Core Platform Services makes the federated infrastructure available to the users by connecting the resources logically and by providing - among other services - access mechanisms, monitoring tools, documentation and support. The second layer of software and services comprises the software tools, libraries, frameworks, APIs and programming models developed and made available by the SP7 partners that are mostly also usable without a computing time allocation for an HPC system.

First layer: Core Platform Services

The Core Platform Services are mainly developed, deployed and maintained by members of WP7.5 "HPC Platform: integration and operations". The column "status" compares the status at the end of M30 with the status in M18.

Software/Service	Description	Available at	Status
Account management	 HPC Platform users with a computing time allocation for at least one HPC system have the same HPC Platform account (bp0xxxx) reserved for them at all systems. The accounts are activated only for the systems for which the user has a valid computing time allocation. The account management is based on a LDAP infrastructure with a central HPC Platform LDAP server currently hosted at EPFL and slave servers at all HPC sites. The HPC Platform accounts are linked to the HBP accounts managed in the central OIDC server at EPFL that are e.g. required to login to the Collaboratory. Currently HPC Platform accounts are created on demand. The implementation of an automated account management has already started: A team of WP7.5 members from all HPC sites agreed on an account management workflow. The implementation will in the end allow 	HPC Platform accounts are created on request (contact form in Guidebook website or by sending an email to <u>hbp-hpc-platform@fz-</u> <u>juelich.de</u>) Work on a web form (see Computing time allocation) in the Collaboratory has started	Unchanged from the user's point of view; The backend is improving by the on-going implementatio n of the account management workflow

Table 1: HPC Platform Architecture: Core Platform Services





	requesting an HPC Platform account based on an existing computing time allocation directly from the Collaboratory. First tests with users started in M29. More information: <u>https://hbp-hpc-platform.fz-juelich.de/?page_id=66</u> Responsible: T7.5.1, T7.5.2, T7.5.3, T7.5.4, T7.5.6		
Cloud storage	The Cloud storage offered by KIT is an S3 Object Storage with currently 460 TB available for the HBP. It can be accessed through UNICORE, REST API, S3 clients and Java/Python APIs. S3 clients: <u>http://wiki.scc.kit.edu/lsdf/index.php/S3_on_WOS</u> Responsible: T7.5.5	UNICORE, REST API, S3 clients and APIs	Available since M18
Computing & storage services	 The four supercomputers integrated in the Platform are for users with a valid computing time allocation (see Annex K: Access to supercomputers). These compute resources can be accessed using SSH, via UNICORE clients, the UNICORE REST API or the UNICORE Portal. The supercomputers are operated in batch mode; interactive sessions are usually possible but the number of concurrent sessions is limited. High performance parallel storage is linked to the supercomputers (GPFS or Lustre). This storage can be accessed from the command line (see Annex D: Summary - Service IT Resource Planning for details) or via UNICORE (REST API, UNICORE Portal or UNICORE clients). WP7.5 is testing AFM, which is a GPFS caching features that allows data sharing across sites. Depending on the results of these tests, AFM might be deployed as a service in the HPC Platform. Responsible: T7.5.1, T7.5.2, T7.5.3, T7.5.4, T7.5.6 	SSH, UNICORE (clients, REST API or Portal)	Unchanged
Computing time allocation (support form)	Users that would like to start using HPC for their research but without much experience in this field will need support in applying for computing time. Therefore, a support request form is integrated in the HPC Collab in the	HPC Collab in the Collaboratory: <u>https://collab.</u>	Prototype integrated in M28





	Collaboratory. The form contains fields to specify which system the user would like to use, for which purpose, how much computing time will be needed, and to provide additional information. The requests are sent to the HPC Platform Team that will then get in contact with the users to support them in choosing the best suited HPC system, a call for computing time and in writing the application. Responsible: T7.5.7 with support from T7.5.1, T7.5.2, T7.5.3, T7.5.4, T7.5.6	humanbrainproject.eu/ #/collab/264/nav/6676	
Documentation (Guidebook)	<text></text>	HPC Collab in the Collaboratory or https://hbp-hpc- platform.fz-juelich.de/	Website published in M24





	Responsible: T7	.6.1						
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			Human Brain Project."	2015				
	Responsible: T7	.5.1, T7.5.2, ⊺	Г7.5.3, Т	7.5.4, T7.5.	7			
Support	The HPC Platfo forwards them t HPC Platform S Setting up a tick Responsible: T7	rm Manageme to relevant ex support Team ket system is a .6.1	nt Team perts if n will be also planr	answers al ecessary. A established ned for the b	requests rec the beginning and take thi beginning of S0	eived and g of SGA1 a s role ove GA1.	it Contact form in HPC collab and Guidebook er. or by email to <u>hbp-hpc- platform@fz-juelich.de</u>	Contact form integrated in Guidebook in M27
UNICORE	UNICORE (Unifo suite providing	rm Interface seamless and	to Compu secure a	iting Resour Iccess to HF	ces) is a Grid C, file system	middlewa ns and oth	re Installed at all HPC er systems and KIT Cloud	UNICORE is continuously





	resources. Its services include job submission and management, file access, data transfer, data and metadata management, cloud storage access and more. Clients can access the UNICORE services through both SOAP web services and a REST API. The development of the REST API was driven by the requests from HBP users. User authentication and authorisation is integrated with other HBP systems such as the OIDC for user authentication and the HPC LDAP servers for authorisation.	storage	updated
	More information: <u>https://hbp-hpc-platform.fz-juelich.de/?page_id=60</u> Responsible: T7.5.7		
UNICORE Portal	The UNICORE Portal is a generic web interface to the UNICORE grid middleware, providing seamless and secure access to HPC, file systems and other resources. User functions include job submission and management, storage access, data transfer and more. User authentication is integrated with the HBP OIDC server. It is integrated into the HPC Collab in the Collaboratory.	HPC Collab in the Collaboratory	Deployed on 25 May 2015 (M20), continuously updated





	COLLABORATORY	HOME COLLARS HELP FE	DMCK				0	
			III HPC					
	Nerryston ()	Workspace .	UNICORE Paniel		eon - ma	Columnation	• •	
	Chemiers HPG Platfore training	<u>U</u> NIC⊕RE	Logged ac Anna	Lührs	<u>s</u> 1			
	Autores to HPC systems Currentscore UN CORES Press? Doctoring unsurrentschon hystems 3 Lubben	Home Create Job My Jobs My Sites	🕘 Create job 🛛 😋 View jobs 🛛 🙀 Data M	Latest activiti	es	Konstanting		
	There (101%pp) (balling) w Pattopper HEFC Pattore status data for 1110 marcents	Data Manager	UNICORE Portal V2.1 deployed OS jun 2016 UNICORE Portal V2 available for HDP 14 Sep 2015	2	Feb 25. PM Anna Li Feb 24, 1134 & Anna Li	ner and a second		
			Internal reliase of the UNICORE Portal for the HPC Platform OS Apr 2015			Aming	>	
			55. 1. 22			Projevanos	>	
	More informat <u>https://hbp-h</u> Responsible: 1	tion: <u>pc-platform</u> 17.5.7	.fz-juelich.de/?page_id=64					
UNICORE workflow engine	The UNICORE control constr workflow exec steps can be maps the user	workflow er ructs (for-ea cution is pos executed o r's accounts	ngine allows defining compl ach, while, if-then-else, e sible thus enabling user int n the same or on differen on the internally used one	ex w tc.). eract nt re and	orkflov Also ion. Tł source takes	ws including pausing the ne workflow s. UNICORE care of the	UNICORE Rich Client (graphical workflow editing, workflow submission and monitoring);	Integrated in M28
	data moveme	nt between s	systems.				UNICORE command line	
	More informat https://hbp-h	ion: pc-platform	.fz-juelich.de/?page_id=767	7			client and REST API (submission and	
	Responsible: 1	Γ7.5.7					monitoring)	
Visualisation systems: booking	HBP users can and at EPFL	n book the (tiled displa	visualisation systems at R y wall) using a web form	WTH integ	Aache grated	n (aixCAVE) in the HPC	<u>https://hbp-hpc-</u> platform.fz-	Integrated in M29





form	Platform Guidebook and the HPC Collab that queries all information relevant for visiting one of the sites to use the high-fidelity systems for visualising and working with the user's data sets.	juelich.de/?page_id=44 2 or
	Responsible: WP7.3 with support from T7.6.1	<u>https://collab.</u> <u>humanbrainproject.eu/</u> #/collab/264/nav/4604

More detailed information about the infrastructure of the HPC Platform and related core services can be found in the "Infrastructure" section of the HPC Platform Guidebook: <u>https://hbp-hpc-platform.fz-juelich.de/?page_id=32</u>

Second layer: Software & Services

The Software & Services layer provides the users of the HPC Platform with tools and libraries that are important for working with HPC systems and that are specific to, or adopted for, the requirements of neuroscience. Some of the tools are written for standard computers and thus also serve users without computing time allocation. Where reasonable, the tools are also integrated into the Collaboratory. More details about the software and services can be found in Annex B: Software and Services Included in this Platform Release and in the HPC Platform Guidebook. The table below lists all new features and updates that were developed and deployed after the internal Platform Release in M18. It also provides information about the target systems for every software package.

Table 2: New software features added after M18 release

Software/Service	New features developed after M18	Tested and installed on	Related Milestones	Tasks involved
Cube	 Externally funded: New version 4.3.3 Derived metrics support Visual plugins Improved performance and scalability 	Linux clusters (Intel, Arm), IBM BlueGene, Cray, K computer	MS137	Т7.2.4
Deflect Client Library	Improved DesktopStreamer	Tiled display walls	MS139, MS141	T7.3.1





	Auto-discovery of DisplayCluster walls			
DisplayCluster	Improved interaction and UI	Tiled display walls	MS139, MS141	T7.3.1
DLB	Interactive-simulation basic mechanism (monitoring information from node usage, use job manager APIs to submit several applications in a job)	MareNostrum III, JUQUEEN	MS135, MS136	T7.2.3
Equalizer	Qt5 supportBug fixes	Tiled display walls	MS141	T7.3.1
Extrae	 New version 3.2.1 (3rd November 2015) Support for MPI3 immediate collectives Use Intel PEBS to sample memory references 	MareNostrum III, JUQUEEN	MS135, MS136	T7.2.4
FLAT	No new features	Pico	MS143	T7.4.1
HCFFT	More possible types transformationsGeneral optimisation	Tested under Linux	MS138	T7.2.5
InDiProv	No new features	Running on server-side	MS141	T7.3.4
Livre	 Support for 4D (temporal) volumes Event-driven rendering ZeroEQ and web service support for major parameters Streaming support via Monsteer Offline rendering 		MS139	T7.3.1
MonetDB	Python integration	Fedora, Ubuntu, Windows, Mac, FreeBSD,	MS143,	T7.4.4





	Representation of arrays inside MonetDBMonetDB as a standalone library (MonetDBLite)	CentOS, RHEL, Solaris	MS144
Monsteer	Loose coupling between simulators and client applications for streaming and computational steering		MS139, T7.3.1 MS141
MSPViz	New software (added to HPC Platform after M18)	Platform independent	MS139, T7.1.3, MS140 T7.3.2, T7.3.3, T7.3.4
NeuroLOTs	 First application based on the library developed that allows the user to tune parameters of the mesh generation process Enabled generated mesh extraction from the GPU 	Supported OS: Windows 7/8.1, GNU/Linux (tested on Ubuntu 14.04) and Mac OSX Target systems: High fidelity displays, desktop computers, notebooks	MS139 T7.3.2
NeuroScheme	 Added filtering and sorting Selection capabilities improved Integration with tiled display wall Advances on the integration with other tools of WP7.3 using ZEQ 	Supported OS: Windows 7, Windows 8.1, Linux (tested on Ubuntu 14.04) and Mac OSX Target systems: Desktop computers, notebooks, tablets	MS139, T7.3.2 MS140
OmpSs	 New version 15.06 Socket aware (scheduling taking into account processor socket) Reductions (mechanism to accumulate results of tasks more efficiently) 	MareNostrum III, JUQUEEN, BlueBrain IV	MS135, T7.2.4 MS136

Human Brain Project



	 Work sharing (persistence of data in the worke mechanisms 	r)			
Paraver	 New version 4.6.0 (3rd February 2016) Automatic workspaces on trace loading Scalability improvements for traces with more than 64 rows Support for wxWidgets 3 Traces with same hierarchy can be combined in thanalysis External tools integration 	MareNostrum BlueBrain IV 4K	III,	MS135, MS136	T7.2.4
PyCOMPSs	 New COMPSs features in M26: Runtime Persistent workers: workers can be deployed of computing nodes and persist during all the application lifetime, thus reducing the runtime overhead. The previous implementation workers based on a per task process is straupported. Enhanced logging system Interoperable communication layer: different inter-nodes communication protocol is supported by implementing the Adaptor interface (JavaGA and NIO implementations already included) Simplified cloud connectors interface JClouds connector 	MareNostrum BlueBrain IV on ne of ill nt ed	III,	MS135, MS136	T7.2.4





	 Added constraints support 			
	 Enhanced methods support 			
	 Lists accepted as a task's parameter type 			
	 Support for user decorators 			
	• Tools			
	 New monitoring tool: with new views, as workload and possibility of visualising information about previous runs 			
	 Enhanced tracing mechanism 			
	Simplified execution scripts			
	 Simplified installation on supercomputers through better scripts 			
	In M30 the basic support for multi-scale simulations (see SP7-UC-003) will be delivered.			
PyramidalExplorer/ NeuroFiReS	Enabled loading more general dataImprovements on the visualisation and interaction	Supported OS: Windows 7/ 8.1, Linux (tested on Ubuntu 14.04) and Mac OSX	MS139	T7.3.2
		Target systems: Desktop computers, notebooks		
Remote Connection Manager (RCM)	No new features	CINECA supercomputers (in particular FERMI and Pico)	MS147	T7.5.4
RTNeuron	 Qt5 GUI Very high-resolution off-screen screenshots Streaming and steering support through Monsteer 		MS139, MS140	T7.3.1





	Better interoperability with NeuroSchemeIPython notebook integration			
RUBIK	New software (added to HPC Platform after M18)	Pico	MS143	T7.4.1
Scalasca	 New version 2.2.2 (externally funded): Power8, ARM64, and Intel Xeon Phi support Pthread and OpenMP tasking support Improved analysis Prototype OmpSs support 	Linux clusters (Intel, Arm), IBM BlueGene, Cray, K computer	MS137	T7.2.4
Score-P	 Externally funded: New version 1.4.2; version 2.0 currently in beta Power8, ARM64, and Intel Xeon Phi support Pthread and OpenMP tasking support Prototype OmpSs support 	Linux clusters (Intel, Arm), IBM BlueGene, Cray, K computer	MS137	T7.2.4
SCOUT	No new features	Pico	MS143	T7.4.1
тоисн	New software (added to HPC Platform after M18)	Pico	MS143	T7.4.1
TRANSFORMERS	New software (added to HPC Platform after M18)	Pico	MS143	T7.4.4
T-Storm	New schemes for tracking different stream correlation metrics (using LSH indexing)	Local TUC cluster	MS143	T7.4.2
UG4	New software (added to HPC Platform after M18)	JUQUEEN, Hazel Hen, Ranger (UT)	MS138	T7.2.5
VisNEST	No new features	Target systems: high	MS140	T7.3.4





			fidelity visualisation platforms, immersive visualisation hardware, desktop computers		
ViSTA	New ViSTA release (1.15) on Sour http://sourceforge.net/projects/vistavrtoolkit/ See release notes for details	rceForge:	Operating systems: Windows, Linux Target systems: High Fidelity Visualisation Platforms, Immersive Visualisation Hardware, desktop computers	MS139	T7.3.4
VIOLA	New software (added to HPC Platform after M18)		Web-based visualisation tool	MS140	T7.3.4
ZeroBuf	 Zero-copy Zero-serialise Zero-hassle protocol buffers 			MS141	T7.3.1
ZeroEQ	http::ServerZeroBuf supportSession filtering			MS141	T7.3.1





Annex B: Software and Services Included in this Platform Release

Product/Software Package/Service name: Cube

Cube, which is used as performance report explorer for Scalasca and Score-P, is a generic tool for displaying a multi-dimensional performance space.

Metadata

Table 3: Export from Collaboratory Software Catalog: Cube

Category	application
Tags	parallel-application-performance-analysis
	HPC
	supercomputers
	performance-analysis
	<u>sp7</u>
Partners	Forschungszentrum Jülich GmbH <u>JUELICH</u>
	German Research School for Simulation Sciences GmbH <u>GRS</u>
Maintainers	JSC group "Programming Environments and Performance Analysis" (Bernd MOHR)
Contributors	Felix WOLF (in the past)
Homepage	http://www.scalasca.org/software/cube-4.x
Documentation	http://www.scalasca.org/software/cube-4.x/documentation.html
Support	<u>scalasca@fz-juelich.de</u>





Source Code	http://www.scalasca.org/software/cube-4.x/download.html
Download Page	http://www.scalasca.org/software/cube-4.x/download.html
License	New BSD 3-Clause
Current Version	4.3.3
All Versions	4.3.3

Description

Cube, which is used as performance report explorer for Scalasca and Score-P, is a generic tool for displaying a multi-dimensional performance space consisting of the dimensions

- 1. Performance metric,
- 2. Call path, and
- 3. System resource.

Each dimension can be represented as a tree, where non-leaf nodes of the tree can be collapsed or expanded to achieve the desired level of granularity. In addition, Cube can display multi-dimensional Cartesian process topologies.

The Cube 4.x series report explorer and the associated Cube4 data format is provided for Cube files produced with the Score-P performance instrumentation and measurement infrastructure or with Scalasca version 2.x trace analyser (and other compatible tools). However, for backwards compatibility, Cube 4.x can also read and display Cube 3.x data.

Cube is part of a larger set of tools for parallel performance analysis and debugging developed by the "Virtual Institute - High Productivity Supercomputing" (VI-HPS) consortium. Further documentation, training and support are available through VI-HPS:

- High-level Tool Descriptions: VI-HPS Tools Guide and http://www.vi-hps.org/tools/
- Index to VI-HPS tool documentation: http://www.vi-hps.org/training/doc/
- Training classes: VI-HPS Tuning Workshops
- Course material: <u>http://www.vi-hps.org/training/material/</u>

Product/Software Package/Service name: Deflect Client Library





Deflect is a C++ library to develop applications that can send and receive pixel streams from other Deflect-based applications, for example DisplayCluster.

Metadata

 Table 4: Export from Collaboratory Software Catalog: Deflect Client Library

Category	Library
Tags	<u>sp7</u> <u>visualisation</u>
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	EPFL Visualisation Team (Stefan EILEMANN)
Contributors	TACC (contact Stefan EILEMANN, EPFL for details)
Homepage	https://github.com/BlueBrain/Deflect
Documentation	https://bluebrain.github.io/
Support	bbp-open-source@googlegroups.com
Source Code	https://bluebrain.github.io/
Download Page	https://github.com/BlueBrain/Deflect
License	BSD
Current Version	0.5
All Versions	0.5





Description

Deflect is a C++ library to develop applications that can send and receive pixel streams from other Deflect-based applications, for example DisplayCluster. The following applications are provided which make use of the streaming API:

- DesktopStreamer: A small utility that allows the user to stream the desktop.
- SimpleStreamer: A simple example to demonstrate streaming of an OpenGL application.





Product/Software Package/Service name: DisplayCluster

DisplayCluster is a software environment for interactively driving large-scale tiled displays.

Metadata

Table 5: Export from Collaboratory Software Catalog: DisplayCluster

Category	Application		
Tags	<u>sp7</u> <u>display-wall</u> <u>visualisation</u>		
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>		
Maintainers	EPFL Visualisation Team		
Contributors	TACC (contact Stefan EILEMANN, EPFL for details)		
Homepage	https://github.com/BlueBrain/DisplayCluster		
Documentation	https://bluebrain.github.io/		
Support	bbp-open-source@googlegroups.com		
Source Code	https://bluebrain.github.io/		
Download Page	https://github.com/BlueBrain/DisplayCluster		
License	BSD		
Current Version	0.5		
All Versions	0.5		





Description

DisplayCluster is a software environment for interactively driving large-scale tiled displays. It provides the following functionality:

- View media interactively such as high-resolution imagery, PDFs and video.
- Receive content from remote sources such as laptops, desktops or parallel remote visualisation machines using the Deflect Client Library.





Product/Software Package/Service name: DLB

DLB is a library devoted to speedup hybrid parallel applications.

Metadata

Table 6: Export from Collaboratory Software Catalog: DL	rt from Collaboratory Software Ca	atalog: DLB
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Category	Library
Tags	sp7 HPC load-balancing
Partners	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion BSC
Maintainers	BSC Programming Models Group
Contributors	BSC Programming Models Group
Homepage	https://pm.bsc.es/dlb
Documentation	https://pm.bsc.es/dlb
Support	pm-tools@bsc.es
Download Page	https://pm.bsc.es/dlb
License	LGPL
Current Version	1.1
All Versions	1.1





Description dynamic load balancing

DLB is a library devoted to speedup hybrid parallel applications. And at the same time DLB improves the efficient use of the computational resources inside a computing node. The DLB library will improve the load balance of the outer level of parallelism by redistributing the computational resources at the inner level of parallelism. This readjustment of resources will be done at dynamically at runtime. This dynamism allows DLB to react to different sources of imbalance: Algorithm, data, hardware architecture and resource availability among others.





Product/Software Package/Service name: Equalizer

Equalizer is a parallel rendering framework to create and deploy parallel, scalable OpenGL applications.

Metadata

Table	7:	Export from	Collaborator	v Software	Catalog:	Equalizer
1 010 10				,	eacers.	

Category	Library
Tags	<u>sp7</u>
	<u>visualisation</u>
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	TACC
Homepage	https://github.com/Eyescale/Equalizer
Documentation	https://eyescale.github.io/
Support	bbp-open-source@googlegroups.com
Download Page	https://github.com/Eyescale/Equalizer
License	LGPL
Current Version	1.8
All Versions	1.8





Description



Equalizer is a parallel rendering framework to create and deploy parallel, scalable OpenGL applications. It provides the following major features to facilitate the development and deployment of scalable OpenGL applications:

- Runtime Configurability: An Equalizer application is configured automatically or manually at runtime and can be deployed on laptops, multi-GPU workstations and large-scale visualisation clusters without recompilation.
- Runtime Scalability: An Equalizer application can benefit from multiple graphics cards, processors and computers to scale rendering performance, visual quality and display size.
- Distributed Execution: Equalizer applications can be written to support cluster-based execution. Equalizer uses the Collage network library, a cross-platform C++ library for building heterogeneous, distributed applications.

Support for Stereo and Immersive Environments: Equalizer supports stereo rendering head tracking, head-mounted displays and other advanced features for immersive Virtual Reality installations.





Product/Software Package/Service name: Extrae

Extrae is an instrumentation and measurement system gathering time stamped information of the events of an application.

Metadata

	Table 8:	Export fr	om Collabora	tory Software	Catalog: Extrae
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Category	Tool		
Tags	parallel-application-performance-analysis HPC supercomputers performance-analysis sp7		
Partners	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion BSC		
Maintainers	BSC Performance Tools Group		
Contributors	BSC Performance Tools Group		
Homepage	http://www.bsc.es/computer-sciences/extrae		
Documentation	http://www.bsc.es/computer-sciences/performance-tools/documentation		
Support	tools@bsc.es		
Download Page	http://www.bsc.es/computer-sciences/performance-tools/downloads		
License	LGPL		
Current Version	3.2.1		





All Versions 3.2.1

Description

Extrae is an instrumentation and measurement system gathering time stamped information of the events of an application. It is the package devoted to generate Paraver trace files for a post-mortem analysis of a code run. It uses different interposition mechanisms to inject probes into the target application in order to gather information about the application performance.




Product/Software Package/Service name: FLAT

A disk-based spatial index for dense data sets.

Metadata

Table 9: Export from Collaboratory Software Catalog: FL	9: Export from Collaboratory Software C	Catalog: FLA
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Category	Tool				
Tags	<u>sp7</u> <u>data-analytics</u> <u>spatial-indexing</u>				
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>				
Maintainers	darius.sidlauskas@epfl.ch				
Contributors	<u>farhan.tauheed@epfl.ch</u> <u>t.heinis@imperial.ac.uk</u>				
Homepage	http://dias.epfl.ch/BrainDB				
Documentation	http://dias.epfl.ch/BrainDB#flat-doc				
Source Code	https://git.epfl.ch/repo/fst.git				
License	Missing				
Current Version	v1.01				
All Versions	1.01 v1.01				





Description



To compile:

\$ cd build && cmake ../cmake && make

To build FLAT index:

\$./bin/FLATGenerator --inputfile data-file.bin --outputprefix flat

To query the built index:

\$ FLAT --queryfile query-file.txt --outputprefix flat

By default, FLAT outputs the result size of each query to the console while the full result is written to files. More details: http://dias.epfl.ch/BrainDB#usage





Product/Software Package/Service name: HCFFT

HCFFT (Hyperbolic Cross Fast Fourier Transform) is a software package to efficiently treat high-dimensional multivariate functions.

Metadata

Table 10: Export from Collaboratory Software Catalog: HCFFT

Category	Library
Tags	<u>sp7</u> <u>fast-fourier-transform</u> <u>multivariate-functions</u>
Partners	Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V. <u>FG</u>
Maintainers	Jan HAMAEKERS, Fraunhofer SCAI
Contributors	Jan HAMAEKERS, Fraunhofer SCAI Christian NEUEN, Fraunhofer SCAI
Support	http://hcfft.org/get-hcfft.html
License	Free for non-commercial purpose
Current Version	1.0
All Versions	1.0

Description

HCFFT (Hyperbolic Cross Fast Fourier Transform) is a software package to efficiently treat high-dimensional multivariate functions. The implementation is based on the fast Fourier transform for arbitrary hyperbolic cross / sparse grid spaces.





Product/Software Package/Service name: InDiProv

This server-side tool is meant to be used for the creation of provenance tracks in context of interactive analysis tools and visualisation applications.

Metadata

Table 11: Export from Collaboratory Software Catalog: InDiProv

Category	Tool					
Tags	sp7 provenance-tracking visualisation interactive-analysis					
Partners	heinisch-Westfälische Technische Hochschule Aachen <u>RWTH</u>					
Maintainers	RWTH Aachen University					
Contributors	RWTH Aachen University					
Homepage	https://github.com/hbpvis					
Documentation	https://github.com/hbpvis					
Support	weyers@vr.rwth-aachen.de					
Source Code	https://github.com/hbpvis					
License	undefined					
Current Version	1.0					





All Versions 1.0

Description

This server-side tool is meant to be used for the creation of provenance tracks in context of interactive analysis tools and visualisation applications. It is capable of tracking multi-view and multiple applications for one user using this ensemble. It further is able to extract these tracks from the internal data base into a XML-based standard format, such as the W3C Prov-Model or the OPM format. This enables the integration to other tools used for provenance tracking and will finally end up in the Collaboratory.





Product/Software Package/Service name: Livre

Largescale Interactive Volume Rendering Engine.

Metadata

Table 12: Export from Collaboratory Software Ca	Catalog: Livre
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Category	Tool					
Tags	open-source sp7 visualisation					
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>					
Maintainers	EPFL Visualisation Team					
Contributors	University of Zurich					
Homepage	https://bbpcode.epfl.ch/browse/code/viz/Livre/					
Documentation	https://bbp.epfl.ch/documentation/code/Livre-0.2/index.html					
Support	https://bbpteam.epfl.ch/project/issues/browse/LIV					
Source Code	https://bbpcode.epfl.ch/code/viz/Livre					
License	LGPL					
Current Version	0.4.0					
All Versions	0.4.0					





Description

Livre is an out-of-core rendering engine that has the following features:

- Distributed rendering using Equalizer parallel rendering framework
- Octree based out-of-core
- Visualisation of pre-processed UVF format volume data sets.
- Real-time voxelisation and visualisation of surface meshes using OpenGL 4.2 extensions.
- Real-time voxelisation and visualisation of Blue Brain Project (BBP) morphologies.
- Real-time voxelisation and visualisation of local-field potentials in BBP circuit.
- Multi-node, multi-GPU rendering.





Product/Software Package/Service name: MonetDB

MonetDB with R and Python integration, SciQL query language for array processing and a loader for .bam files

Metadata

Table 13: Export from Collaboratory Software Catalog: MonetDB

Category	Tool					
Tags	database					
	data-analytics					
	DBMS					
	data-management					
	<u>sp7</u>					
Partners	tichting Centrum voor Wiskunde en Informatica <u>CWI</u>					
Maintainers	DA group of CWI					
Contributors	DA group of CWI					
Homepage	https://www.monetdb.org/					
Documentation	https://www.monetdb.org/Documentation					
Support	users-list@monetdb.org					
Source Code	<u>ssh://hg@dev.monetdb.org/MonetDB</u>					
License	Mozilla Public License, v. 2.0					
Current Version	11.22.0					





All Versions 11.22.0

MnetDB 5, V11.22.0 MonetDB 5, V11.22.0

Description



Users can download MonetDB using the command

hg clone ssh://hg@dev.monetdb.org/MonetDB

Afterwards, they should compile and install it following the instructions found in the README file included in the MonetDB directory. The BAT loader, the Python and R integration are all included in the default branch. More information about them can be found in the following pages

- <u>https://www.monetdb.org/Documentation/Extensions/LifeScience/load</u>
- <u>https://www.monetdb.org/Documentation/UserGuide/MonetDB-R</u>
- <u>https://www.monetdb.org/content/embedded-r-monetdb</u>
- https://www.monetdb.org/Documentation/Manuals/SQLreference/Programming/Python

To use SciQL, one should first update to the SciQL-2 branch (hg update -r SciQL-2) and then compile and build the MonetDB. More information about SciQl can be found here <u>http://www.scilens.org/Resources/SciQL.html</u>.





Product/Software Package/Service name: Monsteer

Interactive Supercomputing tools and library.

Metadata

Table 14: Export from Collaboratory S	Software Catalog: Monsteer
---------------------------------------	----------------------------

Category	Library
Tags	<u>computing</u> <u>open-source</u> sp7
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	EPFL Visualisation Team
Homepage	https://bbpcode.epfl.ch/browse/code/viz/Monsteer/
Documentation	https://bbp.epfl.ch/documentation/code/Monsteer-0.2/index.html
Support	https://bbpteam.epfl.ch/project/issues/browse/VIZTM
Source Code	https://bbpcode.epfl.ch/code/viz/Monsteer
License	lgpl
Current Version	0.2.0
All Versions	0.2.0





Description

Monsteer is a library for Interactive Supercomputing in the neuroscience domain. Monsteer facilitates the coupling of running simulations (currently NEST) with interactive visualisation and analysis applications. Monsteer supports streaming of simulation data to clients (currently only spikes) as well as control of the simulator from the clients (also known as computational steering). Monsteer's main components are a C++ library, an MUSIC-based application and Python helpers.





Product/Software Package/Service name: MSPViz

MSPViz is a visualisation tool for the Model of Structural Plasticity.

Metadata

Table 15: Export from Collaboratory	Software Catalog: MSPViz
-------------------------------------	--------------------------

Category	tool
Tags	<u>sp7</u> <u>visualisation</u>
Partners	Universidad Politécnica de Madrid <u>UPM</u> Forschungszentrum Jülich GmbH <u>JUELICH</u> Rheinisch-Westfälische Technische Hochschule Aachen <u>RWTH</u> Universidad Rey Juan Carlos <u>URJC</u>
Maintainers	<u>UPM</u>
Contributors	UPM, URJC, RWTH, JUELICH
Homepage	http://gmrv.es/mspviz
Support	juanpedro.brito@upm.es
Download Page	http://gmrv.es/mspviz
License	Missing License
Current Version	0.1
All Versions	0.1





Description

MSPViz is a visualisation tool for the Model of Structural Plasticity. It uses a visualisation technique based on the representation of the neuronal information through the use of abstract levels and a set of schematic representations into each level. The multilevel structure and the design of the representations constitutes an approach that provides organised views that facilitates visual analysis tasks.





Product/Software Package/Service name: NeuroLOTs

NeuroLOTs is a set of tools and libraries that allow creating neuronal meshes from a minimal skeletal description.

Metadata

Table	16:	Export	from	Collaboratory	/ Software	Catalog:	NeuroLOTs
IUDIC		Export		contaboratory	Solution	cuturos.	ILCUI OLO I J

Category	Tool
Tags	<u>sp7</u> <u>visualisation</u>
Partners	Universidad Rey Juan Carlos <u>URJC</u>
Maintainers	Pablo TOHARIA, URJC
Contributors	Pablo TPHARIA, URJC
Support	pablo.toharia@urjc.es
License	Missing License
Current Version	0.1
All Versions	0.1

Description

NeuroLOTs is a set of tools and libraries that allow creating neuronal meshes from a minimal skeletal description. It generates soma meshes using FEM deformation and allows to interactively adapt the tessellation level using different criteria (user-defined, camera distance, etc.)





Product/Software Package/Service name: NeuroScheme

NeuroScheme is a tool that allows users to navigate through circuit data at different levels of abstraction using schematic representations for a fast and precise interpretation of data.

Metadata

Table 17: Export from Collaboratory Software Catalog: NeuroScheme

Category	Tool
Tags	<u>sp7</u> <u>visualisation</u>
Partners	Universidad Rey Juan Carlos <u>URJC</u>
Maintainers	Pablo TOHARIA, URJC
Contributors	Pablo TOHARIA, URJC
Support	pablo.toharia@urjc.es
License	Missing License
Current Version	0.1
All Versions	0.1

Description

NeuroScheme is a tool that allows users to navigate through circuit data at different levels of abstraction using schematic representations for a fast and precise interpretation of data. It also allows filtering, sorting and selections at the different levels of abstraction. Finally it can be coupled with realistic visualisation or other applications using the ZeroEQ event library developed in WP 7.3.





Product/Software Package/Service name: OmpSs

OmpSs is a fine-grained programming model oriented to shared memory environments, with a powerful runtime that leverages low-level APIs (e.g. CUDA/OpenCL) and manages data dependencies (memory regions).

Metadata

Table 18: Export from Collaboratory Software Catalog: OmpSs

Category	Library
Tags	<u>sp7</u> <u>HPC</u> <u>programming-model</u> compiler
Partners	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion <u>BSC</u>
Maintainers	BSC Programming Models Group
Contributors	BSC Programming Models Group
Homepage	https://pm.bsc.es/ompss
Documentation	https://pm.bsc.es/ompss
Support	pm-tools@bsc.es
Download Page	https://pm.bsc.es/ompss-downloads
License	LGPL
Current Version	15.06





All Versions 15.06

Description



OmpSs is a fine-grained programming model oriented to shared memory environments, with a powerful runtime that leverages low-level APIs (e.g. CUDA/OpenCL) and manages data dependencies (memory regions). It exploits task level parallelism and supports asynchronicity, heterogeneity and data movement.

The new version 15.06 provides the following new features as compared to version 15.04 that was part of the HBP-internal Platform Release in M18:

- Socket aware (scheduling taking into account processor socket)
- Reductions (mechanism to accumulate results of tasks more efficiently)
- Work sharing (persistence of data in the worker) mechanisms





Product/Software Package/Service name: Paraver

Paraver is a very flexible data browser for performance analysis results.

Metadata

rubic iv. Export nom conuboratory solution catalog, rubicri	Table 19:	Export from	Collaboratory	/ Software	Catalog:	Paraver
---	-----------	--------------------	---------------	------------	----------	---------

Category	Tool
Tags	performance-analysis
	performance-visualisation
-	parallel-application-performance-analysis
Partners	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion <u>BSC</u>
Maintainers	BSC Performance Tools Group
Contributors	BSC Performance Tools Group
Homepage	http://www.bsc.es/computer-sciences/performance-tools/paraver
Documentation	http://www.bsc.es/computer-sciences/performance-tools/documentation
Support	tools@bsc.es
Download Page	http://www.bsc.es/computer-sciences/performance-tools/downloads
License	LGPL
Current Version	4.6.0
All Versions	4.6.0





Description

Paraver is a very flexible data browser. The metrics used are not hardwired on the tool but can be programmed. To compute them, the tool offers a large set of time functions, a filter module, and a mechanism to combine two timelines. This approach allows displaying a huge number of metrics with the available data. The analysis display allows computing statistics over any timeline and selected region, what allows correlating the information of up to three different time functions. To capture the expert's knowledge, any view or set of views can be saved as a Paraver configuration file. Therefore, re-computing the same view with new data is as simple as loading the saved file. The tool has been demonstrated to be very useful for performance analysis studies, giving much more details about the applications behaviour than most performance tools available.





Product/Software Package/Service name: PyCOMPSs

PyCOMPSs is the Python binding of COMPSs, (COMP Superscalar) a coarse-grained programming model oriented to distributed environments, with a powerful runtime that leverages low-level APIs (e.g. Amazon EC2) and manages data dependencies (objects and files).

Metadata

Table 20: Export from Collaboratory Software Catalog: PyCOMPSs

Category	Library
Tags	<u>sp7</u> <u>HPC</u> <u>programming-model</u>
Partners	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion BSC
Maintainers	BSC Workflows and Distributed Computing Group
Contributors	BSC Workflows and Distributed Computing Group
Homepage	http://compss.bsc.es/
Documentation	http://www.bsc.es/computer-sciences/grid-computing/comp-superscalar/downloads-and-documentation
Support	support-compss@bsc.es
Download Page	http://compss.bsc.es/
License	Apache v2.0
Current Version	1.3
All Versions	1.3





Description



PyCOMPSs is the Python binding of COMPSs, (COMP Superscalar) a coarse-grained programming model oriented to distributed environments, with a powerful runtime that leverages low-level APIs (e.g. Amazon EC2) and manages data dependencies (objects and files). From a sequential Python code, it is able to run in parallel and distributed.





Product/Software Package/Service name: PyramidalExplorer/NeuroFiReS

NeuroFiReS is a library for performing search and filtering operations using both data contents and metadata.

Metadata

Table 21: Export from Collaboratory Software Catalog: NeuroFiReS

Category	Library
Tags	<u>sp7</u>
	<u>search-and-filter</u>
	data-management
Partners	Universidad Rey Juan Carlos <u>URJC</u>
Maintainers	Pablo TOHARIA, URJC
Contributors	Pablo TOHARIA, URJC
Support	pablo.toharia@urjc.es
License	Missing License
Current Version	0.1
All Versions	0.1

Description

NeuroFiReS is a library for performing search and filtering operations using both data contents and metadata. These search operations will be tightly coupled with visualisation in order to improve insight gaining from complex data. A first prototype (named spineRet) for searching and filtering over segmented spine data has been developed.





Product/Software Package/Service name: Remote Connection Manager (RCM)

The Remote Connection Manager (RCM) is an application that allows HPC users to perform remote visualisation on Cineca HPC clusters.

Metadata

Table 22: Export from Collaboratory Software Catalog: Remote Connection Manager (RCM)

Category	Application
Tags	<u>sp7</u> <u>remote-visualisation</u>
	<u>HPC</u>
	<u>visualisation</u>
Partners	Consorzio Interuniversitario Cineca <u>CINECA</u>
Maintainers	Roberto MUCCI & Luigi CALORI, CINECA
Homepage	http://www.hpc.cineca.it/content/remote-visualization-rcm
Documentation	http://www.hpc.cineca.it/content/remote-visualization-rcm
Support	superc@cineca.it
License	Missing License
Current Version	1.2
All Versions	1.2

Description

The Remote Connection Manager (RCM) is an application that allows HPC users to perform remote visualisation on Cineca HPC clusters.





The tool offers to

- Visualise the data produced on Cineca's HPC systems (scientific visualisation);
- Analyse and inspect data directly on the systems;
- Debug and profile parallel codes running on the HPC clusters.

The graphical interface of RCM allows the HPC users to easily create remote displays and to manage them (connect, kill, refresh).





Product/Software Package/Service name: RTNeuron

RTNeuron is a tool for the interactive visualisation and media production of cortical column simulation results.

Metadata

Table 23: Export from Collaboratory Software Catalog: RTNeuron

Category	Tool
Tags	<u>sp7</u>
	visualisation
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	EPFL Visualisation Team
Homepage	https://bbpcode.epfl.ch/browse/code/viz/RTNeuron/
Documentation	https://bbp.epfl.ch/documentation/code/RTNeuron-2.8/index.html
Support	https://bbpteam.epfl.ch/project/issues/browse/BBPRTN
Source Code	https://bbpcode.epfl.ch/code/viz/RTNeuron
License	Proprietary, LGPL planned
Current Version	2.8.0
All Versions	2.8.0

Description

RTNeuron is a tool for the interactive visualisation and media production of cortical column simulation results.





Product/Software Package/Service name: RUBIK

A time series indexing tool which enables scalable threshold queries on massive collections of time series data.

Metadata

Table 24: Export from Collaboratory Software Catalog: RUBIK

Category	Tool
Tags	sp7 data-query data-management data-analysis
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	<u>eleni.tziritazacharatou@epfl.ch</u>
Contributors	<u>t.heinis@imperial.ac.uk</u> <u>eleni.tziritazacharatou@epfl.ch</u>
Homepage	http://dias.epfl.ch/BrainDB
Documentation	http://dias.epfl.ch/BrainDB#rubik-doc
Source Code	https://git.epfl.ch/repo/rubik.git
License	Missing
Current Version	0.9
All Versions	0.9





Description



RUBIK is a time series indexing tool, which enables scalable threshold queries on a collection of time series. Given the user input, which should be a threshold for the observation value as well as an upper and lower bound for time, and the dataset to be queried, RUBIK returns all the time series values that are above the given threshold for the specified time range.

To build RUBIK, just run the provide script:

```
$ ./build.sh
```

Usage:

First, to import data into RUBIK, use the following command:

<pre>\$ ImportDataRUBIK nb_timesteps</pre>	input_data	folder_path	output_data	folder_path	grid_timesteps
input_data: folder	containing time	series in csv	files		
output_data: output	binary folder :	for time series	s clusters		
grid_timesteps: num	ber of timestep:	s for each time	e series		

Next, you can build RUBIK by running:







```
--source_data: binary time series clusters folder (output of ImportRUBIK)
--grid_timesteps: number of timesteps for each time series
--grid voltagebins: number of voltage bins used (must be power of two)
Finally, times series can be queried as follows:
$ QueryRUBIK --index_prefix prefix_path --start_time start_time --end_time end_time \
--voltage-gt voltage_value --grid_timesteps nb_timesteps \
--grid_voltagebins nb_voltage_bins --multiple_runs nb_runs
-i,--index_prefix: path prefix for the index (output of BuildRUBIK)
-t,--start_time: lower time bound for query
-u,--end_time: upper time bound for query
--grid_timesteps: number of timesteps for each time series
--grid_voltagebins: number of voltage bins used (the same as in building)
-s,--multiple_runs: define how many times the query should be executed (for performance
measurements only)
Textet with you can be be provided exempted
```

To start with, you can run the provided example:

./run_example.sh

The example script will:

- import in the binary data format the clustered time series (folder data_test_bin)
- build RUBIK data structure in the folder (folder quadtree_index)
- execute example queries on them

More details: <u>http://dias.epfl.ch/BrainDB#usage</u>

Product/Software Package/Service name: Scalasca





Scalasca is a software tool that supports the performance optimisation of parallel programs by measuring and analysing their runtime behaviour.

Metadata

Table 25: Export from Collaboratory Software Catalog: Scalasca

Category	Tool
Tags	performance-analysis sp7 parallel-application-performance-analysis HPC
Partners	Forschungszentrum Jülich GmbH <u>JUELICH</u>
Maintainers	JSC group "Programming Environments and Performance Analysis" (Bernd Mohr)
Contributors	Felix WOLF, GRS Aachen
Homepage	http://www.scalasca.org/software/scalasca-2.x
Documentation	http://www.scalasca.org/software/scalasca-2.x/documentation.html
Support	<u>scalasca@fz-juelich.de</u>
Download Page	http://www.scalasca.org/software/scalasca-2.x/download.html
License	New BSD 3-Clause
Current Version	2.2.2
All Versions	2.2.2





Description



Scalasca is a software tool that supports the performance optimisation of parallel programs by measuring and analysing their runtime behaviour. The analysis identifies potential performance bottlenecks - in particular those concerning communication and synchronisation - and offers guidance in exploring their causes.

Scalasca targets mainly scientific and engineering applications based on the programming interfaces MPI and OpenMP, including hybrid applications based on a combination of the two. The tool has been specifically designed for use on large-scale systems including IBM Blue Gene and Cray XT, but is also well suited for small- and medium-scale HPC platforms. The software is available for free download under the New BSD open-source license.

Scalasca is part of a larger set of tools for parallel performance analysis and debugging developed by the "Virtual Institute - High Productivity Supercomputing" (VI-HPS) consortium. Further documentation, training and support are available through VI-HPS.

- High-level Tool Descriptions: VI-HPS Tools Guide and http://www.vi-hps.org/tools/
- Index to VI-HPS tool documentation: <u>http://www.vi-hps.org/training/doc/</u>
- Training classes: VI-HPS Tuning Workshops
- Course material: <u>http://www.vi-hps.org/training/material/</u>





Product/Software Package/Service name: Score-P

The Score-P measurement infrastructure is a highly scalable and easy-to-use tool suite for profiling, event tracing, and online analysis of HPC applications.

Metadata

Table 26: Export from Collaboratory Software Catalog: Score-P

Category	Tool
Tags	<u>performance-analysis</u> <u>sp7</u> parallel-application-performance-analysis
Partners	Technische Universitaet Dresden <u>TUD</u> Forschungszentrum Jülich GmbH <u>JUELICH</u>
Maintainers	<u>Jülich Supercomputing Centre (Bernd Mohr)</u> TU Dresden
Contributors	RWTH AachenGRS AachenTU MünchenTU DarmstadtGNS BraunschweigUniv. of Oregon
Homepage	http://www.score-p.org/
Documentation	http://www.score-p.org/





Support	support@score-p.org
Download Page	http://www.score-p.org/
License	New BSD 3-Clause
Current Version	1.4.2
All Versions	1.4.2

Description



The Score-P measurement infrastructure is a highly scalable and easy-to-use tool suite for profiling, event tracing, and online analysis of HPC applications. Score-P is developed under a BSD 3-Clause (Open Source) License and governed by a meritocratic governance model.

Score-P offers the user a maximum of convenience by supporting a number of analysis tools. Currently, it works with Periscope, Scalasca, Vampir, and Tau and is open for other tools. Score-P comes together with the new Open Trace Format Version 2, the Cube4 profiling format and the Opari2 instrumenter.

Score-P is part of a larger set of tools for parallel performance analysis and debugging developed by the "Virtual Institute - High Productivity Supercomputing" (VI-HPS) consortium. Further documentation, training and support are available through VI-HPS.

- High-level Tool Descriptions: VI-HPS Tools Guide and http://www.vi-hps.org/tools/
- Index to VI-HPS tool documentation: <u>http://www.vi-hps.org/training/doc/</u>
- Training classes: VI-HPS Tuning Workshops
- Course material: <u>http://www.vi-hps.org/training/material/</u>





Product/Software Package/Service name: SCOUT

A structure-aware method for prefetching data along interactive spatial query sequences.

Metadata

Table 27: Export from Collaboratory Software Catalog: SCUL	Table	27: Export fro	m Collaboratory	/ Software	Catalog:	SCOUT
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Category	Tool	
Tags	<u>sp7</u> <u>data-query</u> <u>data-analytics</u> <u>data-management</u>	
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>	
Maintainers	darius.sidlauskas@epfl.ch	
Contributors	<u>farhan.tauheed@epfl.ch</u> <u>t.heinis@imperial.ac.uk</u>	
Homepage	http://dias.epfl.ch/BrainDB	
Documentation	http://dias.epfl.ch/BrainDB#scout-doc	
Source Code	https://git.epfl.ch/repo/fst.git	
License	Missing	
Current Version	1.03	
All Versions	v1.02	





v1.03		
1.03		
v1.01		

Description



Though SCOUT has a command line interface too (and is very efficient when query file contains spatial query sequences), its main advantages are observed when it is used within the BBP SDK with exploratory user queries (e.g., during visualisation).

To compile:

\$ cd build && cmake ../cmake && make

To run:

\$./bin/SCOUT --queryfile query-file.txt --outputprefix flat

Note: user's data set has to be pre-indexed with FLAT.

More details: <u>http://dias.epfl.ch/BrainDB#usage</u>





Product/Software Package/Service name: TOUCH

In-memory spatial join algorithm that uses hierarchical data-oriented space partitioning, thereby keeping both its memory footprint and the number of comparisons low.

Metadata

Table 28: Export from Collaboratory Software Catalog: TOUCH

Category	Tool
Tags	sp7 spatial-join spatial-indexing data-management
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	<u>darius.sidlauskas@epfl.ch</u>
Contributors	<u>farhan.tauheed@epfl.ch</u> <u>t.heinis@imperial.ac.uk</u>
Homepage	http://dias.epfl.ch/BrainDB
Documentation	http://dias.epfl.ch/BrainDB#touch-doc
Source Code	https://git.epfl.ch/repo/fst.git
License	Missing
Current Version	0.94
All Versions	0.9





0.94	
0.91	
0.93	
0.92	

Description






To compile:

\$ cd build && cmake ../cmake && make

Given two input files with spatial objects, TOUCH can be used to efficiently find intersecting (touching) points between them as follows:

```
$ TOUCH --datasetA arg --datasetB arg [--logfile filename] [--outfile arg] [--epsilon e] [--runs
arg]
     [--localjoin arg] [--base arg] [--partitions arg] [--partitioningtype arg]
    --datasetA: filename containing dataset A
    --datasetB: filename containing dataset B
    --logfile: log filename (default: SJ.txt)
    --outfile: output file (default: touches.out)
    --epsilon: max distance still forming a touch (default: 1.5)
    --runs: number of runs; for performance measurements (default: 1)
    --localjoin: local join algorithm used; 0 - nested loop; 1 - plane sweep (default: 1)
    --base: base (default: 2)
    --partitions: number of partitions (default: 4)
    --partitioningtype: type of partitioning; 0 - arbitrary; 1 - hilbert; 2 - x-axis sort; 3 -
STR (default: 3)
```

More details: <u>http://dias.epfl.ch/BrainDB#usage</u>





Product/Software Package/Service name: TRANSFORMERS

A very robust (w.r.t. data distributions) disk-based (i.e., I/O efficient) spatial join technique.

Metadata

Table 29: Export from Collaboratory Software Catalog: TRANSFORMERS

Category	Tool
Tags	sp7 data-query data-management data-analysis
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	mirjana.pavlovic@epfl.ch
Contributors	<u>t.heinis@imperial.ac.uk</u> <u>mirjana.pavlovic@epfl.ch</u>
Homepage	http://dias.epfl.ch/BrainDB
Documentation	http://dias.epfl.ch/BrainDB#transformers-doc
Source Code	https://git.epfl.ch/repo/transformers.git
License	Missing
Current Version	0.91
All Versions	0.9





0.91

Description



TRANSFORMERS is a method that achieves robust spatial joins by identifying local variations in data distributions and adapting its strategy and the data layout on the fly accordingly. It employs a join method based on data-oriented partitioning when joining areas of substantially different local densities, whereas it uses big partitions (as in space-oriented partitioning) when the densities are similar, while seamlessly switching among these two strategies and the role that each of the two data plays at run-time.

To compile:

```
$ cd RTREE/ && make
```

```
$ cd ../TRANSFORMERS/bin && cmake ../cmake && make
```

To run:

```
$ ./TransformersJoin --datasetA arg --datasetB arg [--resultFile arg]
```

--datasetA: filname containing dataset A

--datasetB: filename containing dataset B

--resultFile: output file (default: Transformers Results)

More details: <u>http://dias.epfl.ch/BrainDB#usage</u>





Product/Software Package/Service name: T-Storm

T-Storm is a platform for supporting scalable real-time analytics of massive sets of voluminous time-series.

Metadata

Table 30: Export from Collaboratory Software Catalog: T-Storm

Category	Tool
Tags	<u>sp7</u> <u>time-series-analysis</u>
Partners	Technical University of Crete <u>TUC</u>
Maintainers	Minos GAROFALAKIS Odysseas PAPAPETROU Nikolaos PAVLAKIS
Contributors	Minos GAROFALAKIS Odysseas PAPAPETROU Nikolaos PAVLAKIS
Support	npavlakis@softnet.tuc.gr
License	Apache Storm (open source)
Current Version	0.1
All Versions	0.1





Description

T-Storm is a platform for supporting scalable real-time analytics of massive sets of voluminous time-series. The platform is constructed over the Storm parallel dataflow engine, and supports both vertical scalability (fully utilising high-end servers and multi-core systems) and horizontal scalability (scaling across a cluster of physical machines or even incorporating virtual cloud resources).

The current version of T-Storm enables efficient maintenance of the highly correlated time-series in linear space and near-linear computational complexity. In practice, computational complexity depends on the input time-series. This functionality is, for example, useful to identify the pairs of neurons that fire in a correlated manner. In future versions, T-Storm will enable a wide range of continuous time-series analytics. These will include single-stream analytics, such as maintaining sliding-window summaries and statistics, but also cross-stream analytics, such as continuous clustering and classification of the time series. Future versions will also support an Application Programming Interface and a high-level user interface, e.g., via R language for statistical computing.





Product/Software Package/Service name: UG4

UG4 is a powerful software framework for the simulation of complex PDE based systems on massively parallel computer architectures.

Metadata

Table 31:	Export from	Collaboratory	Software	Catalog:	UG4
-----------	-------------	---------------	----------	-----------------	-----

Category	Application
Tags	sp7 numerical-solver partial-differential-equations HPC
Partners	Johann Wolfgang Goethe Universität Frankfurt am Main <u>UFRA</u>
Maintainers	Konstantinos XYLOURIS
Homepage	http://gcsc.uni-frankfurt.de/simulation-and-modelling/ug4
Documentation	http://gcsc.uni-frankfurt.de/simulation-and-modelling/ug4
Support	konstantinos.xylouris@gcsc.uni-frankfurt.de
Download Page	http://gcsc.uni-frankfurt.de/simulation-and-modelling/ug4
License	LGPL
Current Version	1.0
All Versions	1.0





Description

UG4 is a powerful software framework for the simulation of complex PDE based systems on massively parallel computer architectures.





Product/Software Package/Service name: VisNEST

VisNEST is a tool for visualising neural network simulations of the macaque visual cortex.

Metadata

Table	32:	Export	from	Collaboratory	/ Software	Catalog:	VisNEST
Tubic	52.	Export		contaborator	Joitmaic	cutulog.	

Category	Tool
Tags	<u>sp7</u> <u>visualisation</u> <u>interactive-analysis</u>
Partners	Rheinisch-Westfälische Technische Hochschule Aachen <u>RWTH</u>
Maintainers	RWTH Aachen
Support	weyers@vr.rwth-aachen.de
License	Missing License
Current Version	1.0
All Versions	1.0

Description

VisNEST is a tool for visualising neural network simulations of the macaque visual cortex. It allows for exploring mean activity rates, connectivity of brain areas and information exchange between pairs of areas. In addition, it allows exploration of individual populations of each brain area and their connectivity used for simulation.

Reference paper: Nowke, Christian, Maximilian Schmidt, Sacha J. van Albada, Jochen M. Eppler, Rembrandt Bakker, Markus Diesrnann, Bernd Hentschel, and Torsten Kuhlen. "VisNEST—Interactive analysis of neural activity data." In Biological Data Visualization (BioVis), 2013 IEEE Symposium on, pp. 65-72. IEEE, 2013.





Product/Software Package/Service name: ViSTA

The ViSTA Virtual Reality Toolkit allows the integration of virtual reality (VR) technology and interactive, 3D visualisation into technical and scientific applications.

Metadata

Table 33: Export from Collaboratory Software Catalog: ViSTA

Category	Library
Tags	<u>sp7</u> <u>visualisation</u> <u>immersive-environments</u>
Partners	Rheinisch-Westfälische Technische Hochschule Aachen <u>RWTH</u>
Maintainers	RWTH Aachen
Support	info@vr.rwth-aachen.de
Source Code	https://github.com/HBPVIS/Vista
Download Page	http://sourceforge.net/projects/vistavrtoolkit/
License	LGPLv3
Current Version	1.15
All Versions	1.15

Description

The ViSTA Virtual Reality Toolkit allows the integration of virtual reality (VR) technology and interactive, 3D visualisation into technical and scientific applications. The toolkit aims to enhance scientific applications with methods and techniques of VR and immersive visualisation,





thus enabling researchers from multiple disciplines to interactively analyse and explore their data in virtual environments. ViSTA is designed to work on multiple target platforms and operating systems, across various display devices (desktop workstations, powerwalls, tiled displays, CAVEs, etc.) and with various interaction devices.





Product/Software Package/Service name: VIOLA

VIOLA (VIsualizer Of Layer Activity) is a tool to visualise activity in multiple 2D layers in an interactive and efficient way.

Metadata

Table 34: Export from Collaboratory Software Catalog: VIOLA

Category	Tool
Tags	<u>sp7</u> <u>visualisation</u>
Partners	Rheinisch-Westfälische Technische Hochschule Aachen <u>RWTH</u> Forschungszentrum Jülich GmbH <u>JUELICH</u>
Maintainers	<u>Benjamin WEYERS, RWTH Aachen</u> <u>Espen HAGEN, Forschungszentrum Jülich</u> <u>Johanna SENK, Forschungszentrum Jülich</u>
Homepage	https://github.com/HBPVIS/VIOLA
Documentation	https://github.com/HBPVIS/VIOLA/wiki
Support	weyers@vr.rwth-aachen.de
Source Code	https://github.com/HBPVIS/VIOLA
License	Missing License
Current Version	1.0
All Versions	1.0





Description

VIOLA (VIsualizer Of Layer Activity) is a tool to visualise activity in multiple 2D layers in an interactive and efficient way. It gives an insight into spatially resolved time series such as simulation results of neural networks with 2D geometry. The usage example shows how VIOLA can be used to visualise spike data from a NEST simulation (http://nest-simulator.org/) of an excitatory and an inhibitory neuron population with distance-dependent connectivity.





Product/Software Package/Service name: ZeroBuf

ZeroBuf implements zero-copy, zero-serialise, zero-hassle protocol buffers.

Metadata

Category	Library
Tags	<u>sp7</u>
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	EPFL Visualisation Team
Homepage	https://github.com/HBPVIS/ZeroBuf
Documentation	https://github.com/HBPVIS/ZeroBuf
Support	HBPVis@googlegroups.com
Source Code	https://github.com/HBPVIS/ZeroBuf
License	LGPL
Current Version	1.0
All Versions	1.0

Description

ZeroBuf implements zero-copy, zero-serialise, zero-hassle protocol buffers. It is a replacement for FlatBuffers, resolving the following shortcomings:





- Direct get and set functionality on the defined data members
- A single memory buffer storing all data members, which is directly serialisable
- Usable, random read and write access to the the data members
- Zero copy of the data used by the (C++) implementation from and to the network





Product/Software Package/Service name: ZeroEQ

ZeroEQ is a cross-platform C++ library to publish and subscribe for events.

Metadata

Category	library
Tags	sp7 HPC visualisation
Partners	École Polytechnique Fédérale de Lausanne <u>EPFL</u>
Maintainers	EPFL Visualisation Team
Contributors	RWTH Aachen URJC UPM
Homepage	https://github.com/HBPVis/zeq
Documentation	https://hbpvis.github.io/
Source Code	https://hbpvis.github.io/
License	LGPL
Current Version	0.2
All Versions	0.2





Description

ZeroEQ is a cross-platform C++ library to publish and subscribe for events. It provides the following major features:

- Publish events using zeq::Publisher
- Subscribe to events using zeq::Subscriber
- Asynchronous, reliable transport using ZeroMQ
- Automatic publisher discovery using Zeroconf
- Efficient serialisation of events using flatbuffers





Annex C: Summary - Platform Use Case Status

The HPC Platform specification deliverable D7.7.2 defines 16 use cases for the HPC Platform and links them to the Functional Requirements. These use cases and requirements have been defined at a very early project stage. In order to assess if these use cases still reflect the users' most urgent requirements, the HPC Platform team is in contact with some typical, exemplary user groups from different SPs, that already have computing time allocations for the HPC Platform systems, in order to evaluate and implement their complex workflows together with them. This strategy is beneficial for both, Platform team and users: The users are supported in using the Platform and in implementing and optimising their workflows for HPC. The Platform team gets to know about bugs in Core Platform Services, missing features of these services and about missing links to other Platforms and their services. The projects are described in more detail in Annex J: User Projects.

The first table below describes the status of the use cases as defined in D7.7.2 and if the collaboration with users revealed that an updating of the use cases is potentially necessary. All use cases will be evaluated at the beginning of SGA1 to align them better with the users' requirements and to update the use case descriptions. Since detailed descriptions of the use cases are available in D7.7.2, they are not repeated below.

The second table below shows the relation of the user projects to use cases and functional requirements (a brighter grey value corresponds with a weaker link between use cases/functional requirements and user projects).

Use Case ID	Status/comments	ID of Related Functional Requirements	Related Product/Software Package/Service	TRL at end of Ramp-Up Phase	Contributors
SP7-UC-001		SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006	Account management, Compute & storage services, maybe UNICORE (Portal) Documentation, User Support	TRL 3	WP7.5 T7.6.1
SP7-UC-002	Use case description potentially requires an update to better cover the aspect of interactive supercomputing	SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006	DLB, OmpSs Account management, Compute & storage services, maybe UNICORE (Portal) Documentation, User Support	TRL 4	T7.2.1, T7.2.3, T7.2.3 T7.3.1 T7.5.1 - T7.5.4, T7.5.7 T7.6.1
SP7-UC-003		SP7-FR-001, SP7-FR-002,	PyCOMPSs	TRL 8	т7.2.2

Table 37: Status of HPC Platform Use Cases





SP7-UC-004		SP7-FR-003, SP7-FR-004, SP7-FR-005 SP7-FR-001, SP7-FR-002, SP7-FR-004, SP7-FR-005	Account management, Compute & storage services Documentation, User Support Account management, Computing & storage services Documentation, User Support	TRL 4	WP7.5 T7.6.1 T7.5.1 - T7.5.4 T7.6.1
SP7-UC-005		SP7-FR-002, SP7-FR-004, SP7-FR-005	Account management, Compute & storage services Documentation, User Support	TRL 4	T7.5.1 - T7.5.4 T7.6.1
SP7-UC-006	Use case description potentially requires an update	SP7-FR-002, SP7-FR-004, SP7-FR-005	Cube, Extrae, Paraver, Scalasca, Score-P Account management, Compute & storage services Documentation, User Support	TRL 4	T7.2.4 T7.5.1 - T7.5.4 T7.6.1
SP7-UC-007	Use case description potentially requires an update	SP7-FR-001, SP7-FR-002, SP7-FR-006	DisplayCluster, ViSTA Account management, Visualisation systems booking form Documentation, User Support	TRL 3	WP7.3 T7.5.7 T7.6.1
SP7-UC-008	Use case description potentially requires an update	SP7-FR-001, SP7-FR-002, SP7-FR-006	InDiProv Account management, Compute & storage services, Visualisation systems booking form Documentation, User Support	TRL 3	WP7.3 WP7.5 T7.6.1
SP7-UC-009	Use case description potentially requires an update, e.g. to cover a simulation over a neuronal network rewiring where the user can analyse the evolution of the Model of Structural Plasticity and how inhibition influences the development of	SP7-FR-001, SP7-FR-002, SP7-FR-006	MSPViz, NeuroLOTs, NeuroScheme, RTNeuron Documentation, User Support	TRL 4	T7.3.2 T7.6.1





	new connections in the network.				
SP7-UC-010		SP7-FR-001, SP7-FR-002, SP7-FR-006	PyramidalExplorer/NeuroFiReS Account management, Compute & storage services Documentation, User Support	TRL 4	T7.3.2 T7.6.1
SP7-UC-011	Implemented: Remote visualisation is implemented using VirtualGL for desktop users, using DisplayCluster on high-resolution tiled display walls and Deflect-based streaming to DisplayCluster. All software deliverables are deployed in binary form on the visualisation cluster (ETHZ-CSCS) facility and as source code on github. Use case description potentially requires an update	SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006	DisplayCluster, Remote Connection Manager Account management, Cloud Storage, Compute & storage services Documentation, User Support Livre	TRL 7	WP7.3 WP7.5 T7.6.1
SP7-UC-012		SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007	TOUCH, TRANSFORMERS Account management, Cloud storage, Compute & storage services Documentation, User Support	TRL 4	T7.4.1 WP7.5 T7.6.1
SP7-UC-013		SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007	TRANSFORMERS Account management, Compute & storage services Documentation, User Support	TRL 4	T7.4.1 WP7.5 T7.6.1
SP7-UC-014		SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007	FLAT, RUBIK, SCOUT, TOUCH Account management, Compute & storage services Documentation, User Support	TRL 4	T7.4.1 WP7.5 T7.6.1





SP7-UC-015SP7-FR-001, SP7-FR-002, SP7-FR-007MonetDB Documentation, User SupportTRL 8T7.4.3SP7-UC-016Until end of March, our T-Storm prototype will support strong correlation and anti-correlation patterns both on streaming time series and on stored data. It will employ two different streaming indexes to support a wide variety of correlation measures (Pearson, Euclidean and Cosine, with a possibility of extension to other measures). The first index will be based on randomisation techniques, whereas the second will be based on dimensionality reduction using the Biscrete Fourier transform. A web service will be provided for getting the data in and out of the system. The whole T-Storm platform will be delivered in linux virtual machines that can be hosted at any.SP7-FR-001, SP7-FR-002, SP7-FR-002, SP7-FR-003, SP7-FR-002, SP7-FR-007T-Storm Account management, Compute & mage services Documentation, User SupportTRL 4, maybe TRL 5, without tests by T-R-1SP7-UC-016Until end of services to other measures). The first index will be based on randomisation techniques, whereas the second will be based on dimensionality reduction using the Biscrete Fourier transform. A web service will be provided for getting the data in and out of the system. The whole T-Storm platform will be delivered in linux virtual machines that can be hosted at any.SP7-FR-001, SP7-FR-002, SP7-FR-0						
SP7-UC-016Until end of March, our T-Storm prototype will support strong correlation and anti-correlation patterns both on streaming time series and on stored data. It will employ two different streaming indexes to support a wide variety of correlation measures (Pearson, Euclidean and Cosine, with a possibility of extension to other measures). The first index will be based on randomisation techniques, whereas the second will be based on dimensionality reduction using the Discrete Fourier transform. A web service will be provided for getting the data in and out of the system. The whole T-Storm platform will be delivered in Linux virtual machines that can be hosted at any compatible server.SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007T-Storm Account management, Compute & mage services Documentation, User SupportTRL 4,T7.4.2Trout without tests by real usersTo other measures, Pearson, Euclidean and out of the system. The whole T-Storm platform will be delivered in Linux virtual machines that can be hosted at any compatible server.SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-000, SP7-FR-007To storm Account management, Compute & mage services Documentation, User SupportTo data mage services mage services Documentation, User SupportTo data mage services mage services Documentation, User SupportTo data mage services mage service without tests by real usersTo data mage services mage serviceTo data mage service mage serviceT	SP7-UC-015		SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007	MonetDB Documentation, User Support	TRL 8	T7.4.3 T7.6.1
Lice case description requires an undate	SP7-UC-016	Until end of March, our T-Storm prototype will support strong correlation and anti-correlation patterns both on streaming time series and on stored data. It will employ two different streaming indexes to support a wide variety of correlation measures (Pearson, Euclidean and Cosine, with a possibility of extension to other measures). The first index will be based on randomisation techniques, whereas the second will be based on dimensionality reduction using the Discrete Fourier transform. A web service will be provided for getting the data in and out of the system. The whole T-Storm platform will be delivered in Linux virtual machines that can be hosted at any compatible server.	SP7-FR-001, SP7-FR-002, SP7-FR-003, SP7-FR-006, SP7-FR-007	T-Storm Account management, Compute & storage services Documentation, User Support	TRL 4, maybe TRL 5 without tests by real users	T7.4.2 WP7.5 T7.6.1

	SP7-UC-001	SP7-UC-002	SP7-UC-003	SP7-UC-004	SP7-UC-005	SP7-UC-006	SP7-UC-007	SP7-UC-008	SP7-UC-009	SP7-UC-010	SP7-UC-011	SP7-UC-012	SP7-UC-013	SP7-UC-014	SP7-UC-015	SP7-UC-016	SP7-FR-001	SP7-FR-002	SP7-FR-003	SP7-FR-004	SP7-FR-005	SP7-FR-006	SP7-FR-007
User project 1																							
User project 2																							
User project 3																							

Table 38: Relation of user projects to use cases and functional requirements





All SP7 use cases will be evaluated and updated at the beginning of SGA1. For these use cases that are not linked to any of the user projects it will be investigated if this is due to the choice of the projects or because they are actually not reflecting the actual requirements of neuroscientists. In addition, users' requirements that are currently not part of any of the 16 use cases will be used to define additional use cases and functional requirements.





Annex D: Summary - Service IT Resource Planning

Supercomputers are limited resources shared by several communities. Thus scientists need to apply for HPC compute and storage resources, and the applications are evaluated in a scientific and technical peer-review to allow for a fair distribution of the resources. Since the HBP does not own a supercomputer, the same applies to users of the HPC Platform. The following table describes which compute and storage resources are theoretically - subject to successful applications - available to the HPC Platform users.

More details about the application process and the upcoming calls for computing time are described in Annex K: Access to supercomputers.

More details about the compute and storage resources integrated in the HPC Platform are available in the HPC Platform Guidebook: https://hbp-hpc-platform.fz-juelich.de/?page_id=32

Resource	TRL	Data Storage Capacity available	Data Access Protocol(s)	Compute Resource(s) Available	Location of Resource	Compute Access Protocol(s)
JUQUEEN (IBM Blue Gene/Q system)	9	GPFS Home: 1.8 PB (total), 10 TB (user) Scratch: 5.3 PB (total) Archive: 1.2 PB (total) Data: 2.7 PB (total; requires additional application by user) (Shared between all systems at JSC)	SCP, UFTP	28 racks with 28,672 nodes and 458,752 cores IBM PowerPC® A2	Jülich Supercomputing Centre (JUELICH)	SSH, UNICORE Job scheduler: LoadLeveler
BlueBrain IV (IBM Blue Gene/Q system)	9	GPFS 128 TB of BlueGene Active Storage (BGAS) 4 PB shared filesystem	SCP, rsync	4 racks with 65,536 nodes IBM PowerPC® A2	Hosted by Swiss National Supercomputing Centre (ETHZ-CSCS)	SSH, UNICORE Job scheduler: Slurm
MareNostrum III (IBM iDataPlex system)	9	GPFS 2 PB disk storage Home, scratch and project directories	SCP, SFTP	52 racks with 3,056 main nodes and 42 heterogeneous nodes Main nodes (3,056 nodes): 2x Intel SandyBridge-EP E5- 2670/1600 20M 8-core at 2.6 GHz	Barcelona Supercomputing Centre (BSC)	SSH, UNICORE Job scheduler: LSF

Table 39: Resources available in the HPC Platform





				Xeon Phi nodes (42 nodes): 2x Intel SandyBridge-EP E5- 2670/1600 20M 8-core at 2.6 GHz 2x Xeon Phi 5110 P		
FERMI (IBM Blue Gene/Q system)	9	GPFS Home: 50 GB (project) Scratch: 900 TB (total), no project quota	SCP, SFTP	10 racks with 10,240 nodes and 163,840 cores IBM PowerPC® A2	Cineca	SSH, UNICORE Job scheduler: LoadLeveler
		Archive available				
Cloud S3 storage	7	460 TB available for HBP	Data access protocols: UNICORE, REST API Available S3 clients: <u>http://wiki.scc.kit.edu/lsdf/index.php/S3_on_</u> <u>WOS</u>		Karlsruhe Institute for Technology (KIT)	

The four supercomputers JUQUEEN (JUELICH-JSC), BlueBrain IV (hosted by ETHZ-CSCS), MareNostrum III (BSC) and FERMI (CINECA) are fully integrated into the HPC Platform. This means that they are integrated into the Authentication and Authorisation Infrastructure and into UNICORE. The feedback received from users of the HPC Platform after the internal Platform release has shown that in addition to these four systems, they also applied or plan to apply for computing time for three additional systems hosted because of these systems' architecture. Therefore, the integration of these systems into the HPC Platform has already started. They will become available as part of the Platform at the beginning of SGA1. The new systems and a brief overview of their architecture are provided in the table below. They will be included in the Guidebook as soon as their integration is finished.

Due to the availability of three additional systems it has been decided to drop the "HBP labels" that were until now used for the first four supercomputers in the Platform, i.e. "HBP Supercomputer" for JUQUEEN, "HBP Development System" for BlueBrain IV, "HBP Molecular Dynamics Supercomputer" for MareNostrum III and "HBP Massive Data Analytics Supercomputer" for FERMI.

Table 40: Additional supercomputers that will become part of the HPC Platform at the beginning of SGA1

Resource	TRL	Data Storage Capacity available	Data Access Protocol(s)	Compute Resource(s) Available	Location of Resource	Compute Access Protocol(s)
JURECA	9	GPFS Home: 1.8 PB (total), 10 TB (user)	SCP, UFTP	1872 nodes with 2 Intel Xeon E5-2680 v3 Haswell CPUs	Jülich Supercomputing Centre (JUELICH)	SSH, UNICORE Job scheduler: Slurm

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		Scratch: 5.3 PB (total) Archive: 1.2 PB (total) Data: 2.7 PB (total)* (Shared between all systems at JSC)		75 of them are additionally equipped with 2 two NVIDIA K80 GPUs 12 visualisation nodes with 2 NVIDIA K40 GPUs each		
Piz Daint (Cray XC30)	9	GPFS, Lustre (scratch) 2.5 PB system storage capacity Home: 86 TB (total), 10 GB (user) Project: 3.2 PB (total), 5 TB (group) Scratch: 2.7 PB (total), no quota Store: 2.6 PB (total), quota per contract	GridFTP	5,272 nodes with one Intel® Xeon® E5-2670 and one NVIDIA® Tesla® K20X	Swiss National Supercomputing Centre (ETHZ-CSCS)	SSH, UNICORE Job scheduler: Slurm
Pico	9	GPFS Home: 50 TB (total), 50 GB (quota) Scratch: 300 TB (total), no quota Archive available	SCP, SFTP	66 compute nodes (20 cores/node): Intel Xeon E5 2670 v2 @ 2.5 GHz 2 visualisation nodes (20 cores/node): Intel Xeon E5 2670 v2 @ 2.5 GHz 2 GPU NVIDIA K40 2 Big Mem nodes (16 cores/node): Intel Xeon E5 2650 v2 @ 2.6 GHz 1 GPU NVIDIA K20 4 BigInsight nodes (16 cores/node): Intel Xeon E5 2650 v2 @ 2.6 GHz 32 TB of local disk	Cineca	SSH, UNICORE Job scheduler: PBS





Annex E: Summary - Service Technology Readiness Levels (TRLs) Metrics

Platform Core Services

The target user count for the services below is difficult to determine since it depends a lot on the HPC demands of HBP researchers and of the general neuroscience community (after the release in M30). The number of projects that get computing time in an allocation period naturally limits the numbers of users of a supercomputer. Because of that, and since the systems are run in batch mode, the number of concurrent users is not an issue. The accounting mechanisms established at the HPC centres can deal with the usual number of users expected for the HPC systems.

The guidebook website and the web forms, e.g. for requesting support or access to the visualisation systems, are lightweight so that the number of concurrent users is also not a problem on the server side. Because of the purpose of these forms it is also unlikely that many users concurrently fill them out at the same time.

Product/Software Package/Service	Technology Readiness Level (TRL1-9)	Target User Count (TRL6+)	SLA Defined (TRL7+)	SLA Monitored (TRL7+)	SLA Enforced (TRL7+)	Comments
Account management	7	N/A	No	No	No	
Cloud storage	7	2000 concurrent connections	No	No	No	Limit of 2000 concurrent connections (uploads/downloads) to the back-end storage (1000 per WOS node)
Computing & storage services	9	N/A	Yes	Yes	Yes	
Computing time allocation (support form)	5 (request form) 9 (allocation processes)	N/A	No (request form) Yes (allocation processes)	No (request form) Yes (allocation processes)	No (request form) Yes (allocation processes)	The support request form has a TRL of 5. The underlying allocation processes established at the HPC centres and in PRACE have a TRL of 9.
Documentation (Guidebook)	6	N/A	N/A	N/A	N/A	The target user count for the Guidebook is hard to estimate since this website provides information on

Table 41: TRL of Platform Core Services





many levels and its usage and number of page visits depends a lot on how many users the HBP infrastructure in general will have in the next months and years.

Monitoring service	7	N/A	No	No	No	
Support	6	N/A	N/A	N/A	N/A	The HPC user support at the HPC centres has a TRL of 9. The TRL of 6 only refers to the specific, additional support offered to the HPC Platform users.
UNICORE	8	50	No	No	No	More testing under nominal load (~50 users) is expected
UNICORE Portal	7	10	No	No	No	UNICORE Portal is not a mandatory part of the core infrastructure. It is intended for a limited number of users and particular use cases.
UNICORE workflow engine	8	5	No	No	No	UNICORE Workflow engine is not a mandatory part of the core infrastructure. It is intended for a limited number of users and particular use cases.
Visualisation systems: bo form	oking 3-4	N/A	N/A	N/A	N/A	Integrated in M29

Legend:

Target User Count (TRL6+) - Target user counts (concurrent service users).

SLA Defined - The software documentation defines some Quality of Service metrics in the service documentation. These metrics may or may not be enforced by the service itself. The service has not been tested to adhere to the documented QoS metrics.

SLA Monitored - The Quality of Service metrics are monitored by a monitoring service.

SLA Enforced - The Quality of Service metrics are enforced by implementing service. If the SLA Definition indicates on 3 API/request/sec/user, there are suitable mechanisms implemented in the service to ensure these limits are not exceeded.





Annex F: Backlog (Remaining bugs and new features to be added)

Bugs

Platform Core Services

Table 42: Known bugs of Platform Core Services

Software/Service	Bug	Short Description	Related Use Case(s) or FR(s)	Status & Comments
Cloud storage	UNICORE Portal access to Cloud	There was a UNICORE issue with creating a new Storage Management System (SMS) from the UNICORE portal (only possible from the UNICORE clients). This was necessary to access the S3 storage via the portal.	SP7-FR-002, SP7-FR-006	Solved in UNICORE Portal release v2.1

Software and Services

Table 43: Known bugs of software and services

Software/Service	Bug	Related Use Case(s) or FR(s)	Status & Comments
Cube	No known or reported bugs	SP7-UC-006 SP7-FR-005 (installation of performance tools)	Open issues and special requirements documented in file "OPEN_ISSUES" packaged with software distribution
Deflect Client Library	No known or reported bugs		List of known issues: <u>https://github.com/BlueBrain/Deflect/issue</u> <u>S</u>
DisplayCluster	No known or reported bugs	SP7-UC-007, SP7-UC-011	List of known issues: <u>https://github.com/BlueBrain/DisplayCluste</u>





		SP7-FR-001	<u>r/issues</u>
DLB	No known or reported bugs	SP7-UC-002	BSC uses internal TRAC for bug reports
Equalizer	No known or reported bugs		List of known issues: https://github.com/Eyescale/Equalizer/issu es
Extrae	No known or reported bugs	SP7-UC-006 SP7-FR-005	An internal shared document is used for reporting bugs
FLAT	No known or reported bugs	SP7-UC-014 SP7-FR-007	
HCFFT	No known or reported bugs		
InDiProv	See HBPVis group on GitHub (issue list) https://github.com/HBPVIS/InDiProv	SP7-UC-008	
Livre	List of known bugs and issues: https://github.com/BlueBrain/Livre/issues?q =is%3Aissue+is%3Aopen+label%3Abug	SP7-UC-011	
MonetDB	MonetDB Server crashes on concurrent schema operations	SP7-UC-015 SP7-FR-007	
Monsteer	No known or reported bugs		List of known issues: <u>https://github.com/BlueBrain/Monsteer/issu</u> <u>es</u>
MSPViz	No known or reported bugs	SP7-UC-009 SP7-FR-001, SP7-FR-002, SP7-FR-006	
NeuroLOTs	No known or reported bugs	SP7-UC-009	





NeuroScheme	No known or reported bugs	SP7-UC-009	
OmpSs	No known or reported bugs	SP7-UC-002 SP7-FR-005	BSC uses internal TRAC for bug reports
Paraver	No known or reported bugs	SP7-UC-006 SP7-FR-005	BSC uses internal bug tracker
PyCOMPSs	No known or reported bugs	SP7-UC-003 SP7-FR-005	BSC uses internal TRAC for bug reports
PyramidalExplorer/ NeuroFiReS	No known or reported bugs	SP7-UC-010	
Remote Connection Manager (RCM)	No known or reported bugs	SP7-UC-011	
RTNeuron	No known or reported bugs	SP7-UC-009	
RUBIK	No known or reported bugs	SP7-UC-014 SP7-FR-007	
Scalasca	No known or reported bugs	SP7-UC-006 SP7-FR-005 (installation of performance tools)	Open issues and special requirements documented in file "OPEN_ISSUES" packaged with software distribution
Score-P	No known or reported bugs	SP7-UC-006 SP7-FR-005 (installation of performance tools)	Open issues and special requirements documented in file "OPEN_ISSUES" packaged with software distribution
SCOUT	No known or reported bugs	SP7-UC-014 SP7-FR-007	
тоисн	No known or reported bugs	SP7-UC-012, SP7-UC-014	





		SP7-FR-007	
TRANSFORMERS	No known or reported bugs	SP7-UC-012, SP7-UC-013	
		SP7-FR-007	
T-Storm	No known or reported bugs		
UG4	No known or reported bugs		
VisNEST	No known or reported bugs	SP7-FR-001	
ViSTA	No known or reported bugs	SP7-UC-007	For the future a bug tracker integration on
		SP7-FR-001	Gittab is plained
VIOLA	See HBPVis group on GitHub (issue list) https://github.com/HBPVIS/VIOLA		List of known issues: https://github.com/HBPVIS/VIOLA/issues
ZeroBuf	No known or reported bugs		List of known issues: https://github.com/HBPVIS/Zerobuf/issues
ZeroEQ	No known or reported bugs		List of known issues: https://github.com/HBPVIS/zeq/issues

Features

Platform Core Services

Table 44: Planned features for Platform Core Services

Software/Service	Feature	Short Description	Necessary for Use Case(s) or FR(s)	Status & Comments
Account management	Web service for automated HPC project and account creation	A central service for creating HPC projects with a computing time grant in the HPC Platform and adding registered users to these projects from	SP7-UC-001 SP7-FR-001, SP7-FR-002,	Details still need to be discussed in WP7.5.







		the Collaboratory needs to be implemented. The service could be accessed from Collaboratory apps, when principal investigators register their approved HPC projects and add collaborators to their projects or when users apply for becoming members of an HPC project.	SP7-FR-003	account management workflow into the Collaboratory.
	Full implementation of the account management workflow	Deal with account and project deletion and automatic propagation of account data changes such as addresses, SSH keys or project membership. This implementation is expected to be finished towards the end of 2016.	SP7-UC-001 SP7-FR-001, SP7-FR-002, SP7-FR-003	
Cloud storage	Per-user storage quota management	A per-user storage quota management (only per bucket) is not available yet, but DataDirect Networks (DDN, http://www.ddn.com) is working on this feature, which will be available in the next release, planned for the second quarter 2016.	SP7-FR-001, SP7-FR-002, SP7-FR-006	Planned for second quarter of 2016 in collaboration with DDN

Software and Services

Table 45: Planned features of software and services

Software/Service	Feature	Short Description	Necessary for Use Case(s) or FR(s)	Status & Comments
Cube	New features planned but out of the scope of HBP			New developments externally funded
Deflect Client Library	New features planned			No details available
DisplayCluster	New features planned			No details available
DLB	 Holistic Dynamic Resource Management (M18) 	Define and implement different levels of malleability APIs in the different schedulers of the system, so they can exchange information	SP7-UC-002	For more details see WP7.4 workplan for SGA1





	 New scheduling policies for neuroscience application's requirements (M22) 	among themselves towards obtaining a holistic resource management. Generic policies that will be considered (but not limited to) are: optimisation of the execution time for a single application or for a group of applications, minimisation of data movements when executing an application to exploit data locality, maximisation of node utilisation or maximisation of the whole system's throughput. Besides, policies defined from the specific use cases of neuroscience		
		where several HBP simulators will interact) will be also defined, to achieve particular objectives for them.		
Equalizer	Features needed for sort-last rendering in Livre			
Extrae	Java application instrumentation (using AspectJ and JVMTI)	Extrae will include capabilities to instrument automatically Java functions in a Java code, by using the frameworks AspectJ and JVMTI, which enable code interception. Once instrumented, applications will be able to generate trace files and analysed later with the Paraver performance analysis tools.	SP7-UC-006 SP7-FR-005	Included in Extrae implementation roadmap
FLAT	No new features planned			
HCFFT	More variants for dimension- adaptivity			
InDiProv	No new features planned			
Livre	New features planned			No details available
MonetDB	No new features planned in the			





	context of HBP			
Monsteer	Support for closed loop simulations (coupling of robot and brain simulations)			
MSPViz	New features will be developed in SGA1.			On-going modifications to measure the behaviour and detect possible bottlenecks in different visualisation pipelines.
NeuroLOTs	New features will be developed in SGA1.			
NeuroScheme	New features will be developed in SGA1.			
OmpSs	 Efficient reductions in tasks Tasks with automatic checkpoint/restart OmpSs at cluster, with automatic load balance 	Essentially, with reductions results are stored in partial variables to avoid thread contention, and later a final accumulation is done when a synchronisation point is reached. Efficient reductions will be available shortly, and presented to the OpenMP Committee to be introduced in the OpenMP 5.0 standard. In addition, tasks with checkpoint will be investigated (automatic checkpoint/restart of tasks). Finally, the OmpSs version at clusters will be studied to be able to balance the load automatically (send tasks to other nodes via gasnet).	SP7-UC-002 SP7-FR-005	References for the new features mentioned are: <u>http://dx.doi.org/10.1007/978-3-</u> <u>319-24595-9_14</u> and <u>http://dx.doi.org/10.1007/978-3-</u> <u>319-11454-5_1</u>
Paraver	 Timeline view for punctual information Improvements in basic CFGs 	Different enhancements will be performed in order to improve the Quality of Experience from the end user perspective. In particular, not only the graphical user interface will be improved, but also the related documentation	SP7-UC-006 SP7-FR-005	Included in Paraver's development roadmap





	Extend DocumentationEnable zoom in timeline with mouse wheel	and the configuration files which are a common way to work with Paraver.		
PyCOMPSs	 Enhanced support for multi- scale simulations Add scheduling policies Integration of persistent objects Integration with Docker 	We will enhance the support to multi-scale simulations with feedback from the users (September 2016). In addition we will add scheduling policies, which take into account total energy, performance and cost for the execution of a COMPSs application (November 2016), the integration of persistent objects in the runtime (objects that last after the execution is over) (July 2016), and the integration with new Docker container technologies (July 2016).	SP7-UC-003 SP7-FR-005	Included in PyCOMPSs development roadmap, to deliver on next release
PyramidalExplore r/ NeuroFiReS	New features will be developed in SGA1.			Details depend on future funding
Remote Connection Manager (RCM)	No new features planned			
RTNeuron	New features planned			
RUBIK	No new features planned			
Scalasca	New features planned but out of the scope of HBP			New developments externally funded
Score-P	New features planned but out of the scope of HBP			New developments externally funded
SCOUT	No new features planned			
тоисн	No new features planned			





TRANSFORMERS	No new features planned	
T-Storm	No new features planned	
UG4	Improvement in user-friendliness, additional features for scaling studies on large HPC systems.	
VisNEST	Conceptual basis for planned multi- view framework in SGA1	
ViSTA	No new features planned	
VIOLA	New features planned	The choice of new features is user- driven in a co-design approach
ZeroBuf	JSON schema support	
ZeroEQ	HPC machine support Remote management protocol	





Annex G: IPR Status, Ownership and Innovation Potential

Table 46: IRP status, ownership and innovation potential of software and services

Product/Software Package/Service	IPR Status*	Owner(s)	Non-HBP users**	Innovation Potential***
Cube	Open Source	Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH	Installed and used at dozens of HPC centres and companies worldwide	In daily use by application developers and HPC support personal for the performance analysis of HPC applications in general
Deflect Client Library	Open Source		BBP, Kaust, TACC. OSS licensed	Client library for DisplayCluster
DisplayCluster	Open Source		BBP, Kaust, TACC. OSS licensed	Collaborative, interactive tiled display walls for team work on complex data
DLB	Open Source	Barcelona Supercomputing Centre	Other research projects where BSC is taking part	As a general purpose tool, it has huge potential to be applied to many different scenarios outside the HBP
Equalizer	Open Source		Commercial and research users worldwide, e.g. Dassault, University of Zurich, Electronic Visualization Lab at UIC	Any parallel OpenGL application
Extrae	Open Source	Barcelona Supercomputing Centre	Many different stakeholders from BSC (private & public companies, as well as project partners)	As a general purpose tool, it has huge potential to be applied to many different scenarios outside the HBP
FLAT	Open Source	EPFL-DIAS	No non-HBP users	
HCFFT	Free license for non-commercial	Fraunhofer SCAI	Academic license	




	purpose			
InDiProv	Open Source	RWTH Aachen	No non-HBP users	
Livre	Open Source		BBP, University of Zurich	
MonetDB	Open Source	DA group of CWI	Open Source, so anyone can use it	It can be used in any scientific application
Monsteer	Open Source		BBP	Non-commercial framework for interactive supercomputing.
MSPViz	To be defined	Universidad Politécnica de Madrid	No non-HBP users	Yes
NeuroLOTs	To be defined	Universidad Rey Juan Carlos	No non-HBP users	Yes
NeuroScheme	To be defined	Universidad Rey Juan Carlos	No non-HBP users	Yes
OmpSs	Open Source	Barcelona Supercomputing Centre	Many different stakeholders from BSC (private & public companies, as well as project partners)	As a general purpose tool, it has huge potential to be applied to many different scenarios outside the HBP
Paraver	Open Source	Barcelona Supercomputing Centre	Many different stakeholders from BSC (private & public companies, as well as project partners)	As a general purpose tool, it has huge potential to be applied to many different scenarios outside the HBP
PyCOMPSs	Open Source	Barcelona Supercomputing Centre	Many different stakeholders from BSC (private & public companies, as well as project partners)	As a general purpose tool, it has huge potential to be applied to many different scenarios outside the HBP
PyramidalExplorer/ NeuroFiReS	To be defined	Universidad Rey Juan Carlos	No non-HBP users	Yes
Remote Connection Manager	Open Source	Cineca	Cineca HPC users	

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(RCM)				
RTNeuron	Proprietary, open source planned			
RUBIK	Open Source	EPFL-DIAS	No non-HBP users	
Scalasca	Open Source	Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH	Installed and used at dozens HPC centres and companies worldwide	In daily use by application developers and HPC support personal for the performance analysis of HPC applications in general
Score-P	Open Source	JSC, TU Dresden, RWTH Aachen, TU München, TU Darmstadt, GNS Braunschweig	Installed and used at dozens HPC centres and companies worldwide	In daily use by application developers and HPC support personal for the performance analysis of HPC applications in general
SCOUT	Open Source	EPFL-DIAS	No non-HBP users	
ТОИСН	Open Source	EPFL-DIAS	No non-HBP users	
TRANSFORMERS	Open Source	EPFL-DIAS	No non-HBP users	
T-Storm	Open Source	Technical University of Crete, SoftNet Lab	Also employed for financial stream analytics (QualiMaster, EU STREP)	Real-time financial stream analysis
UG4	Open Source	Consortium of developers lead by G-CSC, University of Frankfurt	Yes	Too early to be considered.
VisNEST	Closed Source	RWTH Aachen	Yes	
ViSTA	Open Source	RWTH Aachen	Yes	Yes, non-commercial
VIOLA	Open Source	RWTH Aachen	Yes	





ZeroBuf	Open Source	Open Source: non-HBP users are possible	Non-commercial library for zero- copy serialisable objects
ZeroEQ	Open Source	BBP. OSS licensed	Non-commercial library for pub- sub and web service for all C++ applications

* IPR Status: Open Source, Copyright, Patent, Trade Secret, pre-IPR (i.e. you intend to obtain some form of IPR in the future)

** If this product/software package/service is currently being used outside HBP (e.g. donated, loaned, licensed, sold), please specify by whom.

*** Innovation Potential: Potential practical applications beyond HBP, commercial and/or non-commercial.





Annex H: Quality and testing strategies for software and services

Table 47: Quality and testing strategy for software and services

Software/Service	Software quality and testing strategy
Cube	Continuous integration, automated build testing, manual execution testing, code review
Deflect Client Library	Code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
DisplayCluster	Code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
DLB	Continuous integration using GIT. Jenkins server configured for testing. Each time a push is made to the repository, both compilation and a set of tests are checked, in different machines with different configurations. When everything is correct, a source code pack is generated and uploaded to the website.
Equalizer	Code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
Extrae	Continuous integration with SVN. We include regression tests (to ensure functionality is not broken with changes) and overhead tests (to determine the cost of using Extrae)
FLAT	Manual testing, code reviews, deploying/support on different platforms
HCFFT	Application on model problems
InDiProv	Version control (Git), Open Source, GitHub (<u>https://github.com/HBPVIS/InDiProv</u>)
Livre	Code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
MonetDB	Automated testing





Monsteer	CI of compilation through Jenkins, 100% code reviewed
MSPViz	Continuous integration, code review
NeuroLOTs	Continuous integration, code review
NeuroScheme	Continuous integration, code review
OmpSs	Continuous integration using GIT. Jenkins server configured for testing. Each time a push is made to the repository, both compilation and a set of tests are checked, in different machines with different configurations. When everything is correct, a source code pack is generated and uploaded to the website.
Paraver	Continuous integration (new features always merged to the main branch), manual testing (developers and performance tools group members)
PyCOMPSs	Continuous integration with SVN. New developments made in auxiliary branches in SVN (while developing and debugging). Then, when the capabilities are solid, we add them in the main development branch. We do manual testing (developers) and automated testing (using Jenkins for UnitTests, local tests, VM and package creation tests, cloud tests).
PyramidalExplorer/ NeuroFiReS	Continuous integration, code review
Remote Connection Manager (RCM)	Manual testing
RTNeuron	Code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
RUBIK	Manual testing, code reviews, deploying/support on different platforms
Scalasca	Continuous integration, automated build testing, manual execution testing, code review
Score-P	Continuous integration, automated build testing, manual execution testing, code review





SCOUT	Manual testing, code reviews, deploying/support on different platforms
ТОՍСН	Manual testing, code reviews, deploying/support on different platforms
TRANSFORMERS	Manual testing, code reviews, deploying/support on different platforms
T-Storm	
UG4	We use automatic testing, but the main issue is, that solutions of the generalised model must coincide with solutions already accepted by simpler models in the respecting limit cases.
VisNEST	Version Control (SVN), BuildServer for continuous delivery, Migration to GitLab offering Version Control, BuildServer, Bugtracker etc. planned for the next weeks, User Tests on immersive Hardware
ViSTA	Version Control (SVN), BuildServer for continuous integration, Migration to Git based repository in progress offering Version Control, BuildServer, Bugtracker etc., Partial Tests Harness, User Test on immersive Hardware, Release Definition
VIOLA	OpenSource, Git Version Control
ZeroBuf	High code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs
ZeroEQ	High code coverage using unit and integration tests, enforced 100% test success through Jenkins CI, enforced code review through github PRs





Annex I: User feedback received in M18-M30 for software and services

Table 48: Key feedback received in M18-M30 for software and services

Software/Service	Summary of key feedback received	Additional information
Cube	None	
Deflect Client Library	None	https://github.com/BlueBrain/Deflect/issues
DisplayCluster	Robust, usable feature set compared to alternatives	Feedback received during interactive demonstrations. List of known issues: <u>https://github.com/BlueBrain/DisplayCluster/issues</u>
DLB	Very interesting that balance improvements are transparent to the user. Both code developers and machine owners (vendors) shown little interest in the beginning of the Ramp- Up Phase, but this has significantly changed between M18-M30 (as it is demonstrated by the continuation of this work in SGA- 1).	Feedback received through co-design with code developers and machine owners/vendors. BSC uses a private TRAC as ticket system. Mailing list for users: <u>pm-tools@bsc.es</u>
Equalizer	None	https://github.com/Eyescale/Equalizer/issues
Extrae	The tool enables tracing without changing the source code	Feedback received through co-design with users. BSC-internally shared document for bug tracking. Mailing list for users: <u>tools@bsc.es</u>
FLAT	None	FLAT is currently only used internally.
HCFFT	None	Feedback received by email to the developers.
InDiProv	None	https://github.com/HBPVIS/InDiProv





Livre	None	https://github.com/BlueBrain/Livre/issues
MonetDB	None	
Monsteer	Easy to use alternative for streaming data out of a NEST simulation running on a supercomputer and injecting stimulus modifications	Feedback received by email and in videoconferences with the users. List of known issues: <u>https://github.com/BlueBrain/Monsteer/issues</u>
MSPViz	Currently under user study evaluation. Tested by neuroscientist form JUELICH.	Feedback received in emails, during demos and in meetings with users.
NeuroLOTs	General positive feedback with some issues that need to be tackled	Feedback received in emails and during videoconferences with users.
NeuroScheme	Currently under user study evaluation. Being used at the EPFL's tiled display wall.	Feedback received in emails and during demos.
OmpSs	Main advantage of OmpSs as compared to OpenMP is the higher dynamicity to change the number of threads at runtime. Also some users have shown interest in being able to run OmpSs at Windows platforms (currently not supported).	Feedback received through co-design with users. BSC uses a private TRAC as ticket system. Mailing list for users: <u>pm-tools@bsc.es</u>
Paraver	The tool shows many interesting details and low-level metrics inside a node	Feedback received through co-design with users. Mailing list for users: <u>tools@bsc.es</u>
PyCOMPSs	Very nice tool to create high-level workflows in a programmatical way. Python support is very important in the neuroscience community. Interest in the integration of PyCOMPSs with new datastores, making its usage transparent for end users. Interest in activating/deactivating COMPSs in an easy manner in the code.	Feedback received through co-design with users. BSC uses a private TRAC as ticket system. Mailing list for users: <u>support-compss@bsc.es</u>
PyramidalExplorer/ NeuroFiReS	Positive feedback, developed using user-centred design	Feedback received in continuous contact with users, mainly by email.





Remote Connection Manager (RCM)	None		
RTNeuron	None		
RUBIK	None		RUBIK is currently only used internally.
Scalasca Score-P	•	Tool support helped scaling CoreNeuron to full JUQUEEN at an Extreme Scaling Workshop @ JUELICH- JSC, developers returned to 2nd workshop with multiple codes Developers used the tools for multiple applications, which resulted in multiple feature requests and support inquires Tool support helped scaling CoreNeuron to full JUQUEEN at an Extreme Scaling Workshop @ JUELICH- JSC, developers returned to 2nd workshop with multiple codes Developers used the tools for multiple applications, which resulted in multiple feature requests and support inquires	 HBP users were in continuous contact with JUELICH-JSC by email and several Skype calls HBP users attended the Extreme Scaling Workshop at JUELICH-JSC Developers made feature requests and asked for support via mailing lists Mailing list: scalasca@fz-juelich.de HBP users were in continuous contact with JUELICH-JSC by email and several Skype calls HBP users attended the Extreme Scaling Workshop at JUELICH-JSC Developers made feature requests and asked for support via mailing lists HBP users attended the Extreme Scaling Workshop at JUELICH-JSC Developers made feature requests and asked for support via mailing lists Mailing list: support@score-p.org
SCOUT	None		SCOUT is currently only used internally.
ТОՍСН	None		TOUCH is currently only used internally.
TRANSFORMERS	None		TRANSFORMERS is currently only used internally.
T-Storm	None		
UG4	None		





VisNEST	None	
ViSTA	None	Tracking on GitLab planned Mailing list: <u>vista-dev@lists.rwth-aachen.de</u>
VIOLA	Suitable approach for layered neural simulation model, especially addressing the web-based implementation	Feedback received through co-design with users. List of known issues: <u>https://github.com/HBPVIS/VIOLA/issues</u>
ZeroBuf	None	List of known issues: <u>https://github.com/HBPVIS/Zerobuf/issues</u>
ZeroEQ	Easy to use, robust, patches for new platforms	Feedback received through github pull requests and during interactive demos
		List of known issues. <u>https://github.com/hbr/vis/2eq/issues</u>





Annex J: User Projects

The user projects are collaborations between HBP users that have HPC computing time allocations and relevant scientists and developers of the HPC Platform. The projects represent different neuroscientific research areas varying from simulations of spiking neural networks to data analysis and image processing.

The user projects are beneficial for both the HPC Platform and its users: The HPC Platform receives direct feedback on bugs, missing but required features, and links to other SPs that need to be improved. This also helps to verify the use cases that were defined in the HPC Platform Specification Deliverable D7.7.2 (M6). The users are supported in integrating their workflows into the HPC Platform and in using the supercomputers, which allows them to use their computing time allocations as efficiently and effectively as possible.

The user projects were defined in December 2015. The implementation of the projects started in January 2016. It is planned to have first parts of the projects finished by the end of the Ramp-Up Phase. Other parts depend on developments that will only become available in the course of SGA1 so that work on the projects will continue in SGA1. As an example the implementation of a provenance tracking for UNICORE workflows is developed outside the HBP; a first release is currently scheduled for summer 2016. The collaborations between users and HPC Platform will become even stronger in SGA1 as some of the users involved in the projects will become members of SP7 in SGA1 to allow for an even better collaboration.

The first three user projects are fully described (see below for details). The definition of another two projects started in February 2016. The topics of these projects will be "Data mining for characterising disease pathways" (collaboration with SP8) and a circuit simulation based on Neuron (collaboration with SP6). The implementation will start as soon as these projects are fully described, which includes among other points requirements from both sites, i.e. HPC Platform and users, issues to be solved, potential solutions, and a timeline for the implementation. The HPC Platform Guidebook will be updated with the descriptions of these additional use cases soon.

It is expected that more projects will be started in the context of the Co-Design Projects (CDP) at the beginning of SGA1. The HPC Platform will mainly contribute to the following CDPs and support the scientists in using HPC:

- CDP1 "Development of Whole Mouse Brain Model and related Mouse Brain Atlas"
- CDP3 "Multi-Level Human Brain Atlas"
- CDP5 "Plasticity, Learning and Development: Modelling the Dynamic Brain"

The CDPs will need supercomputers for processing and analysing datasets and for brain simulations. The specific requirements of the CDPs will be taken into account for the future development of the HPC Platform.





Project 1: Comparative data analysis between experiment, HPC and neuromorphic systems (NEST-SpiNNaker-Elephant)

Collaborating SPs and scientists:

- SP5: Michael DENKER, Sonja GRÜN, Pietro QUAGLIO, Vahid ROSTAMI, Alper YEGENOGLU (JUELICH)
- SP6: Markus DIESMANN, Jakob JORDAN, Johanna SENK (JUELICH)
- SP7: WP7.3 (Benjamin WEYERS, RWTH) and WP7.5 (mainly Carsten KARBACH and Bernd SCHULLER (JUELICH), Cristian MEZZANOTTE (ETHZ))
- SP9: David LESTER, Andrew ROWLEY (UMAN), Andrew DAVISON (CNRS), Björn KINDLER (UHEI)

Leadership: Sonja GRÜN (scientific lead) and Bernd SCHULLER (technical lead)

A NEST-Elephant demo organised by members from SP5 and SP6 at the HBP Summit 2015 successfully showed how a NEST simulation and a subsequent analysis of the results with Elephant could be started through the Collaboratory. However, simulation and analysis were not yet running on a system like HPC or neuromorphic (NMS) hardware. Members from SP7 presented in another demo at the same Summit how a job on an HPC system could be started from the Collaboratory through the integrated UNICORE Portal.

The goal of this project is to combine these two demos, i.e. to implement as a first use case a workflow that allows to start a NEST simulation through the Collaboratory on different backends (HPC or NMS) and to analyse the results with Elephant. This way it can be evaluated for the first time if the HPC and the NM implementations of NEST lead to the same results when simulating the same model. An additional, more complex use case of this project will be to also analyse experimental data and to compare it with simulation results.

The implementation of this user project will happen in two phases (see figures below). The implementation of the first use case is planned for the next couple of months (end of the Ramp-Up Phase and beginning of SGA1); the second use case will be implemented in a second step and merged with the overall workflow.

The HPC Platform is working on the implementation and/or improvement of the following points that are important for this project:

- Provenance tracking for entire workflows started from the Collaboratory and running on HPC systems
- Mechanism for uploading (experimental) datasets and for transferring results from NM systems to an HPC storage (for analysing large datasets) or to the storage of a Collab (for analysing smaller datasets) for the analysis with Elephant
- Visualisation of the analysis results
- Using the UNICORE REST API for starting HPC jobs from the Collaboratory





It is also planned to investigate using PyCOMPSs (WP7.2) as a parallelisation engine to enable trivial parallelisation of advanced analysis routines, which would allow the analysis of significantly larger datasets directly on a supercomputer.



Figure 2: NEST-Elephant workflow implementation phase 1







Figure 3: NEST-Elephant workflow implementation phase 2





Project 2: UNICORE-based 3D-Polarized Light Imaging and data sharing workflow

Collaborating SPs and scientists:

- SP2: Markus AXER and his Fibre Architecture group (JUELICH)
- SP7: WP7.5 (mainly Oliver BÜCKER, André GIESLER, Carsten KARBACH, Bernd SCHULLER (JUELICH), Cristian MEZZANOTTE (ETHZ))

Leadership: Markus AXER (scientific lead) and Oliver BÜCKER (technical lead)

3D-Polarized Light Imaging (3D-PLI) is a technique used to extract the orientation of nerve fibres at micrometre scale. Two different setups at the Institute of Neuroscience and Medicine (INM-1), Forschungszentrum Jülich are being used for the imaging.

A human brain is cut into about 2500 sections that are imaged using 3D-PLI microscopy, which results in about 1.3 micron pixel size and 80,000 x 100,000 pixels per section. The polarisation filters used in the imaging process are rotated 18 times so that 18 different images per section are available. The mentioned resolution and the 18 images result in a memory consumption of about 750 GB/section for the raw data, which is then transferred to the storage of the HPC systems at Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich. The supercomputer JURECA is used to run the complex workflow that extracts the fibre orientations (3D vector per pixel) from the raw data. This analysis is not based on staining on the images but it uses the birefringence of the myelin sheaths that shield the axons of nerve fibres. Most tools in the workflow are developed at Forschungszentrum Jülich in the Fibre Architecture group led by Markus AXER and in close collaboration with Oliver BÜCKER and the Simulation Laboratory Neuroscience (both JSC). To speed up the workflow, it has been implemented using the UNICORE workflow engine (supported by André GIESLER, JSC), which allows analysing a section in the order of hours instead of weeks.

The goal of this use case project is now to integrate the existing UNICORE workflow (see figure below) into the infrastructure of the HBP. The HPC Platform is working on the implementation and/or improvement of the following points that are important for this project:

- Using the UNICORE provenance tracking mechanism (under development at JSC) and linking it with the Collaboratory mechanisms,
- Establishing access mechanisms to the HPC storage for non-HPC users to enable sharing of results.

It is planned to have the access mechanisms ready before the end of the Ramp-Up Phase. A first release of the UNICORE provenance tracking is planned for summer 2016; the Fibre Architecture group already started preparing workflow and tools for it. The viewer integration is planned for the beginning of SGA1; a locally running viewer is already available.









Figure 4: UNICORE-based Polarized Light Imaging workflow





Project 3: Machine learning workflow and interactive supercomputing for high-resolution image datasets

Collaborating SPs and scientists:

- SP5: Timo DICKSCHEID, Philipp GLOCK (JUELICH)
- SP7: WP7.5 (mainly André GIESLER, Björn HAGEMEIER (JUELICH), Cristian MEZZANOTTE (ETHZ))

Leadership: Timo DICKSCHEID (scientific and technical lead)

The goal of this project is the implementation of a workflow for texture analysis in high-resolution imaging data for the brain atlas that is based on machine learning. It is part of a larger analysis workflow, i.e. the results of this project are intermediate results of the larger workflow and not meant to be provided directly to "end users". The results must be quality-checked by humans before they can be processed further in the larger workflow. It is planned to realise this manual interaction through a web-based viewer. It can also be used to improve the learning algorithm. When the result is approved, it should be possible to signal this to the larger workflow so that it can continue automatically.

The HPC Platform is working on the implementation and/or improvement of the following points that are important for this project:

- Required infrastructure: storage that is accessible for the HPC system on which the data is produced, for the viewer and for web server(s) used to transfer the data
- Integrating a viewer for HDF5 files that serve as the main file format for high-resolution
- Investigating the viewer integration into the Collaboratory
- Provenance tracking of the workflow using the UNICORE provenance tracking as soon as this is available and linked to the other provenance tracking mechanisms in the HBP

The access mechanisms to HPC storage will be implemented in the next months. The implementation of the UNICORE workflow is planned to start in March. The provenance tracking based on UNICORE can only be implemented starting in summer 2016 when the UNICORE provenance tracking mechanism is deployed. For the machine learning implementation, usage of PyCOMPS will be assessed.





Annex K: Access to supercomputers

The supercomputers that are part of the HPC Platform are publicly funded and thus scientists do not need to pay for using them. Since the users of such HPC systems are demanding more compute resources than actually available - core hours are a limited resource - the HPC centres have application processes in place that distribute resources to these projects that can benefit most from using them. SP7 is ready to support users in writing their applications and in getting started with HPC.

The application for HPC resources usually consists of the following steps. A description of how to start using HPC is available in the Guidebook: <u>https://hbp-hpc-platform.fz-juelich.de/?page_id=732</u>

Computing time application workflow	Support and actions by HPC Platform
(1) A call for proposals is opened, usually including a template to be used for the application. This template both asks for the scientific background and goals of the project, and for the technical details of the software to be used on the HPC system (proof of scalability on the respective system, type of parallelisation, memory consumption, storage consumption, I/O behaviour)	The HPC Platform Guidebook contains a list of all upcoming calls for the integrated systems (see also below). The HPC Platform team is ready to help users decide which system to use and which call to answer. A contact form will be integrated in the HPC Collab before the end of the Ramp-Up Phase that serves as a single point of contact for users who need assistance in applying for HPC resources.
(2) A PI writes an application for the project using the template provided and submits it to the HPC site.	The experts of all four HPC sites are ready to provide support in writing the application.
Prerequisite: The PI needs to get access to the system before submitting an application to port the application and to gather the information requested for the call, e.g. the scaling behaviour of the application; see below for details.	The HPC Platform training programme also contains a section with introductions to HPC that can be helpful for users without much experience in HPC (<u>https://hbp-hpc-platform.fz-juelich.de/?tribe_events_cat=hpc-intro</u>).
(3) The HPC site organises an independent, scientific and technical peer-review of all applications. It is expected that successful projects both will lead to scientific progress and make efficient use of the HPC resources.	In this step the HBP scientists' projects are treated like any other project.
(4) The PIs are informed within a couple of days or weeks (depending	The HPC Platform team creates HPC Platform projects and accounts

Table 49: Workflow of computing time applications





on the call and the review process) if their applications were successful. PIs of projects granted with HPC resources get a project ID and user accounts for the HPC system at the beginning of the allocation period.	using the bp0 naming scheme instead of standard project accounts. If the same person has computing time allocations for more than one system of the HPC Platform, the same bp0 account will be activated on all these systems.
	A Collaboratory app is under development that can be used by the PI to create the HPC project and for requesting accounts for the users of the computing time allocation.

Most of the HPC sites offer different types of calls for proposals, with different eligibility criteria, resources to be distributed and project durations. They are organised directly by the site, by country-specific or international organisations like PRACE (Partnership for Advanced Computing in Europe). The table below describes for all four HPC systems currently integrated in the HPC Platform which calls are available, what are the eligibility criteria, and when and how often the calls are open. More information are available in the Guidebook: <a href="https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://hbp-https://https://https://hbp-https://htttps://https://https://https://https/https/htttps://https/

Table 50	Calls for	^r computing	time for	· HPC	systems
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HPC system	Calls available	Eligibility	Resources	Next calls' deadlines
JUQUEEN	VSR/JARA-HPC	Researchers affiliated with Forschungszentrum Jülich and/or RWTH Aachen; National and international collaborators possible	260 million core hours (total)*	Two calls per year, each with a project duration of twelve months, starting 1 st May and 1 st November. Next call for proposals is open from 25 th January 2016 till 29 th February 2016. The call for the November allocation period will
	NIC	German PI;	900 million core hours in total for NIC and GCS call*	open end of July 2016 and close end of August 2016.
	GCS Large Scale	collaborators possible	NIC: <35 million core hours/project*	The calls for JUQUEEN are synchronised.
			GCS: >35 million core hours/project*	

Human Brain Project

Co-funded by the European Union



	PRACE	No restriction	Currently not available for	JUQUEEN	
BlueBrain IV	 As of today, the workflow to get access to the HBP Development System BlueBrain IV is still paper based, i.e. users need to fill out forms. A web-based solution will be implemented in the near future. The application workflow consists of the following two steps: Request for a new project from a PI. In case the applicant is neither a Blue Brain Project (BBP) employee nor already accredited: Request to be accredited in order to become eligible to participate in a project on BlueBrain IV. 				
	All information is currently provided an internal wiki page as it is so far expected that collaborators request access to t BBP facilities because they are already working with some members of the Blue Brain Project.				
MareNostrum III	PRACE	No restriction.	About 120 million core hours per call	Two calls per year, each with a project duration of 12 months.	
			(total)	The first call opens in February, the allocation starts in September.	
				The second call opens in September, the allocation starts in March of the following year.	
				The PRACE calls for all sites are synchronised.	
	RES Spanish collaborator recommended	About 34 million core hours per call (total)	The RES access in managed in 3 calls per year. Each call provides access to the granted projects for 4 months. The granting periods are the following:		
				• 1 st November till 28 th /29 th February	
				• 1 st March till 30 th June	
				• 1 st July till 31 st October	
				The next period for submitting applications will start on 2 nd March 2016 and will close around 10 th May (the exactly date will be published in the	

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				RES web site on 2 nd March: <u>www.bsc.es/RES</u>)
FERMI	PRACE	No restriction.	About 120 million core hours per call (total)	Two calls per year, each with a project duration of 12 months.
				The first call opens in February, the allocation starts in September.
				The second call opens in September, the allocation starts in March of the following year.
				The PRACE calls for all sites are synchronised.
	ISCRA	Italian PI needed	250 million core hours per call	Class B: Two calls per year with a project duration of 12 months.
			1-10 million core hours for class B projects	Class B calls open from 1 st December till mid January (allocation starts in April) and from mid June till mid July (allocation starts in
			Up to 1 million core hours for class C projects	November).
				Class C projects are received through continuous submission and reviewed once per month (no peer-review). An average period of about 15 days is required for activating the project. For each user it is allowed to have only one class C project each 6 months as PI. The maximum duration is 9 months.
	Small grants	There are calls for small grants to "Class C" above). So far, resource available also to issue some spece HBP topics.	based on a continuous s ses were assigned to HB sific pilot action to acce	ubmission and a regular cut-off every month (see P users directly through direct grants. CINECA is ess specific resources for data analytics related to

*Numbers from end of 2015

Since applying for regular calls already requires some first experience with the system in order to prepare the requested information, all HPC sites also offer test accounts and/or "preparatory access". The HPC Platform team can be contacted to ask for test accounts. The





following table lists all calls for preparatory access. The applications for these calls are also reviewed, but the effort for writing these applications is much smaller than for regular calls. The review mainly assesses if the application can use the requested system at all.

Table 51: Calls for preparatory access to HPC systems

HPC system	Calls available	Eligibility	Resources	Next calls' deadlines	
JUQUEEN	JSC Preparatory Access	Researchers affiliated with Forschungszentrum Jülich and/or RWTH Aachen; German PI; National and international collaborators possible	Up to 100,000 core hours per project including support by a JSC Simulation Lab (Simulation Lab Neuroscience for HBP projects) for a period of up to 4 months and about 2 person-weeks in total	Two calls per year, the application deadlines are beginning of May and beginning of November.	
	PRACE Preparatory Access	No restriction	Prep. Access Type A: 100,000 core hours to be spent within 2 months (for scalability tests)	Continuous submission with four cut-offs per year (beginning of March, June, September, December)	
			Prep. Access Type B: 250,000 core hours to be spent within 6 months (for scalability tests and optimisation by the user)		
			Prep. Access Type C: 250,000 core hours to be spent within 6 months (for scalability tests and optimisation by the user) and up to 6 person months of support by a PRACE expert		
BlueBrain IV	The Blue Brain Project can be contacted to get test access to BlueBrain IV.				
MareNostrum III	PRACE Preparatory Access	No restriction	Prep. Access Type A: 50,000 core hours to be spent within 2 months (for scalability tests)	Continuous submission with four cut-offs per year	
			Prep. Access Type B: 100,000 core hours to be spent within 6 months (for scalability tests and optimisation by the user)	(beginning of March, June, September, December)	
			Prep. Access Type C: 100,000 core hours to be		





			spent within 6 months (for scalability tests and optimisation by the user) and up to 6 person months of support by a PRACE expert	
FERMI	PRACE Preparatory Access	No restriction	 Prep. Access Type A: 100,000 core hours to be spent within 2 months (for scalability tests) Prep. Access Type B: 250,000 core hours to be spent within 6 months (for scalability tests and optimisation by the user) Prep. Access Type C: 250,000 core hours to be spent within 6 months (for scalability tests and optimisation by the user) and up to 6 person months of support by a PRACE expert 	Continuous submission with four cut-offs per year (beginning of March, June, September, December)