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CALIPSOplus JRA2 Meeting
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Outline

Current state of PSI offline computing

PSI HPC user community has access to

- local HPC-Cluster (~900 cores)
  - typically run smaller simulation jobs, but also a lot of high trivially parallel job arrays.
- Supercomputing resources at Swiss National Supercomputing Center (CSCS) - long standing collaboration with PSI co-investing.

PSI synchrotron users almost never used these resources. Reasons:

- external users have to take data home for analysis
- for in-house research the local online-shared resources frequently were still adequate
  - this is now changing with the advent of new detectors
- effort to port needed applications to the cluster environments was prohibitive for the beamline colleagues and internal users. IT did no have manpower for this.

$\rightarrow$ Address the growing need for computing in the DaaS project for building up initial service

Overview

Funding Body	SUC (now *swissuniversities*) is the organization of the heads of the Swiss Universities.
Project name	Data Analysis Service (DAS)
Internal PSI Name	DaaS (Data Analysis as a Service).
Partner institutions	ETHZ/CSCS
Project Duration	04.2015 - 04.2017
Project Managers	Stephan Egli, Derek Feichtinger
Project User-Base Contact	Mirjam van Daalen
Team members	16 (incl. 3 new positions financed by project)

- Alain Studer
- Björn Abt
- Daniel Lauk
- Daniel Webster
- Dmitry Ozerov
- Edgar Barabas
- Hans-Christian Stadler
- Heiner Billich
- Ivan Usov
- Ivano Talamo
- Jan Solca
- Leonardo Sala
- Markus Knecht
- Peter Hüsser
- René Kapeller
- Valeri Markushin

Work Packages

DaaS Science Community oriented WPs

- WP2: Data Analysis Environments for major use cases
- WP4: Integration and development of scientific analysis codes

DaaS SW Infrastructure WPs

- WP1: Common Tools and Services
- WP3: Identity Management, DUO, Authentication and Authorization

DaaS HW Infrastructure oriented WPs

- WP5: Procurement, installation, operation of analysis cluster infrastructure

DaaS Science Community oriented WPs (1)

WP2: Data Analysis Environments for major use cases

Build up *offline analysis environments* for user community. Focus on 4 major use cases (based data volume/throughput.

- MX: macromolecular crystallography
- TOMCAT: X-Ray tomography
- cSAXS: coherent small angle X-ray scattering
- SwissFEL

Software deployment

- *Pmodules* based on environment modules
  - central SW deployment / packaging that can easily be used by users to deploy locally.
- Use of container technology
  - Not central component in DaaS project, but considered as a possibility for difficult SW deployment cases (conflicting SW)

DaaS Science Community oriented WPs (2)

WP4: Integration and development of scientific analysis codes

Development and integration/porting of codes for the major use cases, so that they can profit from the new infrastructure

- Ptychography, 3D SAXS
- Tomography analysis chain
- serial crystallography

DaaS SW Infrastructure WPs

WP1: Common Tools and Services

- Remote Access: nomachine, sigateway (own development allowing tunneling of host:ports groups based on user/group identification through a gateway)
- Remote Transfer: globus Online for bulk, rsync/ssh for concurrent
- Data Catalog: multiple candidates being evaluated

WP3: Identity Management, DUO, Authentication and Authorization (3)

- Consolidation effort of historically grown IdM at PSI
- DUO integration for managing offline users/groups
- Umbrella and other federated authn/z integration
- Investigating Moonshot for non-HTTP

DaaS HW Infrastructure oriented WPs

WP5: Procurement, installation, operation of analysis cluster infrastructure

Start by building up of local cluster and storage infrastructure for enabling offline analysis for all SLS and SwissFEL users in the future.

- using modern standard HW
- leveraging on IBM GPFS for storage and data flows
  - Spectrum Scale also provides interfaces for enabling technologies like Hadoop/Spark and connecting to external storage clouds, so we keep these options open.

Start with this *architecturally conservative approach* (not Cloud), because complexity to be mastered with priority is in area of data management and providing intensive science community support. In this project we want to build a better understanding of the service that is to be provided and progress from there.

WP6: Infrastructure sharing with other institutions

- PoC for using an external Petabyte archive. Leveraging on GPFS features for data flows.
- collaborating with other Swiss projects in this funding framework
- study using offline resources at other sites

PSI strategy

- we are evaluating extending our collaboration with the Swiss National Supercomputing Center (CSCS) and other sites for a part of our offline computing tasks and to be able to cover peak loads. In this context packaging of VMs and containers may become central (q.v. shifter technology from NERSC for containers on Cray).
- Concern in regard to relying on being able to package everything
  - some SW is proprietory (e.g. the MX SW) and there sometimes are technical as well as license related problems. Packaging and maintenance effort may be very high.

List of expertise - some PSI comments (1)

- Project Coordination + workshops
- Use (science) case definition and collation (multiple disciplines, facilities and user/industry) (Scientists) use DaaS use cases: MX, TOMCAT, cSAXS, SwissFEL
- Packaging for applications (SysAdmins) interested in the activity
- Cloud setup and deployment (SysAdmins) currently we are not actively using cloud resources but we are interested in observing the evolution closely
- Configuration of site and test sites (DevOps)
- Port and package applications and examples (~~Software engineer~~) interesting to us for planned collaborations

List of expertise - some PSI comments (1)

- Umbrella authentication (AAI+security) complements well earlier PSI and DaaS efforts, Moonshot
- User portal development (Web engineers) ? Scope is not clear to us
- Definition, development and distribution of mini demonstrator platform to test sites (DevOps)
- Report on results and links to HNSciCloud + EOSC (IT Engineer+SysAdmin+Software+Scientists) What access could Swiss Researchers have to such resources?