THE UNIVERSITY OF QUEENSLAND
AUSTRALIA
CREATE CHANGE

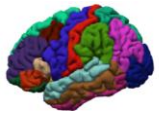
NeuroDesk

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

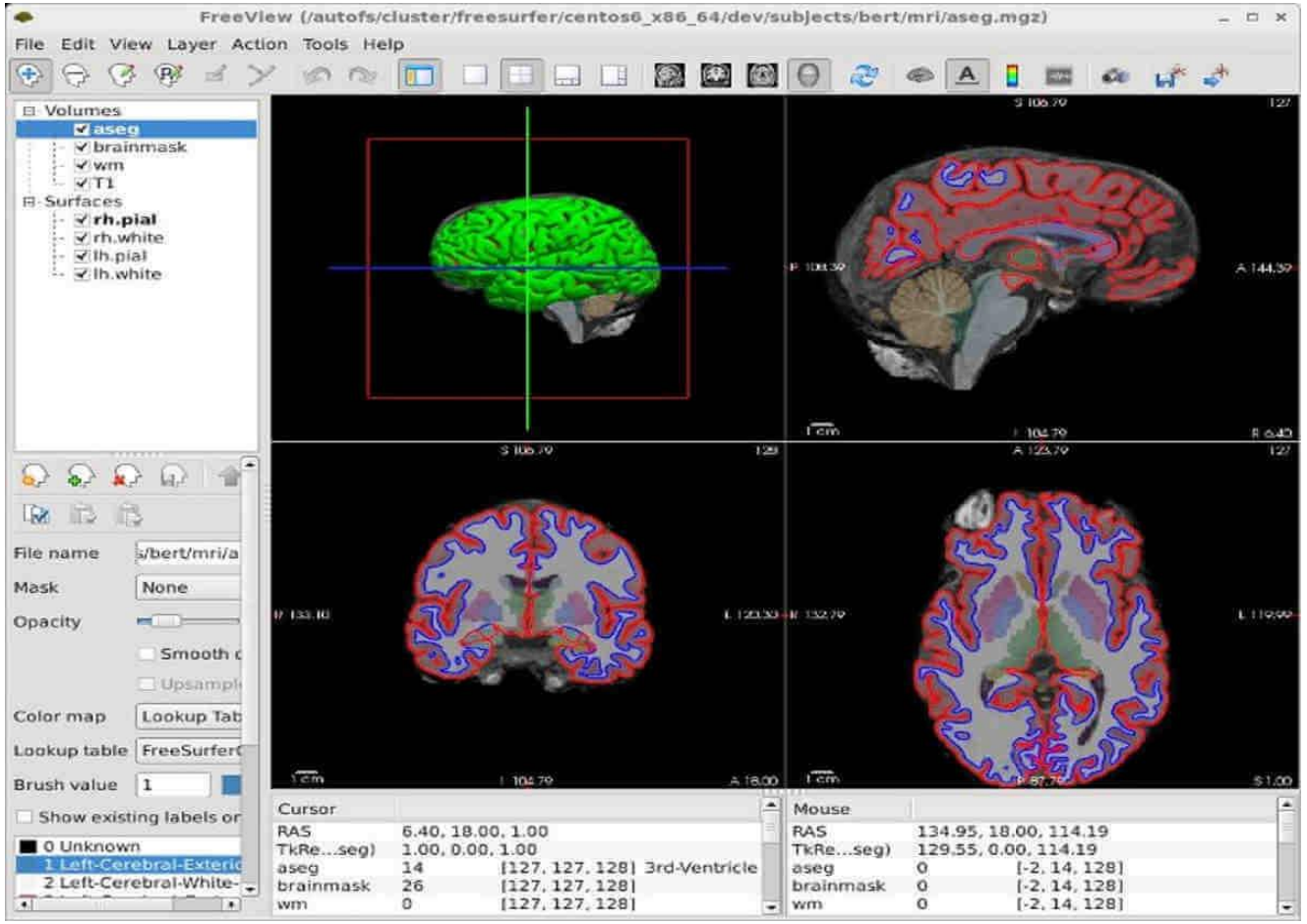
Steffen Bollmann[1,2], **Oren Civier**[2,3], **Aswin Narayanan**[1,2], **Markus Barth**[1,2], **Tom Johnstone**[2,3]

[1]The University of Queensland
[2]Australian National Imaging Facility
[3]Swinburne Neuroimaging, Swinburne University of Technology

Large ecosystem of scientific software …



FreeSurfer



Large ecosystem of scientific software …

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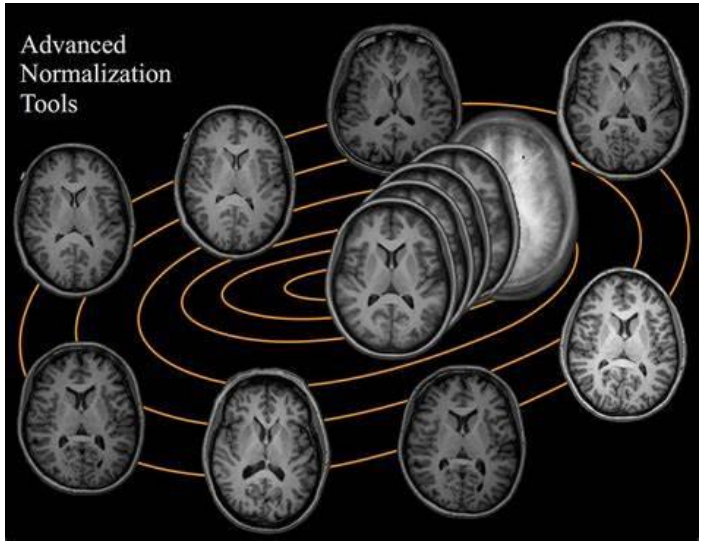
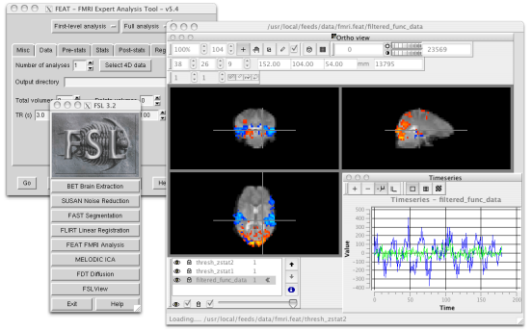
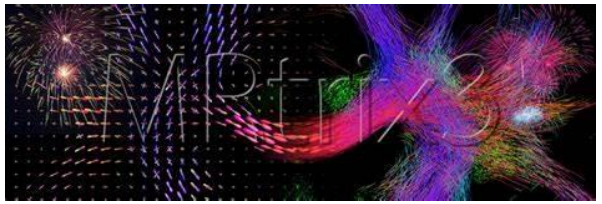




python™

julia



… creating problems for researchers:

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 ccmake .. 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 commend 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:

… creating problems for researchers:

- 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
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… creating problems for researchers:

- Most tools require Linux
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- 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

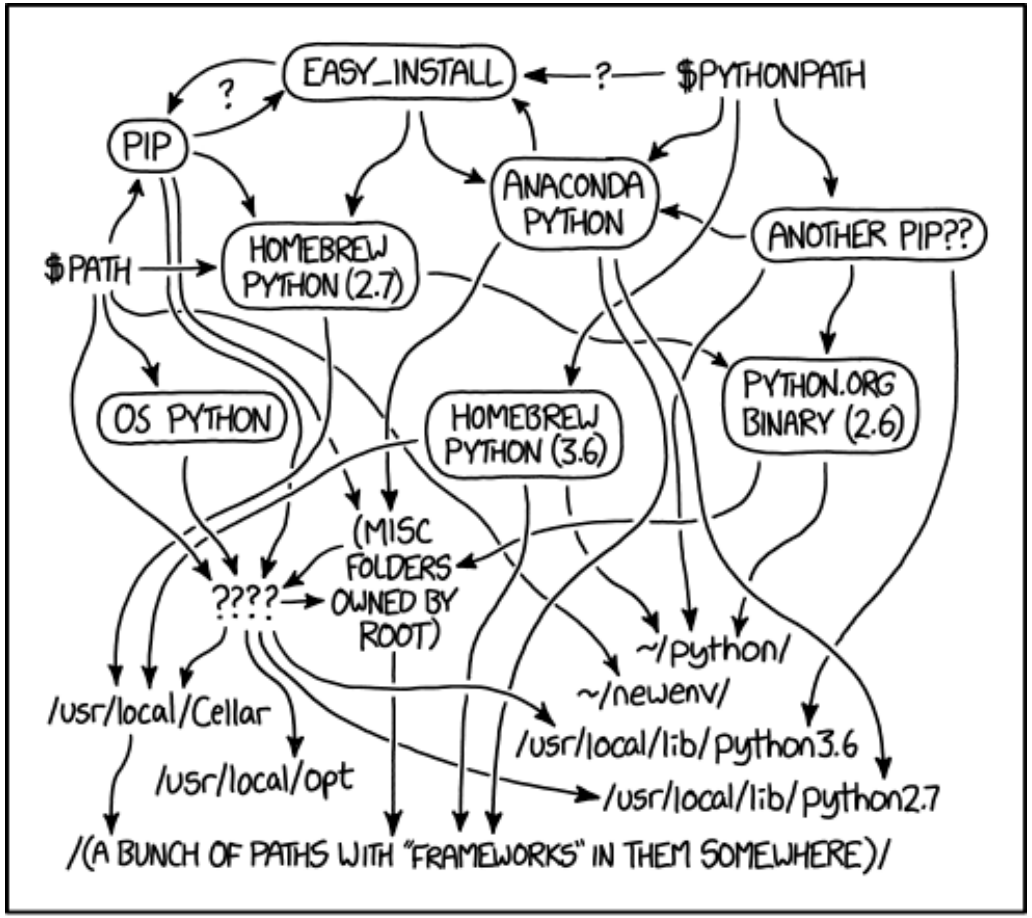
Tristan Glatard[1,2], Lindsay B. Lewis[1], Rafael Ferreira da Silva[3], Reza Adalat[1], Natacha Beck[1], Claude Lepage[1], Pierre Rioux[1], Marc-Etienne Rousseau[1], Tarek Sherif[1], Ewa Deelman[3], Najmeh Khalili-Mahani[1] and Alan C. Evans[1]

```
expf(1.5405185222625732421875000000000)
    =4.667009353637695312500000

expf(1.5405185222625732421875000000000)
    =4.667009830474853515625000
```

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

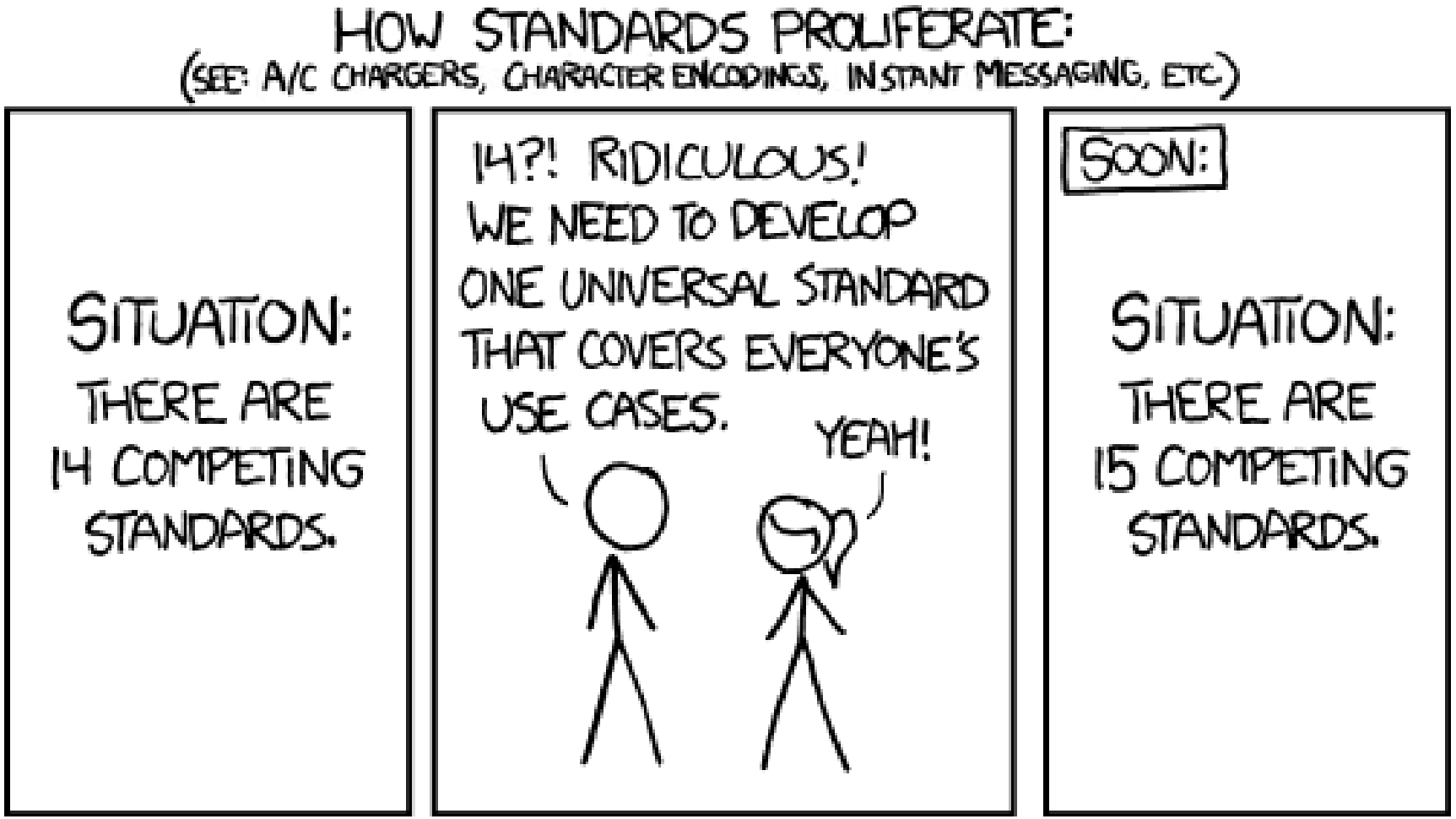
How to help with this…



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

https://xkcd.com/1987/

… but avoid …



https://xkcd.com/927/

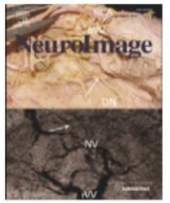
Let's start with a use case

- 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

Contents lists available at SciVerse ScienceDirect

NeuroImage

journal homepage: www.elsevier.com/locate/ynimg



MINC 2.0: A Flexible Format for Multi-Modal Images

*Robert D. Vincent[1], Peter Neelin[2], Najmeh Khalili-Mahani[1], Andrew L. Janke[3], Vladimir S. Fonov[1], Steven M. Robbins[1], Leila Baghdadi[4], Jason Lerch[4,5], John G. Sled[4,5], Reza Adalat[1], David MacDonald[6], Alex P. Zijdenbos[7], D. Louis Collins[1,8] and Alan C. Evans[1]**

[1] McConnell Brain Imaging Centre, Montreal Neurological Institute, McGill University, Montreal, QC, Canada, [2] Intelerad Medical Systems, Montreal, QC, Canada, [3] Center for Advanced Imaging, The University of Queensland, Brisbane, QLD, Australia, [4] Mouse Imaging Centre, The Hospital for Sick Children, Toronto, ON, Canada, [5] Department of Medical Biophysics, University of Toronto, Toronto, ON, Canada, [6] Autodesk Inc., Montreal, QC, Canada, [7] Biospective Inc., Montreal, QC, Canada, [8] Department of Biomedical Engineering, McGill University, Montreal, QC, Canada

frontiers in NEUROINFOR

Nipype: a f
data proce

Krzysztof Gorgolev ***Michael L. Waskom[5,6], Satrajit S. Ghosh[7]***

Let's start with a use case

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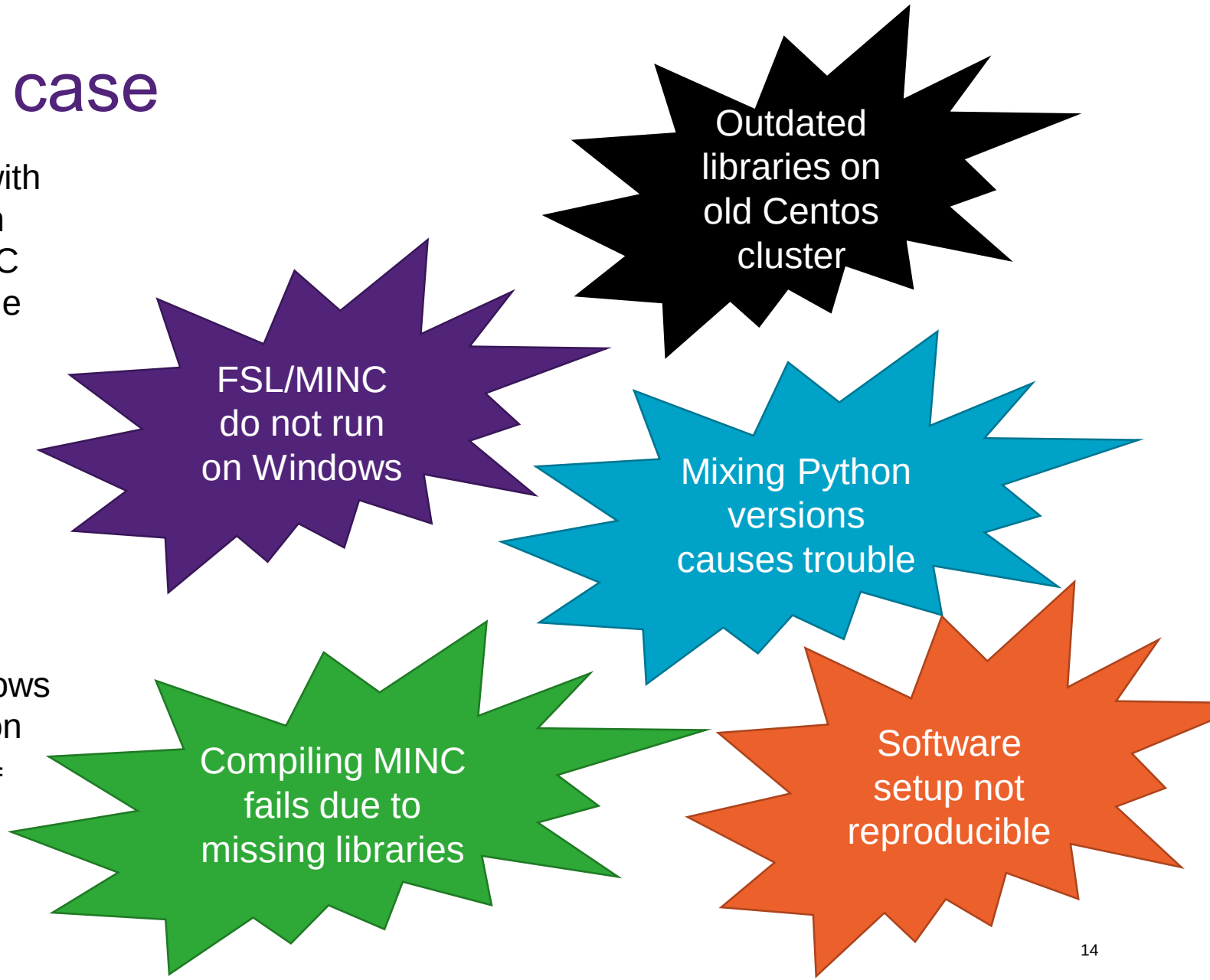
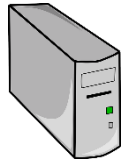


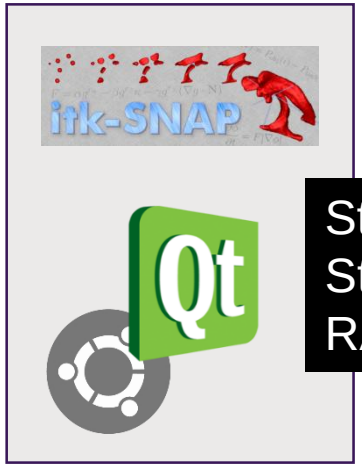
What exists already and how can we combine efforts?

Virtual Machines VS Containers

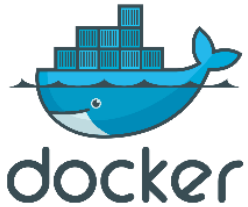
Storage: 10 GB
Startup: 15s
RAM: 4GB

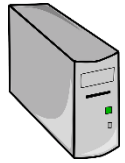


Application	• e.g. itksnap
Libraries	• e.g. QT4
Guest OS	• e.g. Ubuntu 16.04
Hypervisor	• e.g. Virtualbox
Host OS	• e.g. Centos 6
Hardware	• e.g. Dell Precision



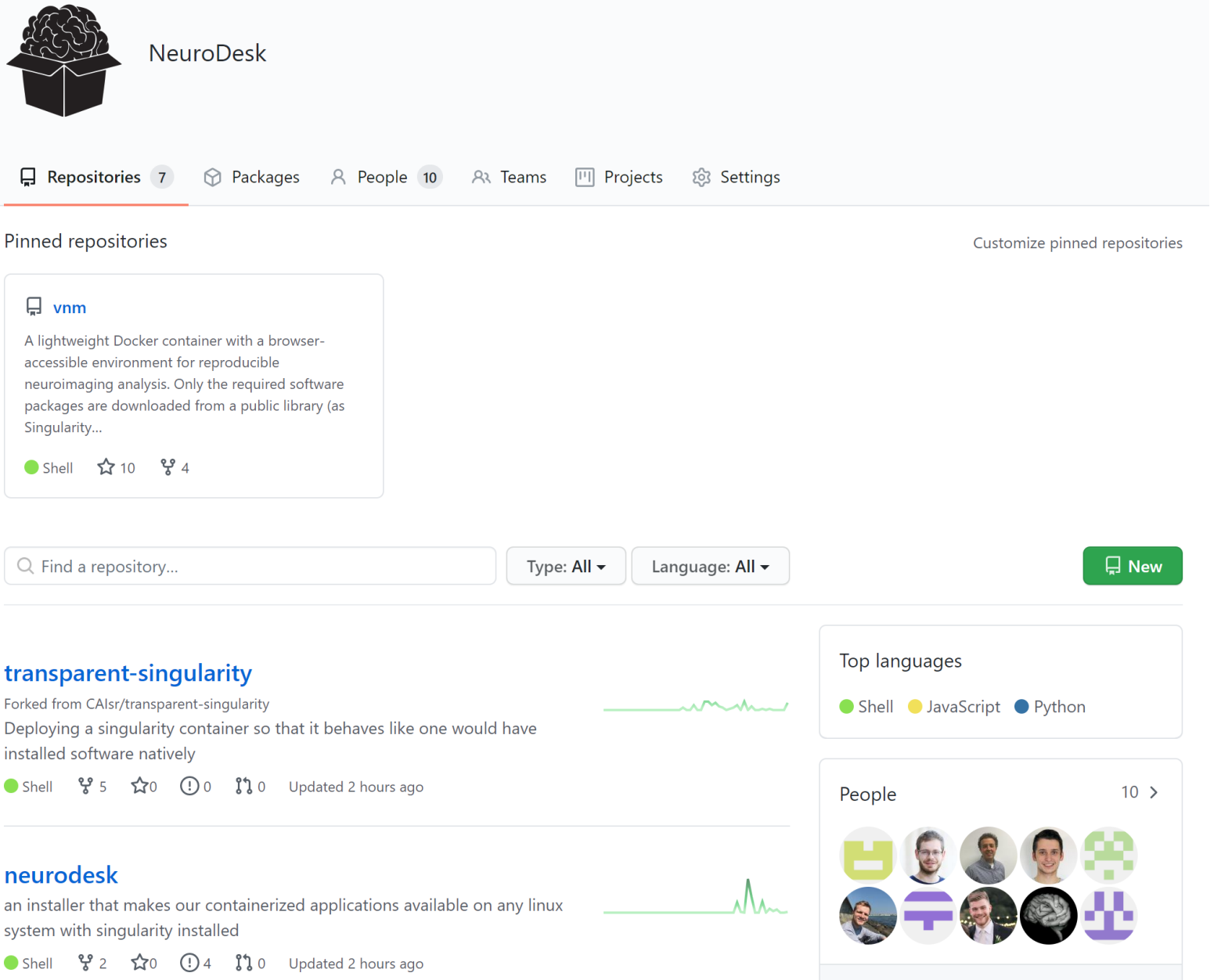
Storage: 0.1 GB
Startup: 0.2 s
RAM: 0.1 GB





NeuroDesk

- Community project
- Started at Organisation for Human Brain Mapping Hackathon

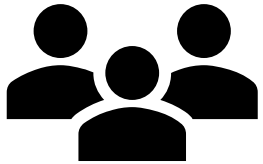


Design principles for NeuroDesk

Linux, Mac, Windows	• Docker
Scale to HPC	• Singularity
Interactive	• Full Linux desktop interface
Lightweight	• Tools are installed on demand
Re-use existing repositories	• NeuroDebian, conda, NeuroDocker

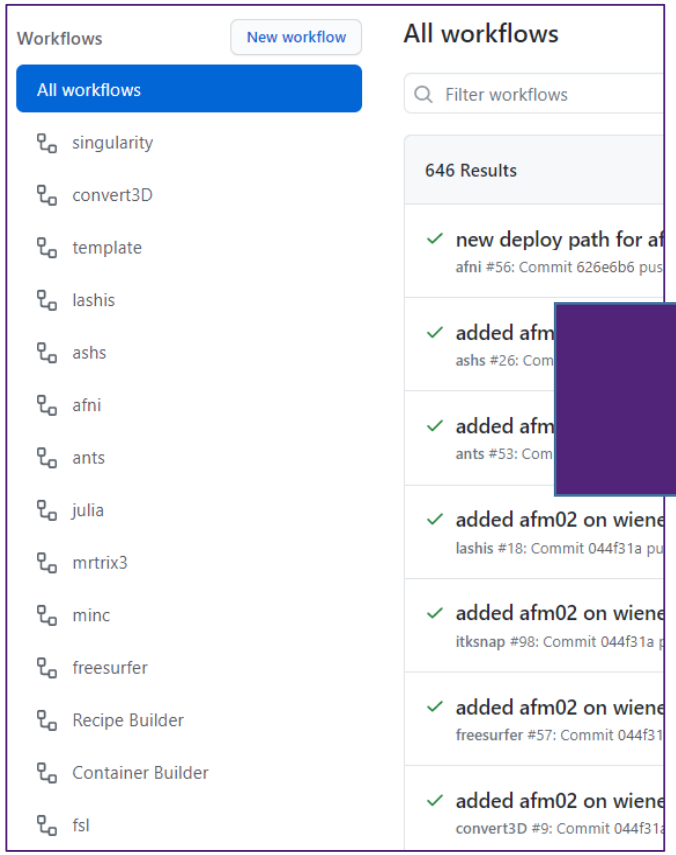
Architecture

Community developing recipes using conda, neurodebian, neurodocker ….



CAID – Automated Container building

Automated container building using github actions

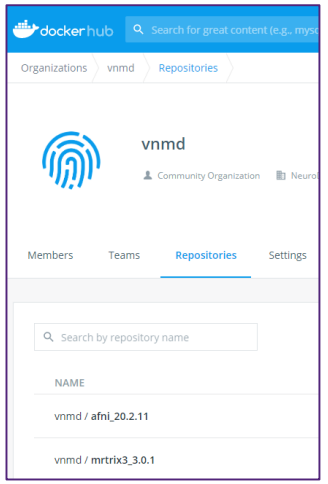


currently available tools:

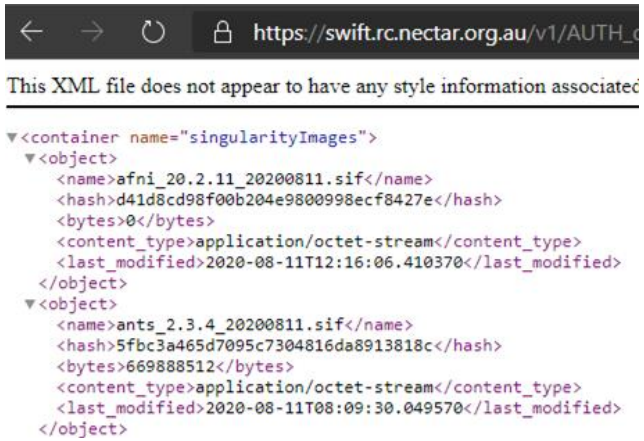
https://github.com/NeuroDesk/caid/packages

- afni passing
- ants passing
- ashs passing
- convert3D passing
- freesurfer passing
- fsl passing
- itksnap passing
- julia passing
- lashis passing
- minc passing
- mrtrix3 passing

Docker

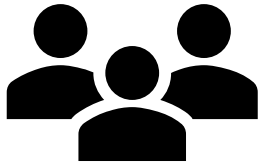


Singularity



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
```

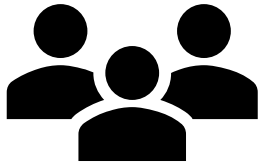
```
neuro@5c2bff15d401:~$ ml fsl
neuro@5c2bff15d401:~$ ml

Currently Loaded Modules:
  1) fsl/6.0.3

neuro@5c2bff15d401:~$ ml freesurfer
neuro@5c2bff15d401:~$ ml

Currently Loaded Modules:
  1) fsl/6.0.3   2) freesurfer/7.1.1
```

```
neuro@5c2bff15d401:~$ which freeview
/vnm/containers/freesurfer_7.1.1_20200924/freeview
neuro@5c2bff15d401:~$ which fslmaths
/vnm/containers/fsl_6.0.3_20200820/fslmaths
```

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

Architecture

Community developing recipes



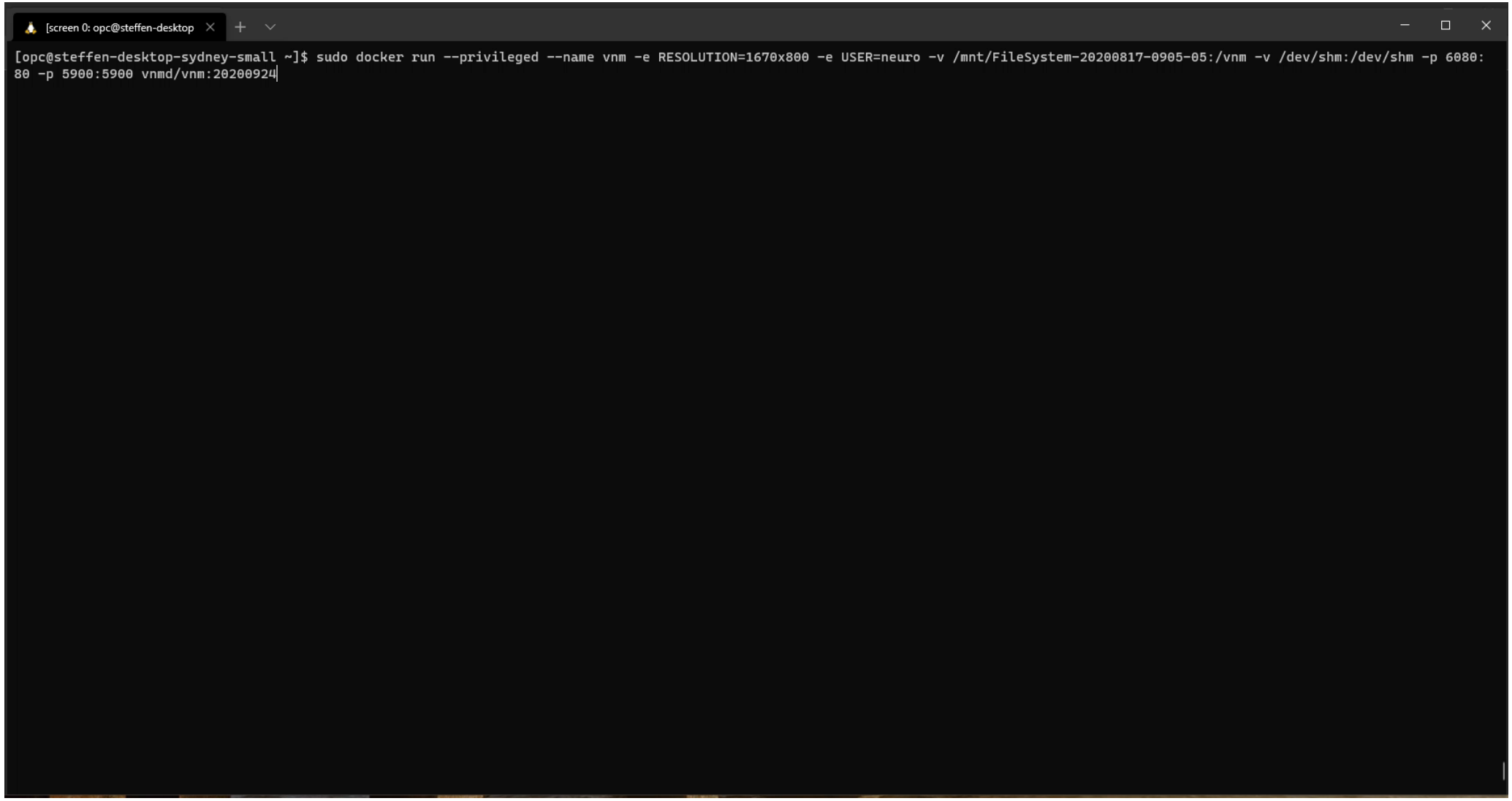
Users on Windows, Mac

CAID – Automated Container building

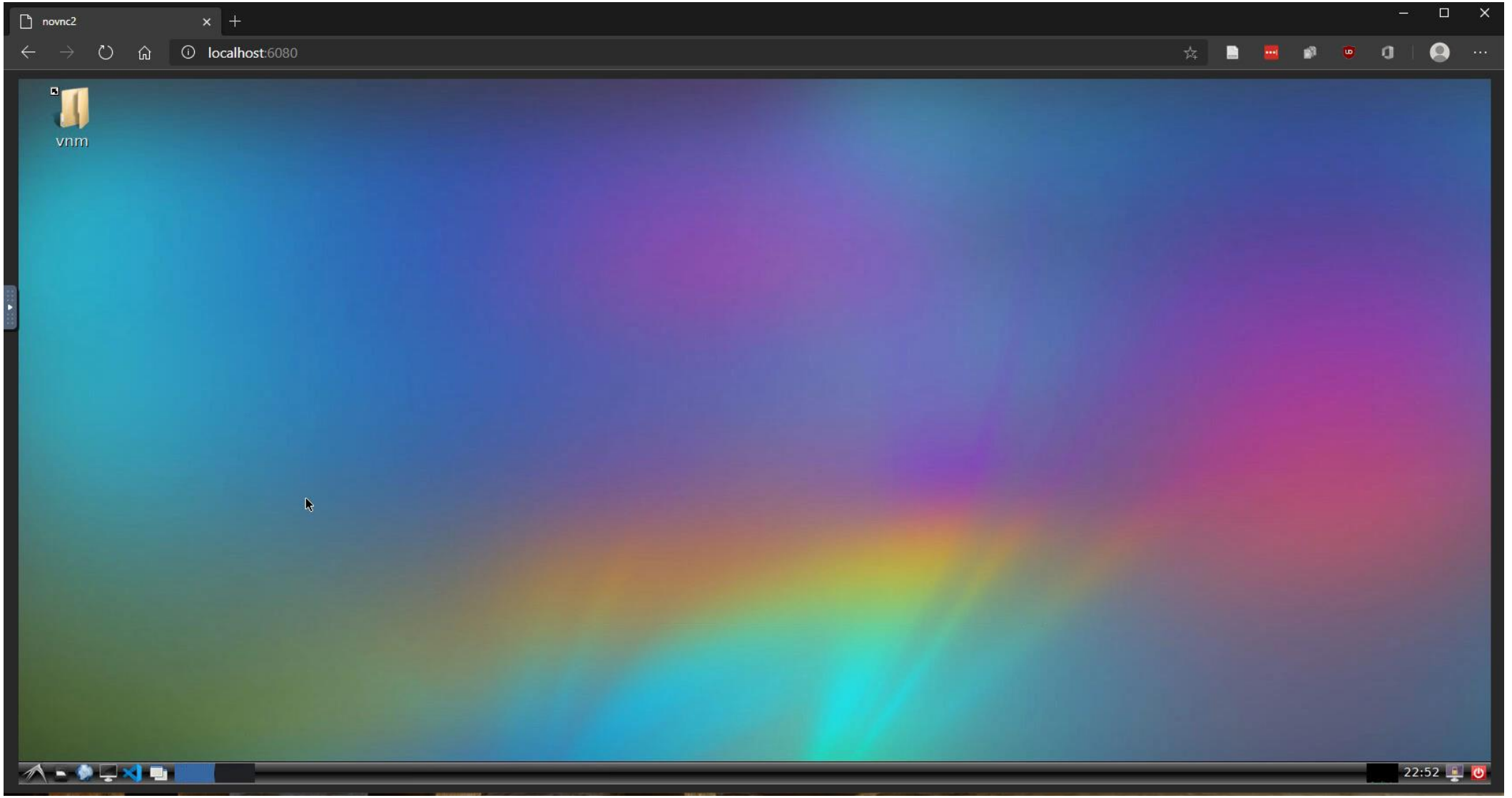
NeuroDesk – Integrating our containers on any Linux OS

VNM – Lightweight Linux Desktop in Docker container

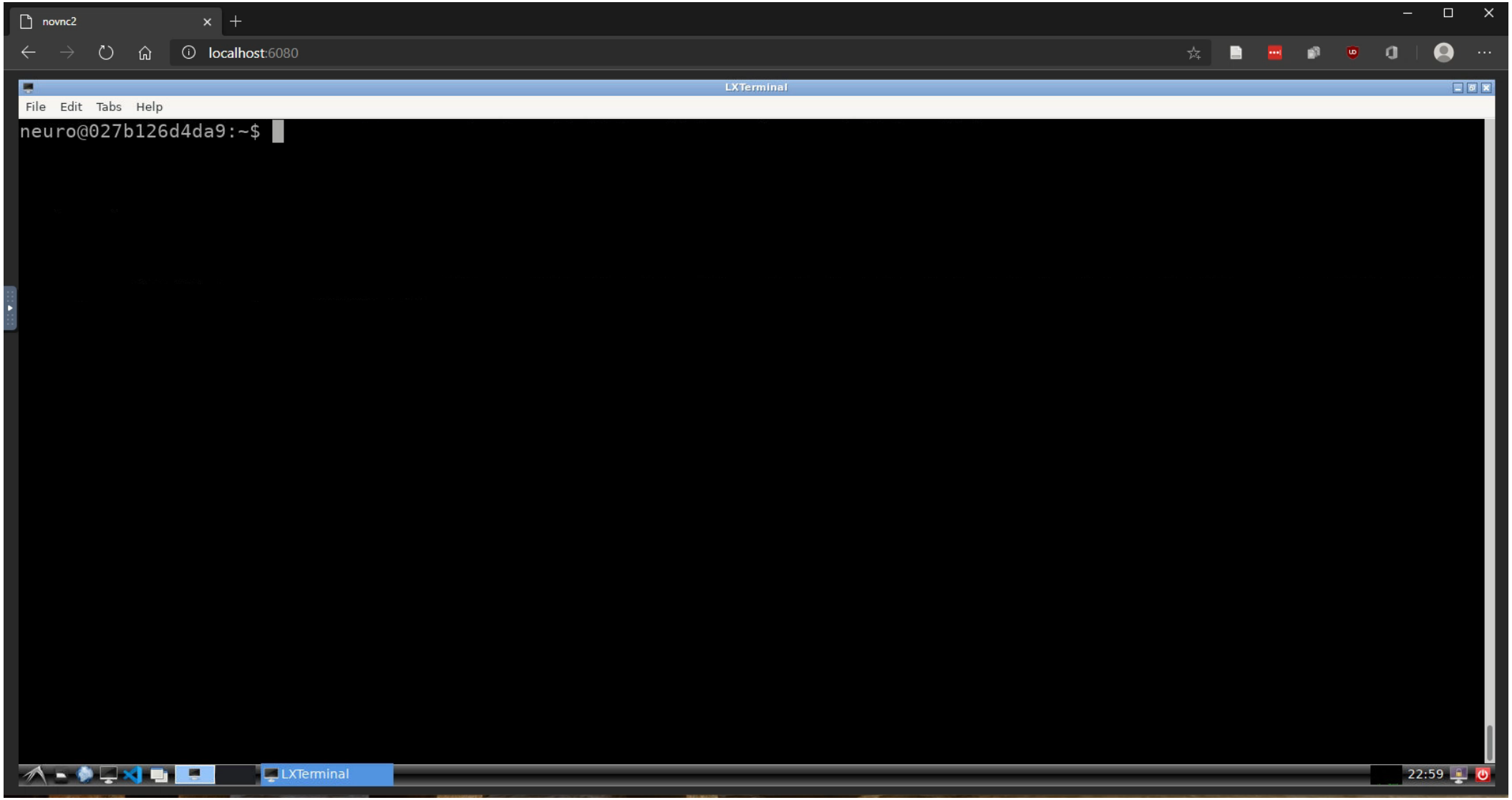
VNM – Interface accessible from any browser ☺



VNM – Containers are installed when needed ☺



VNM – Reproducible/Scriptable via lmod module system ☺



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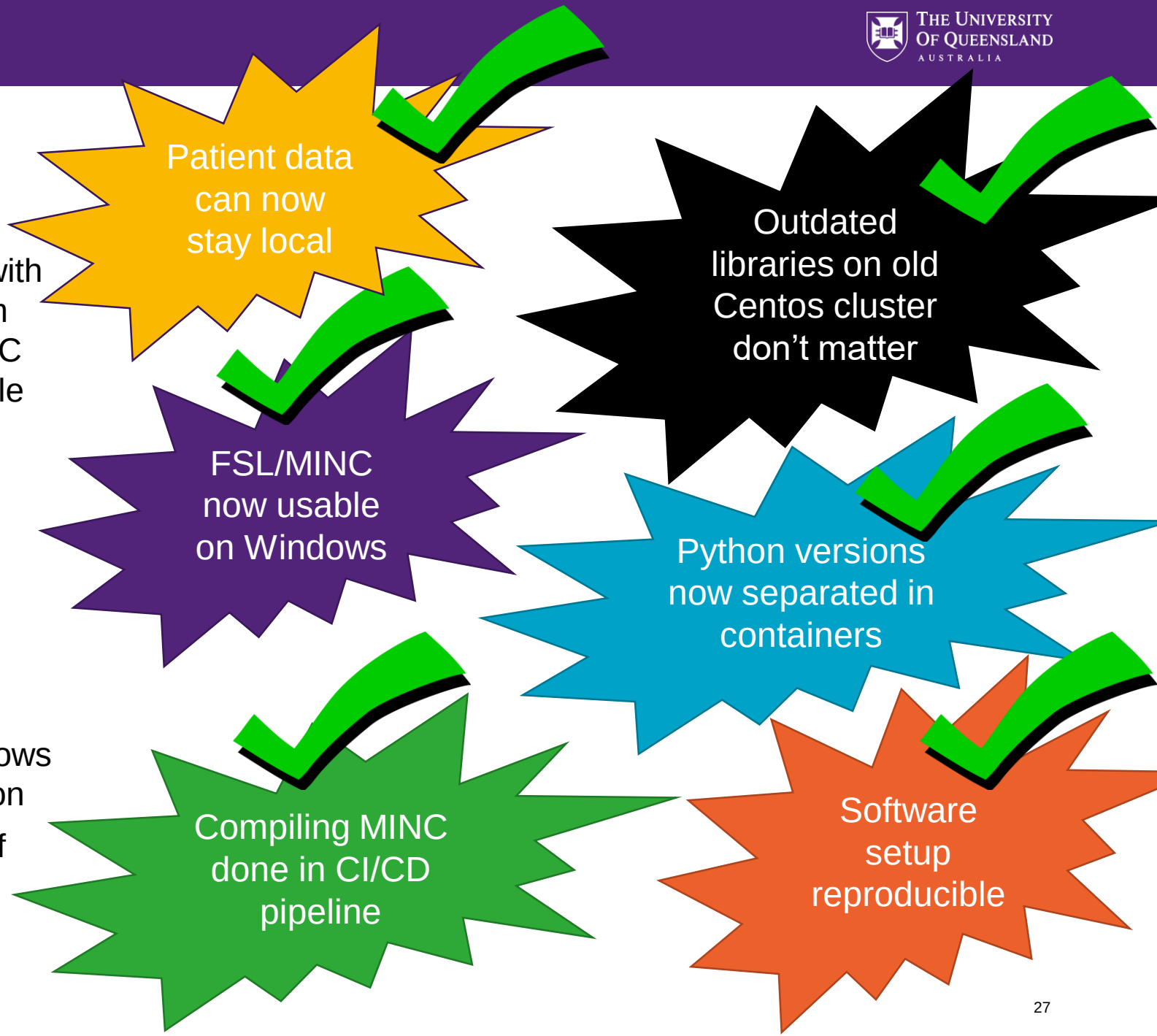
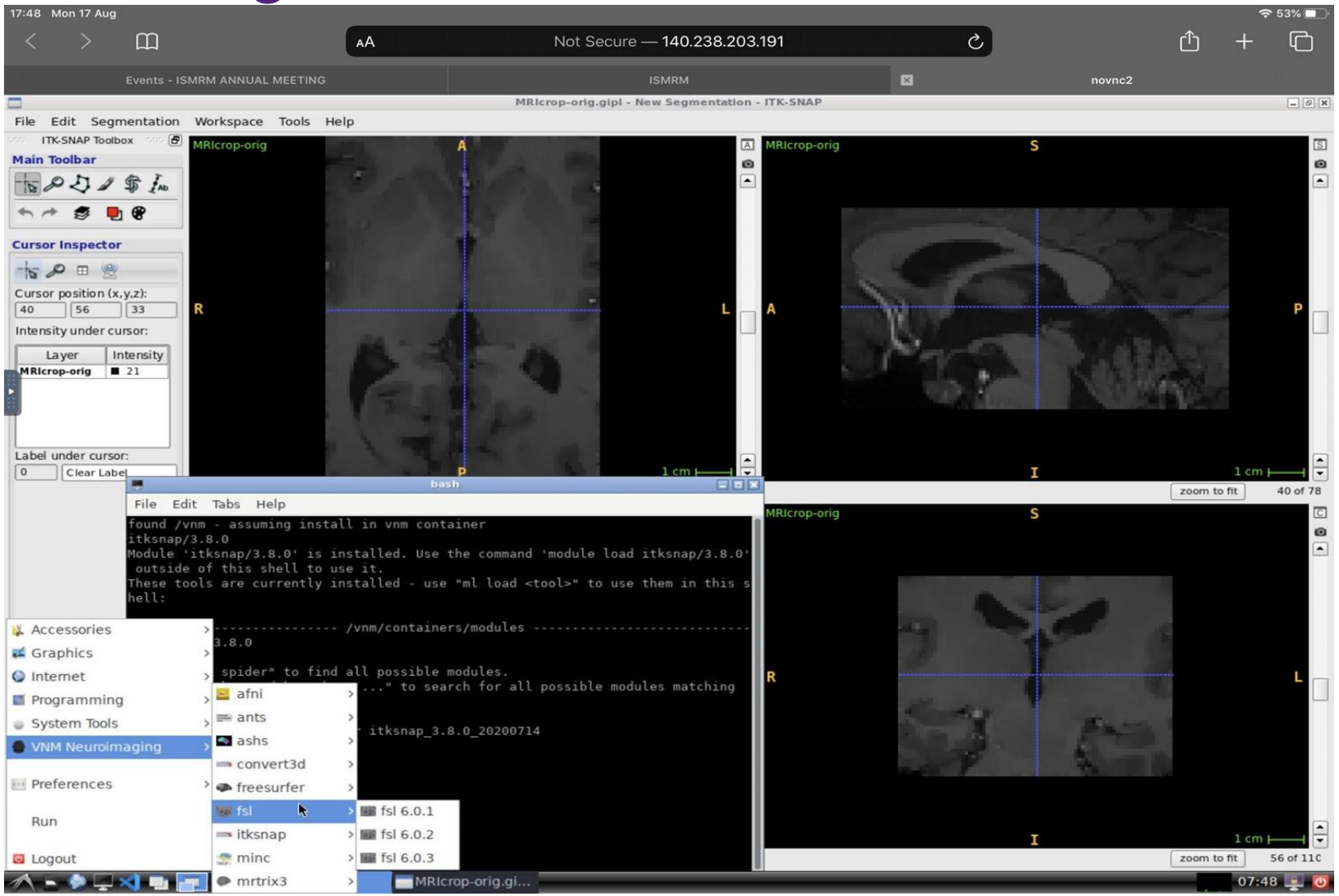


Contributions welcome - github.com/NeuroDesk

- 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

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Swinburne University of Technology