**Notes of MoBrain Competence Centre teleconference**

Meeting date: 8th October, 2015.

Meeting page: <https://indico.egi.eu/indico/conferenceDisplay.py?confId=2665>

Notes written by: Gergely Sipos, Alexandre Bonvin

Attendees:

- Alexandre Bonvin (UU)

- Marco Verlato (INFN)

- Laura del Cano, Jose Miguel de la Rosa Trevin, Jesus Cuenca (Madrid)

- Jerome Revillard (Gnubila)

- Ales Krenek (CESNET)

- Antonio Rosato (CIRMMP)

- Gergely Sipos (EGI.eu)

Discussed topics with key points:

Introduction:

* See Alexandre's slides in the agenda (called 2015-10-08-MoBrain-update.pptx)

GPU applications and portals

* Already experimenting with both GROMACS and AMBER on GPUs
* Integration with GPUs is progressing in three ways:
	+ 'Direct access' to GPUs
	+ Access to GPUs in OpenStack (Slovakian partner)
	+ Experimenting with Docker and then possibly accessing GPUs from Docker containers (to be developed/tested)
* GPUs in EGI: Related session is organised in Bari at the EGI Forum
* Some new portals will be developed in the coming months, which will adapted at a later stage to make use of grid or cloud GPGPU resources
* Related deliverable is due for review at end of February. This deadline can be met. Initial ideas for content to cover in the deliverable:
	+ GPU performance measures
	+ Discoverability of GPUs in EGI
	+ Migration of portals from grid CPUs to GPUs

Cypion in the cloud (Laura)

* See Laura’s slides in the agenda (called cloud-cryoem-20151008.pptx)
* Porting image framework to cloud. Working with EGI FedCloud experts from IFCA, Valencia, CESNET
	+ Two types of VMs are expected at the end in the cloud: (1) framework to develop and run workflows, (2) software that's combined in the workflow
	+ We still need to understand which workflow element we can port to the cloud which we cannot
* Understanding and trying to deal with network bandwith bottleneck with DANTE, Surfsara, CESNET
	+ Transfer of input data into the cloud
	+ I/O requirement of workflow elements
	+ Assume that the data will go from the data generator labs to IT centres (Surfsara is one of them)
* Improving the Crymo user experience in parallel with the cloud porting

Integrating the micro- (WeNMR/INSTRUCT) and macroscopic (NeuGRID4you) virtual research communities (Jerome)

* Discussed possibilities for integration: Install a Liferay front-end, through EGI Marketplace, Using the WestLife VRE as the integrated front-end
* Deliverable is due for review at end of January 2016 and things will become clearer about WestLife and the Maketplace only later
* Makes no sense to implement the Liferay integration if there is a chance that WestLife or Marketpalce makes this obsolete. Suggest delaying this deliverable to when we will be able to decide and use the effort more wisely. Gergely to request this from the Project Office.

BMB Symposium:

* EGI will have an exhibition booth where CC members can demonstrate apps, VMs, tools, frameworks, datasets they put on EGI.
* Antonio will attend the event and is interested to demonstrate. Gergely and Antonio to follow up offline

EGI Forum:

* Will attend: Alex, (Antonio), Andrea, Marco, Gergely
* GPU session by Marco
* WestLife presentation by Alexandre
* Cloud sessions to be attended

Next meeting - on the last week of November. Gergely to setup a doodle