

AlphaFold Workshop

Lesson 16

Revision 1

Petr Kulhánek

kulhanek@chemi.muni.cz

Laboratory of Computational Chemistry
National Centre for Biomolecular Research
Faculty of Science
Masaryk University
Kamenice 5
CZ-62500 Brno

Infinity

MetaCentrum

Temporal Activation

```
(BUSTER) kulhanek@perian:~$ /storage/brno2/home/kulhanek/infinity-start

# ~~~~~ [AMS 8.327.50de04b] ~~
# Site info          ||| metavo |||
# ~~~ User identification~~~~~
# User name   : kulhanek
# User group  : kulhanek [umask: 027 files: rw-r----- dirs: rwxr-x---]
# ACL groups  : compchem
#
# ~~~ Host info ~~~~~ [cached] ~~
# Full host name      : perian.grid.cesnet.cz
# Num of host CPUs    : 8      / Num of host threads : 8
# Host SMP CPU model  : Intel(R) Xeon(R) Gold 6248R CPU @ 3.00GHz [Total memory: 7.8 GB]
# Host arch tokens    : avx, avx2, i386, i686, m64-centos7, m64-deb10, m64-deb9, m64-ub18,
#                       noarch, sse4_1, sse4_2, x86_64
#
# ~~~ Site documentation and support ~~~~~
# Documentation      : https://infinity.ncbr.muni.cz
# Mailing list       : users@infinity.ncbr.muni.cz
# Support e-mail     : support@lcc.ncbr.muni.cz
# ~~~~~

>>> OpenGL renderer: opengl-mesa (llvmpipe (LLVM 4.0, 256 bits) / OpenGL 3.1 Mesa 18.1.7)

[kulhanek@perian ~]$
```

This must be executed in each terminal, where we want to work with Infinity.
Functionality is currently limited.

Permanent Activation

Activation Script:

```
(BUSTER) kulhanek@perian:~$ /software/ncbr/infiboot/infinity-activate
```

```
=====  
Infinity - activation profile ...  
=====
```

```
ERROR: The activation profile is required!
```

```
Usage: /software/ncbr/infiboot/infinity-activate <profile>
```

```
Supported profiles are: ceitec-ams-8.0-robox-pro general  
                        general-ams-8.0 metavo-ams-8.0 metavo-remove
```

Permanent Activation, cont.

Activation Procedure:

```
(BUSTER) kulhanek@perian:~$ /software/ncbr/infiboot/infinity-activate metavo-ams-8.0
```

```
=====  
Infinity - activation profile ... metavo-ams-8.0  
=====
```

```
Activation of Infinity via cluster home directories ...
```

```
>>> /storage/brn011-elixir/home/kulhanek - success.
```

```
>>> /storage/brn012-cerit/home/kulhanek - success.
```

```
>>> /storage/brno4-cerit-hsm/home/kulhanek - success.
```

```
>>> /storage/brno6/home/kulhanek - - no access
```

```
>>> /storage/brno7-cerit/home/kulhanek - success.
```

```
>>> /storage/brno8/home/kulhanek - - no access
```

```
>>> /storage/budejovice1/home/kulhanek - success.
```

```
>>> /storage/praha2-natur/home/kulhanek - success.
```

```
>>> /storage/praha5-elixir/home/kulhanek - success.
```

```
>>> /storage/pruhonicel1-ibot/home/kulhanek - success.
```

```
>>> /storage/vestec1-elixir/home/kulhanek - success.
```

```
All is done.
```

```
WARNING: Please open a new terminal session to complete the Infinity profile metavo-ams-8.0 activation procedure.
```

Permanent Activation, cont.

```
[kulhanek@pes ~]$ ssh perian.ncbr.muni.cz
...
>>> INFO: The source site 'personal' is not allowed to be transferred to this host!
        The default site will be activated.

# ~~~~~ [AMS 8.327.50de04b] ~~
# Site info          ||| metavo |||
# ~~~ User identification~~~~~
# User name   : kulhanek
# User group  : kulhanek [umask: 027 files: rw-r----- dirs: rwxr-x---]
# ACL groups  : compchem
#
# ~~~ Host info ~~~~~ [cached] ~~
# Full host name      : perian.grid.cesnet.cz
# Num of host CPUs    : 8      / Num of host threads : 8
# Host SMP CPU model  : Intel(R) Xeon(R) Gold 6248R CPU @ 3.00GHz [Total memory: 7.8 GB]
# Host arch tokens    : avx, avx2, i386, i686, m64-centos7, m64-deb10, m64-deb9, m64-ub18,
                      noarch, sse4_1, sse4_2, x86_64
#
# ~~~ Site documentation and support ~~~~~
# Documentation   : https://infinity.ncbr.muni.cz
# Mailing list    : users@infinity.ncbr.muni.cz
# Support e-mail  : support@lcc.ncbr.muni.cz
# ~~~~~

>>> OpenGL renderer: opengl-mesa (llvmpipe (LLVM 4.0, 256 bits) / OpenGL 3.1 Mesa 18.1.7)

[kulhanek@perian ~]$
```