

HPC and Cloud Infrastructure for Neuroscientists

Webinar



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www.fenix-ri.eu

Outline

- The ICEI Project
- Fenix Infrastructure
 - Overview
 - Services
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 - Outlook
- Use case example(s)
- Getting support
- Q&A



The ICEI Project

- Interactive Computing E-Infrastructure for the Human Brain Project (HBP)
 - Co-funded by the European Commission, Specific Grant Agreement under the umbrella of the HBP Framework Partnership Agreement
 - Started officially in January 2018
 - 5 Supercomputing centres (PRACE Hosting Members) involved:



The ICEI project carries out coordinated procurements of equipment and R&D services to realise elements of the Fenix Infrastructure



Fenix Infrastructure – Overview

- Federated computing and data services for European researchers
- Data storage and scalable computing resources in close proximity to each other and tightly integrated
- Service-oriented provisioning of resources, aiming to
 - Meet the requirements of various science communities
 - Form a basis for the development and operation of communityspecific platform tools and services
- Federation of infrastructure services to optimize for data locality, enhance availability and broaden variety of services



Fenix Infrastructure – Services

Scalable Computing Services (SCC)

- Massively parallel HPC systems suitable for large-scale brain simulations and high-throughput data analysis tasks
- Interactive Computing Services (IAC)
 - Quick access to single compute servers to analyse and visualise data interactively, or to connect to running simulations using SCC
- Virtual Machine (VM) Services
 - Service for deploying VMs in a stable and controlled environment, e.g. platform services like the HBP Collaboratory
- Active Data Repositories (ACD)
 - Site-local data repositories for storing temporary slave replicas of large data sets (parallel file systems)

Archival Data Repositories (ARD)

Federated data store for long-term storage and sharing of large data sets



Fenix Infrastructure – Available resources

Fenix Infrastructure services are available only at CSCS, yet.
 Overview of available resources:

| Component | Service Type | ICEI Total Allocation (100%) | Available Resources (quarterly) |
|--------------------------|--------------|---------------------------------|------------------------------------|
| Piz Daint Multicore | SCC | 250 nodes | 465'375 node-hrs |
| Piz Daint Hybrid | SCC + IAC | 400 nodes | 744'600 node-hrs |
| OpenStack laaS | VM | 35 servers | 35 servers |
| POSIX, Object and Tape | ARD | 4 PB | 4 PB |
| Low-Latency Storage Tier | ACD | 80 TB | 80 TB |

Resources at other centres will become available within the next months, details are published on the Fenix website: <u>https://fenix-ri.eu/infrastructure/resources/planned-resources</u>



Resources at CSCS – Some details

Piz Daint Multicore

- 2x Intel Xeon E5-2695 v4 (2.10GHz, 18 cores)
- 64 or 128 GByte host memory
- Up to 1431 nodes per job
- Piz Daint Hybrid



- 2x Intel Xeon E5-2690 v3 (2.6 GHz, 12 cores) + 1x NVIDIA P100 GPU
- 64 GByte host + 16 GByte device memory
- Up to 5320 nodes per job
- Archival Data Repository
 - Access via Swift interface
 - Same interface at all sites





Fenix Infrastructure – User access

- Allocation Mechanism for resources that are available within the Fenix Infrastructure, principles:
 - Process follows peer review principles established by PRACE
 - Each user community (e.g. HBP) is responsible for the actual distribution of their share within that community
- HBP is the initial prime and lead user community
 - 25% of available resources are reserved for HBP
 - 15% are provided to European researchers at large via PRACE
 - The remaining 60% are with the respective centre that is providing the resources and are made available to users e.g. via National Calls
- Access for HBP members
 - Flyer "Access to Fenix IT Services for HBP Users" on Fenix website
- Access for non-HBP members
 - **PRACE Tier-0** calls and in the future dedicated **ICEI PRACE Tier-1** calls



Fenix Infrastructure – Outlook

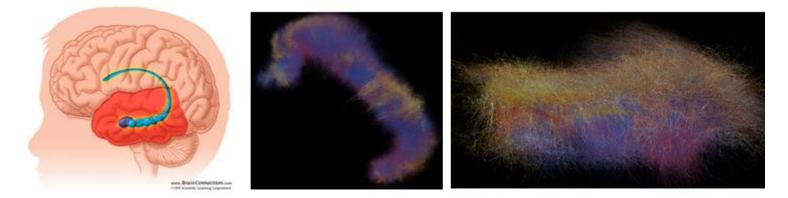
- Infrastructure components that are procured within ICEI are becoming operational at all centres
 - Realisation of federated infrastructure services, including:
 - Authentication and Authorization Infrastructure (AAI)
 - Enabling central user identification and authentication
 - Fenix AAI will provide access to infrastructure services, e.g. storage, while community platforms and services will retain their own authentication and authorization mechanisms
 - Fenix User and Resource Managements Service (FURMS)
 - Central system to manage membership and roles of users within certain stakeholder groups
 - Allows for resource allocation and accounting within these groups
 - Data location and transfer services
 - Enabling users of the Fenix infrastructure to locate and **move their data between centres**
 - Data Mover Service
 - Enabling users to move data between ACDs and ARDs at a single centre

Infrastructure is open to new user communities and centres
FENIX RI

Use case example

Large scale simulations of models: Hippocampus

 Project studies the mechanisms that may contribute to the emergence of higher brain functions at the cellular and behavioural level in the hippocampus (*PI: M. Migliore*)



Required resources of the Fenix Infrastructure:

- **Scalable Computing** Services for running large-scale simulations using Neuron
- Active Data Repositories as temporary storage [write from simulation, read for analysis]
- Interactive Computing Services for analysing data produced by simulations
- Archival Data Repositories for storing final data products

Where to get help

Central point of contact for any support requests:

support@humanbrainproject.eu

- Provides access to all levels of support
 - 1st and 2nd level support at the Fenix sites for technical problems with Fenix services
 - Advanced support by the HBP High-Level Support Team (HLST)
- HLST support includes
 - Guidance and assistance in the preparation of applications for computing and data resources
 - Implementation support for simulation and data analytics workflows, possibly using multiple Fenix services, up to the codevelopment of solutions that benefit other use cases as well



OpenStack SWIFT

Object Store

- This is not a file system (especially not POSIX)
- HTTP-based API in the style of REST
- Manipulation of entities via POST/PUT/GET
- Atomic units: objects; not files
- No byte-granularity access
- https://endpoi.nt/my-project/my-account/a-container/object-1/name-1
 - Endpoints signify installations at different sites
 - Projects and accounts group containers by creator
 - Containers group objects into 'directories'
 - Object names can contain '/', but these hold no meaning
- Sharing Data
 - ACLs can be set for containers
 - Regulate list/read/write access



Archival Data Repository Access

Currently only at CSCS

Obtain an account with the Pollux Infrastructure

https://user.cscs.ch/tools/openstack/#access-to-pollux

Install the OS Swift CLI Client

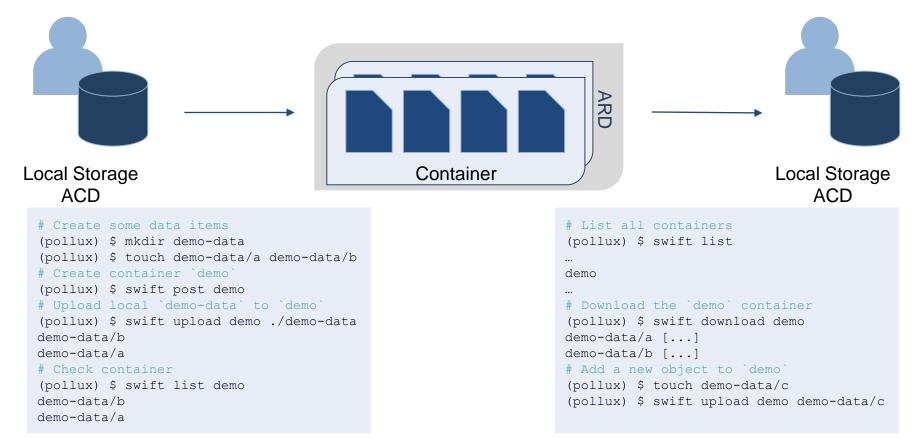
```
# Create a Python Virtual Environment
$ python3 -venv pollux
$ source pollux/bin/activate
# Install the Client
(pollux) $ pip install python-swiftclient python-openstackclient oauthlib python-heatclient
# Get environment script for CSCS Pollux
(pollux) $ curl -0 <u>https://raw.githubusercontent.com/eth-cscs/openstack/master/cli/pollux.env</u>
(pollux) $ deactivate
```

Authenticate

\$ source pollux/bin/activate (pollux) \$ source pollux/pollux.env Username: ******* Password: ******* Choose Project: ** # From here you can use the `swift` command line tool. # `swift` is an alias pre-configured to use your account prefix and the Pollux endpoint. # ! BE AWARE WHEN TRYING TO ACCESS DIFFERENT ENDPOINTS/ACCOUNTS !



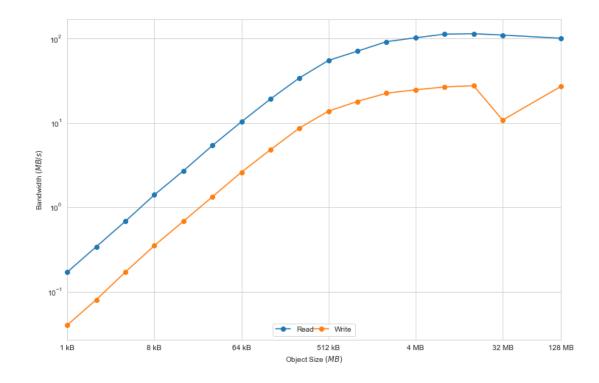
Archival Data Repository Workflow



There is a lot going on behind the scenes! See here for getting started <u>https://wiki.humanbrainproject.eu/bin/view/Collabs/how-to-data-access-and-efficient-io/</u>



ARD - Performance



- CosBench (openio 0.4.1) on a single node (<u>https://github.com/open-io/cosbench</u>)
- JSC Juron to CSCS Pollux
- Concurrent mix of 80% read, 20% write
- Object size relevant for performance, use > 4MB







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