

Einsatz von UNICORE in der Hirnforschung

2017-03-16 | Björn Hagemeyer

Activities in Neuroscience

- SMHB - Supercomputing and Modeling for the Human Brain
- HBP - Human Brain Project

UNICORE



Web Command line GUI API

Clients



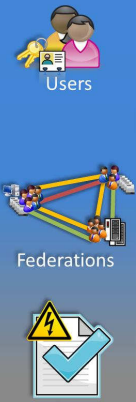
Workflows Jobs Data Management Discovery

Services



Compute Storage

Resources



Users

Federations

Policies

Security

Polarized Light Imaging (PLI)

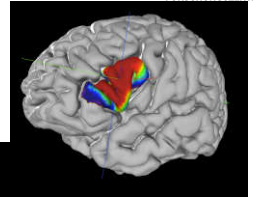
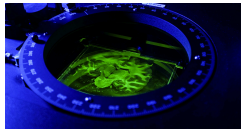
The Method

- Developed at Institute for Neuroscience and Medicine, Forschungszentrum Jülich
- Aim: extract the course of single nerve fibers
- Sections of postmortem human brain, each $70\mu m$
- Imaging the sections under linearly polarized light
 - ~ 1500 sections/brain
 - 30×25 tiles/section
 - 2048×2048 pixels/tile



Polarized Light Imaging (PLI)

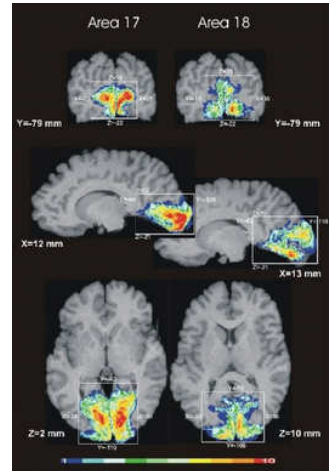
The Workflow



High-throughput brain scans

Jülich/HHU collaboration

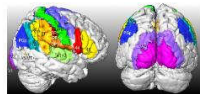
- Goal is to create a 3D brain atlas
- Data acquisition
 - Brain section scans (ex vivo)
 - (~2000 slices, 500GB per slice → 1PB)
 - MRT scans (in vivo)
- Processing: image registrytion, calibration, segmentation, etc.
- Image processing using HPC
- Raw data often re-processed (new algorithms, new software versions)
- Additionally: workflows, metadata, sharing with external partners



Part: Human Brain Project

Human Brain Project

- FET Flagship
- ~10 years, ~1 Billion EURO
- Coordinated by EPFL (Lausanne)
- Huge, multidisciplinary consortium
 - Neuroscience, medicine, physics, IT, philosophy
- <https://www.humanbrainproject.eu>



HBP

Platforms

- The *Neuroinformatics* Platform
- The *Brain Simulation* Platform
- The *High Performance Analytics and Computing* Platform
- The *Medical Informatics* Platform
- The *Neuromorphic Computing* Platform
- The *Neurorobotics* Platform

System Access

User questions

Typical SSH access scenario, multiple machines and sites

- What's my login/password on machine X?
- What LRMS is running on machine X and what are its commands?
- How do I set cores, nodes, memory, etc.?
- Where is my application located?
- Where is my workgroup's data or mine located?

⇒ Particularly difficult for domain scientists

System Access Integration

How can I

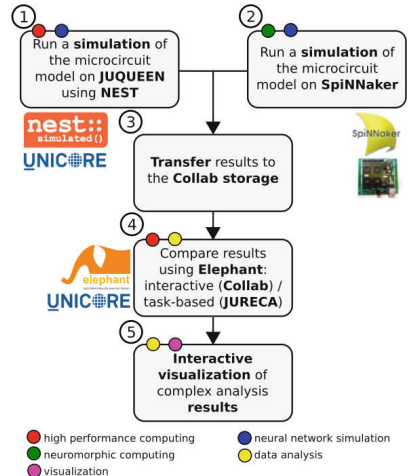
- ... use multiple, heterogeneous systems seamlessly and securely?
- ... manage my job input data and results?
- ... do the above across system boundaries?
- ... integrate HPC and data resources into applications/portals?

NEST

The Neural Simulation Technology Initiative

NEST Simulator

- simulator for spiking neural network models
- focus on the dynamics, size and structure of neural systems



Source: Senk et. al (2017)

Running nest Without UNICORE

- Login via SSH to JUQUEEN
- Manage working directory, code, and input parameters
- Create and submit a LoadLeveler script

Example

```
#job_name = slns_demo
#...
#@bg_size = 32
#@wall_clock_limit = 00:10:00

module load python3/3.4.2
export TMPDIR=$WORK/tmp
export PYTHONPATH=/homeb/slns/slns007/local/opt/...

runjob --ranks-per-node 1 --exp-env ... : /bgsys/.../python3 microcircuit.py
```

Running nest Using UNICORE

- Complexity is now hidden by UNICORE
- User can use a UNICORE Application “NEST”
- User only needs to invoke application and provide relevant data

Example

```
ApplicationName: NEST,  
  
Parameters: [  
  NESTCODE: microcircuit.py, PARAMETERS: parameters.py, ],  
  
Imports: [ ... ],  
  
Resources: { Nodes: 32, Runtime: 1200 }
```

Running nest Using UNICORE

Admin defines UNICORE Application “NEST” for JUQUEEN

Example

```
<idb:IDBApplication>

  <idb:ApplicationName>NEST</idb:ApplicationName>

  <jsdl:POSIXApplication>
    <jsdl:Executable>runjob --ranks-per-node 1 --exp-env ... : .../python3</jsdl:Executable>
    <jsdl:Argument Type="filename">${NESTCODE?}</jsdl:Argument>
    <jsdl:Argument Type="filename"># $PARAMETERS?</jsdl:Argument>
  </jsdl:POSIXApplication>

  <idb:PreCommand>#@environment = COPY_ALL</idb:PreCommand>
  <idb:PreCommand>module load python3/3.4.2</idb:PreCommand>
  <idb:PreCommand>export TMPDIR=$WORK/tmp</idb:PreCommand>
  <idb:PreCommand>export PYTHONPATH=/usr/local/...:$PYTHONPATH</idb:PreCommand>

  <idb:PostCommand>find -name *gdf | xargs zip output.zip</idb:PostCommand>

</idb:IDBApplication>
```

HBP's HPC Platform



Single Sign-On

Unity

- Bridges UNICORE to HBP OIDC infrastructure
- Supports REST and Web clients
- Support for SOAP/WS clients (legacy)

User Management

- Users are granted resources (→ review process)
- User IDs and groups are mirrored to HPC sites (LDAP)
- Access via UNICORE is configured automatically

The screenshot shows the HBP Collaboratory web application. The interface includes a top navigation bar with links like 'Home', 'About', 'News', 'Contact', 'Help', 'Log In', and 'Sign Up'. The main content area is titled 'HBP Collaboratory' and features a 'Where collaboration happens' section. This section contains a list of projects, including 'HBP Collaboratory', 'HBP Collaboratory', 'HBP Collaboratory', and 'HBP Collaboratory'. Each project entry includes a brief description and a link to the project page. Below the project list is a section titled 'Neuroinformatics Platform', which describes the platform's capabilities and provides a list of features. A large 3D brain model is displayed in the bottom right corner of the main content area.

[illegible]

The Collaboratory Applications

- Applications can be added to *collabs*
- One such application is the UNICORE Storage Browser

bjoernh test collab Private Member

Navigation

Overview

Team

Storage

Settings

Task 2.2

My Profile

HPC Storage JURECA

HPC Storage KIT

Job Manager

Workspace

bp000027-Home

HPC-JURECA

bp000027-Home

Name	Content	Created on	Created by
.cache			
.config			
.ssh			
.2012-06-04_Private_Cloud.pdf.metadata			
.bashrc			
.kshrc			
.news_time			
.profile			
.sh_history			
.Xauthority			

Collaboration

1 member - 1 available



This is the very beginning of the current collab's chat. Start using it to collaborate with your team!

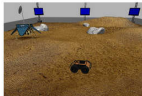
Part: Neurorobotics

Current Goals

Neurorobotics

Workspace

Example experiments



Husky Braitenberg experiment in the SpaceBotCup 2013 arena

This experiment loads the Husky robot from Clearpath Robotics and the arena from the SpaceBotCup 2013. If the user starts the experiment, the Braitenberg vehicle network is executed and the robot will...



Husky Braitenberg experiment with automatically switching screens

This experiment is similar to the Husky Braitenberg one (Husky robot detecting red colour and driving towards it). In this experiment the right screen is turned red automatically after...



iCub Visual Tracking experiment

In this experiment the iCub robot performs a Visual Tracking task in the virtual room environment.

Timeout: 00 00:14:00

Backend availability: 13 / 14

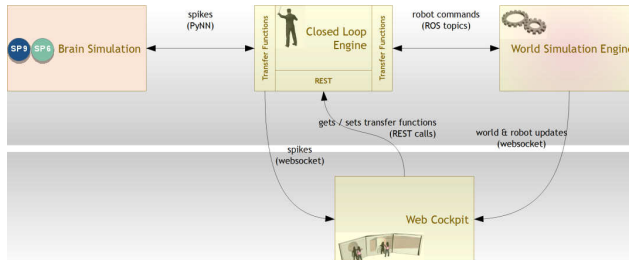
Cluster availability: 6 / 34

+ Launch

Upload custom environment

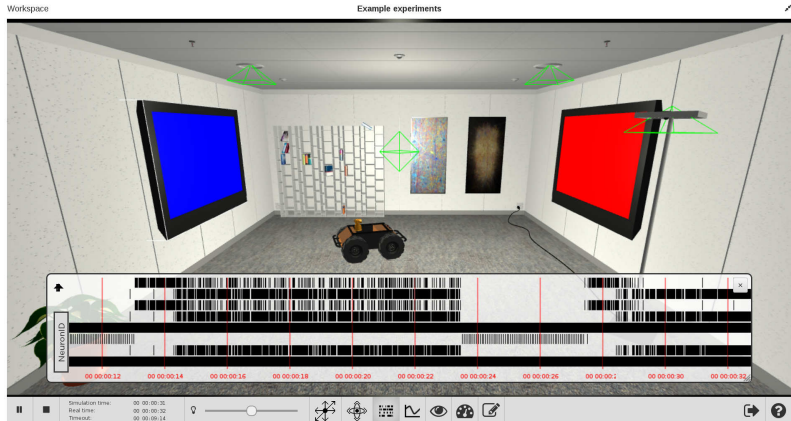
Screenshot of HBP SP10 NRP Example Experiments

NRP Architecture



Axel von Arnim, HBP SP10

NRP Web Cockpit



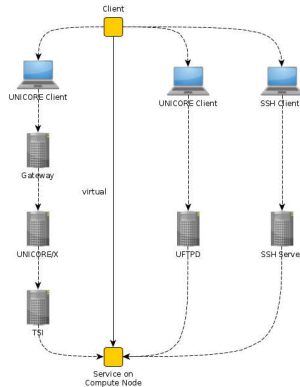
Screenshot of HBP SP10 NRP Husky Braitenberg Experiment

Requirements

- Network tunnel into HPC resources
- Forwarding VNC connections
- Low latency
- Bandwidth?

Architecture Options

- Many hops
- Higher latency expected
- Implementation difficult



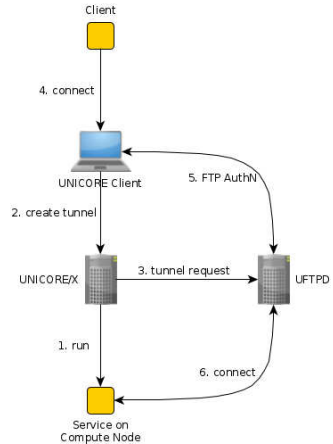
- Fewer hops
- Proven components
- Easier implementation

Own

Implementation

Tunnel Setup

- Same flow as for *ordinary* UFTP connections
- Firewall friendly



Tunnel Setup

UCC

- New create-tunnel command
- Parameter -L resembling SSH syntax
- Source Address can be set via -i
 - Important for NATing or multiple interfaces
- Example:

```
$ ucc run iperf.u -a  
720208ac-7015-49c3-b0c1-9e047b4287be.job  
$ ucc create-tunnel 720208ac-*.job -L 5001:localhost:5001  
Listening on localhost:5001
```

Results

Some (superficial) measurements

Throughput/Bandwidth

- Measured using iperf (submitted as job)
- No noticeable difference to native performance or SSH tunnels

Latency

- Usable for VNC, no noticeable lag

Results

IPerf

- 6 consecutive tests, 2 each using UFTP, SSH, and direct connections
- Server side log

Server listening on TCP port 5001

TCP window size: 85.3 KByte (default)

```
[ 5] local 127.0.0.1 port 5001 connected with 127.0.0.1 port 41246
[ ID] Interval Transfer Bandwidth
[ 5] 0.0-10.8 sec 120 MBytes 93.5 Mbits/sec
[ 7] local 127.0.0.1 port 5001 connected with 127.0.0.1 port 41252
[ 7] 0.0-10.7 sec 119 MBytes 93.4 Mbits/sec
[ 5] local 127.0.0.1 port 5001 connected with 127.0.0.1 port 41253
[ 5] 0.0-11.0 sec 119 MBytes 91.3 Mbits/sec
[ 7] local 127.0.0.1 port 5001 connected with 127.0.0.1 port 41254
[ 7] 0.0-11.0 sec 123 MBytes 93.5 Mbits/sec
[ 5] local 192.168.16.142 port 5001 connected with 134.94.168.32 port 52196
[ 5] 0.0-10.1 sec 112 MBytes 93.6 Mbits/sec
[ 7] local 192.168.16.142 port 5001 connected with 134.94.168.32 port 52200
[ 7] 0.0-10.1 sec 112 MBytes 93.6 Mbits/sec
```

Open Issues

The small print

- Need to deploy full NRP scenario including VirtualGL over VNC
- Currently only a single connection possible after tunnel setup
- Tunnel tear-down needs to be implemented
- It is not as straightforward to implement SSH tunnels as it may seem
- More measurements under various conditions
 - Better abstraction is needed

Summary

- Neuroscience involvement
 - SMHB
 - HBP
- Variety of services for supporting neuroscience
- New use cases lead to new features