NeuroDesk
A cross-platform, flexible, lightweight, scalable, out-of-the-box data analysis environment

Steffen Bollmann\textsuperscript{1,2}, Oren Civier\textsuperscript{2,3}, Aswin Narayanan\textsuperscript{1,2}, Markus Barth\textsuperscript{1,2}, Tom Johnstone\textsuperscript{2,3}

\textsuperscript{1}The University of Queensland
\textsuperscript{2}Australian National Imaging Facility
\textsuperscript{3}Swinburne Neuroimaging, Swinburne University of Technology
Large ecosystem of scientific software …

FreeSurfer
Large ecosystem of scientific software …
Most tools require Linux

… creating problems for researchers:
Most tools require Linux

Tools are not available in standard package systems

(base) uqsbollm@uqsbollm-7952:$ sudo apt install freesurfer
[sudo] password for uqsbollm:
Reading package lists... Done
Building dependency tree
Reading state information... Done
Package freesurfer is not available, but is referred to by another package. This may mean that the package is missing, has been obsoleted, or is only available from another source

E: Package 'freesurfer' has no installation candidate
... creating problems for researchers:

Most tools require Linux

Tools are not available in standard package systems

Compiling from source often a nightmare

Then run `cmake ..` and set `CMAKE_INSTALL_PREFIX` to be the desired directory as the above `cmake` command is ignoring the setting.

```
make -j 4
```

This will fail configuring beast.

Edit `/home/564/sb1053/minc-toolkit-v2/minc-toolkit-v2/BEaST/CMakeLists.txt` and command out `FIND_PACKAGE( NETCDF )` (in two places).

```
run make -j 4 again.
```

This will fail to compile `/home/564/sb1053/minc-toolkit-v2/minc-toolkit-v2/minctools/progs/mincdump/mincdump.h`

Edit this file and replace `enum` with `#define:`
Most tools require Linux

Tools are not available in standard package systems

Compiling from source often a nightmare

Conflicting dependencies

freeview.bin: error while loading shared libraries: libpng12.so.0: cannot open shared object file: No such file or directory
… creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare
- Conflicting dependencies
- Reinstalling tools on different platforms takes time
… creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare
- Conflicting dependencies
- Reinstalling tools on different platforms takes time
- Differing results between software versions
GLIBC 2.5 vs 2.18

Reproducibility of neuroimaging analyses across operating systems

Tristan Glatard¹-², Lindsay B. Lewis¹, Rafael Ferreira da Silva³, Reza Adalat¹, Natacha Beck¹, Claude Lepage¹, Pierre Rioux¹, Marc-Etienne Rousseau¹, Tarek Sherif¹, Ewa Deelman³, Najmeh Khalili-Mahani¹ and Alan C. Evans¹*

• glibc 2.5 vs 2.18 deliver different floating-point results
• leads to significant differences in long pipelines

expf(1.54051852262573242187500000000)
=4.667009353637695312500

expf(1.54051852262573242187500000000)
=4.6670098304748535156250
How to help with this…

https://xkcd.com/1987/

Steffen Bollmann | @sbollmann_MRI | github.com/NeuroDesk
... but avoid ...

How Standards Proliferate:
(See: A/C chargers, character encodings, instant messaging, etc)

Situation:
There are 14 competing standards.

14?! Ridiculous!
We need to develop
one universal standard
That covers everyone's
use cases.

Yeah!

Soon:
Situation:
There are 15 competing standards.

https://xkcd.com/927/
Let’s start with a use case

- Researcher wants to run an analysis with Nipype (Python 3), combining tgv_qsm (Python 2), FSL 6.0.3 (Linux) and MINC 1.9.17
Let’s start with a use case

- Researcher wants to run an analysis with Nipype (Python 3), combining tgv_qsm (Python 2), FSL 6.0.3 (Linux) and MINC 1.9.17 (Prebuilt packages only available for Ubuntu)
- Develop pipeline interactively on Windows 10 notebook
- Test analysis on pilot data on a Linux workstation running Ubuntu 18.04
- Analyse all data on a cluster running ROCKS Centos
- Visualize results interactively on Windows 10 notebook and prepare for publication
- Share analysis pipeline with readers of paper
What exists already and how can we combine efforts?
Virtual Machines VS Containers

- **Application**: e.g. itksnap
- **Libraries**: e.g. QT4
- **Guest OS**: e.g. Ubuntu 16.04
- **Hypervisor**: e.g. Virtualbox
- **Host OS**: e.g. Centos 6
- **Hardware**: e.g. Dell Precision

**Storage**: 10 GB  
**Startup**: 15s  
**RAM**: 4GB

**Storage**: 0.1 GB  
**Startup**: 0.2 s  
**RAM**: 0.1 GB
NeuroDesk

- Community project
- Started at Organisation for Human Brain Mapping Hackathon
Design principles for NeuroDesk

- Docker
- Singularity
- Full Linux desktop interface
- Tools are installed on demand
- NeuroDebian, conda, NeuroDocker

Linux, Mac, Windows
Scale to HPC
Interactive
Lightweight
Re-use existing repositories
Architecture

Community developing recipes using conda, neurodebian, neurodocker ….

CAID – Automated Container building
Automated container building using github actions

currently available tools:

https://github.com/NeuroDesk/caid/packages

- afni passing
- ants passing
- alicc passing
- convert3D passing
- freesurfer passing
- fsl passing
- itkSNAP passing
- julia passing
- lashis passing
- minc passing
- mrtrix3 passing
Architecture

Community developing recipes

CAID – Automated Container building

PowerUsers on Linux, HPC, CVL

NeuroDesk – Integrating our containers on any Linux OS
Combining tools from different Containers using modules

```
neuro@5c2bff15d401:~$ module avail

-------------------------------------------- /vnm/containers/modules --------------------------------------------
freesurfer/7.1.0    fsl/6.0.3    mrtrix3/3.0.1
freesurfer/7.1.1 (D) itksnap/3.8.0
```

```
neuro@5c2bff15d401:~$ which freeview
/vnm/containers/freesurfer_7.1.1_202000924/freeview
```

```
neuro@5c2bff15d401:~$ which fslmaths
/vnm/containers/fsl_6.0.3_20200820/fslmaths
```

```
neuro@5c2bff15d401:~$ cat /vmn/containers/fsl_6.0.3_20200820/fslmaths
#!/usr/bin/env bash
export PWD=`pwd -P`
singularity exec --pwd $PWD /vmn/containers/fsl_6.0.3_20200820/fsl_6.0.3_20200820.sif fslmaths $@
```
Architecture

Community developing recipes

CAID – Automated Container building

NeuroDesk – Integrating our containers on any Linux OS

VNM – Lightweight Linux Desktop in Docker container

Users on Windows, Mac

Community developing recipes

CAID – Automated Container building

NeuroDesk – Integrating our containers on any Linux OS

VNM – Lightweight Linux Desktop in Docker container

Users on Windows, Mac
VNM – Interface accessible from any browser 😊
VNM – Containers are installed when needed 😊
VNM – Reproducible/Scriptable via lmod module system 😊
Our use case

- Researcher wants to run an analysis with Nipype (Python 3), combining tgv_qsm (Python 2), FSL 6.0.3 (Linux) and MINC 1.9.17 (Prebuilt packages only available for Ubuntu)
- Develop pipeline interactively on Windows 10 notebook
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Patient data can now stay local

FSL/MINC now usable on Windows

Compiling MINC done in CI/CD pipeline

Outdated libraries on old Centos cluster don’t matter

Python versions now separated in containers

Software setup reproducible
Contributions welcome - github.com/NeuroDesk

- Software/Container testing
- Singularity registry in Australia
- Simple installer
- More use cases
- Extension to other fields (e.g. Electrophysiology -> ARDC Platforms Program Call “AEDAPT”)
## Acknowledgements

### NEURODESK GITHUB CONTRIBUTORS

<table>
<thead>
<tr>
<th>Username</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>@aswinnarayanan</td>
<td>Aswin Narayanan</td>
</tr>
<tr>
<td>@civier</td>
<td>Oren Civier</td>
</tr>
<tr>
<td>@crnolan</td>
<td>Christopher Nolan</td>
</tr>
<tr>
<td>@geetah05</td>
<td>Geeta Hariharaputran</td>
</tr>
<tr>
<td>@kaczmarj</td>
<td>Jakub Kaczmarzyk</td>
</tr>
<tr>
<td>@MartinGrignard</td>
<td>Martin Grignard</td>
</tr>
<tr>
<td>@meganEJcampbell</td>
<td>MEJ Campbell</td>
</tr>
<tr>
<td>@stebo85</td>
<td>Steffen Bollmann</td>
</tr>
<tr>
<td>@thomshaw92</td>
<td>Thom Shaw</td>
</tr>
</tbody>
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