

Supporting Characterisation Communities with Interactive HPC (Characterisation Virtual Laboratory)

www.cvl.org.au

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Demonstration Outline

What is the CVL (Characterisation Virtual Laboratory) ?

What is a virtual laboratory

What is a workbench?

What do we provide?

What are tools we have developed? What are we reusing?

How do we manage research software? (How do we receive contributions from the community?)

How are we making CVL sustainable (Federation of sites nationally)





What is the CVL?

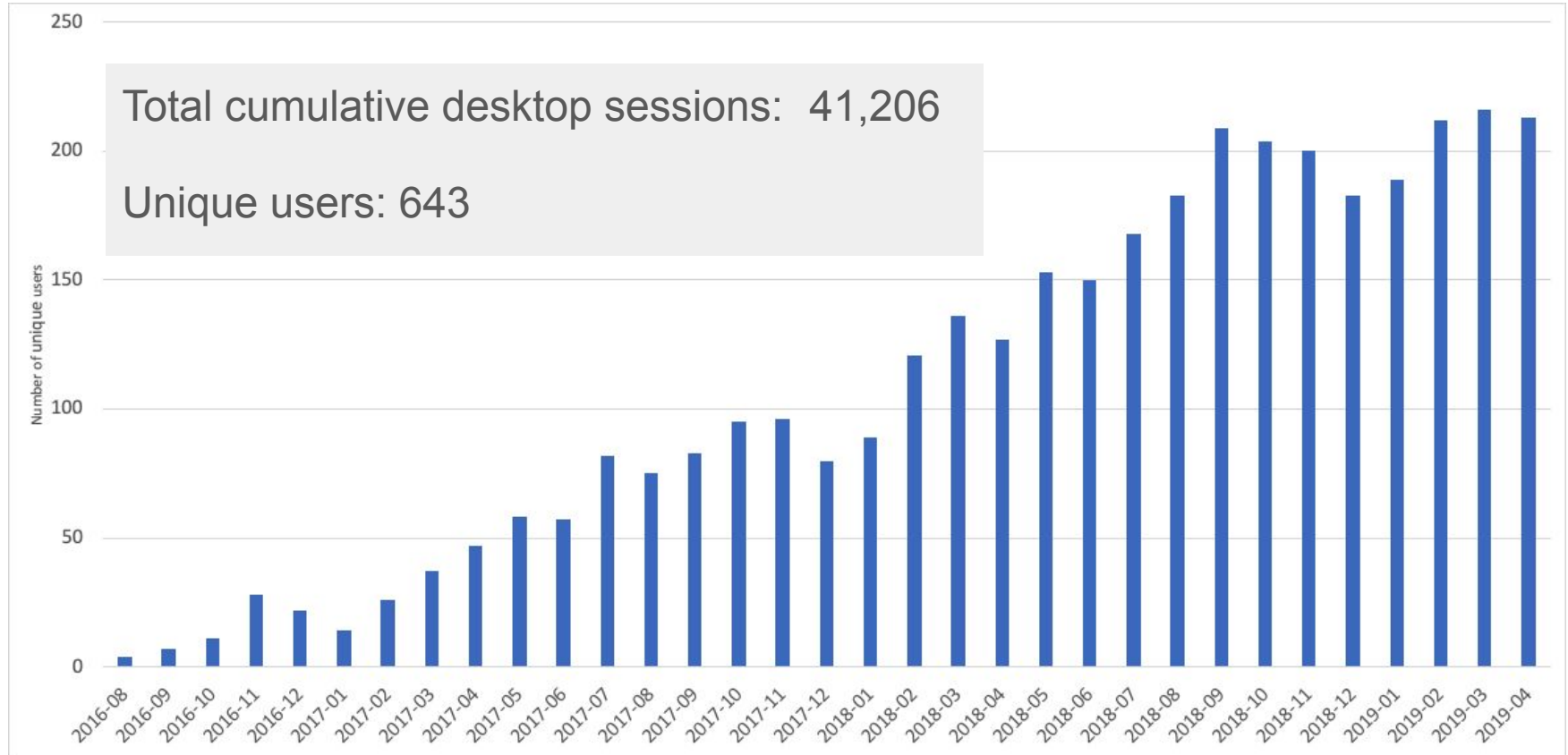
The **Researcher** view:

A single place where you can access your characterisation data and software tools, in a user friendly format.

Project (C-DeVL) view:

A program of work to connect Australian Characterisation instruments with data management environments, tools and analysis pipelines on the Australian research cloud.

CVL Desktop Unique Users per month (CVL@MASSIVE) 08/2016 - 04/2019



What do we provide? (Interactive HPC)

One Caveat

```
$ ping m3.massive.org.au
```

```
PING m3.massive.org.au (118.138.254.157): 56 data bytes
```

```
64 bytes from 118.138.254.157: icmp_seq=0 ttl=45 time=178.006 ms
```

```
64 bytes from 118.138.254.157: icmp_seq=1 ttl=45 time=192.210 ms
```

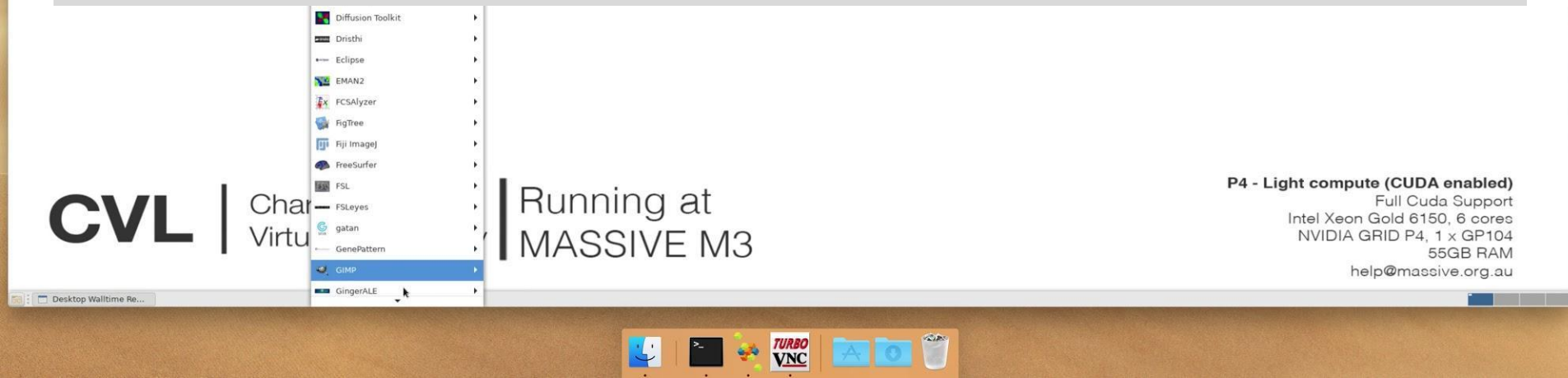
```
64 bytes from 118.138.254.157: icmp_seq=2 ttl=45 time=177.006 ms
```

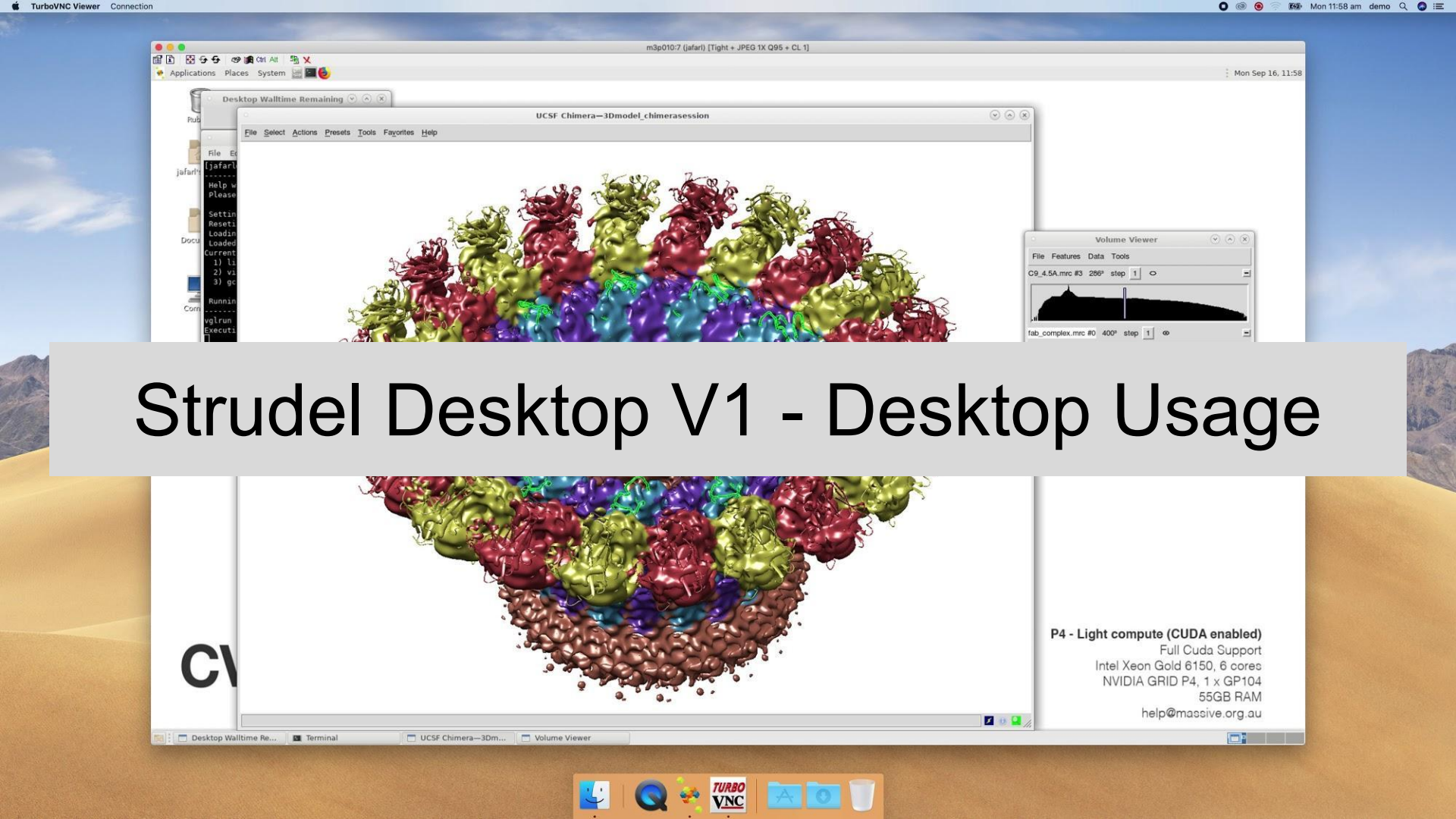
```
64 bytes from 118.138.254.157: icmp_seq=3 ttl=45 time=173.014 ms
```

Live Demo of Strudel Desktop V1



Strudel Desktop V1 - Login process





Strudel Desktop V1 - Desktop Usage

CV

P4 - Light compute (CUDA enabled)

Full Cuda Support
Intel Xeon Gold 6150, 6 cores
NVIDIA GRID P4, 1 x GP104
55GB RAM
help@massive.org.au

desktop.cvl.org.au

Strudel Web

Send feedback

Lance.Wilson@monash.edu

MASSIVE M3

M3 STANDARD DESKTOP

M3 LARGE DESKTOP

M3 Standard Desktop

Launch a desktop

Nodes: 1, Processors: 3

Memory (gb): 13, Time (hours): 4

LAUNCH

Running desktops

You currently have no running desktops.

Server messages

Any messages from the server will be displayed here.

Strudel Web & Desktop

desktop.cvl.org.au

Strudel Web

Applications, Places, System

Applications

- Structural Biology
- Bioinformatics
- Neuroimaging
- Cytometry
- Cryo-Electron Microscopy
- Neutron Beam Imaging
- General Imaging Tools
- Light Microscopy
- General Scientific
- Full List of Apps

Feedback? Please email help@massive.org.au and let us know!

3D Slicer

Aarnet Cloudstor+

adsv

AFNI

Amira

Analyze

Avizo

Beast1

Beast2

Caret

CCP4

Cell Ontology

Cell Profiler

Cell Profiler Analyst

ChimeraX

Chrome

Connectome

Convert3D

Cryo EM processing tool

Cryosparc

CST Studio Suite

Cytoscape

Diffusion Toolkit

Drishti

Eclipse

EMAN2

Created 6 months ago

P6

Desktop Walltime Re...

Projects | cryoSPARC v...

Details

Job Builder

PROJECTS

28 Projects, 53 Workspaces, 1105 Jobs

RECENT PROJECTS

P1: cryosparc_v2_test

Aldolase Arctica

jJM_talos

NEW_GLP

Lance Wilson Admin

M3 Standard Desktop

No CUDA Support (e.g. GCTF, and Caffe)

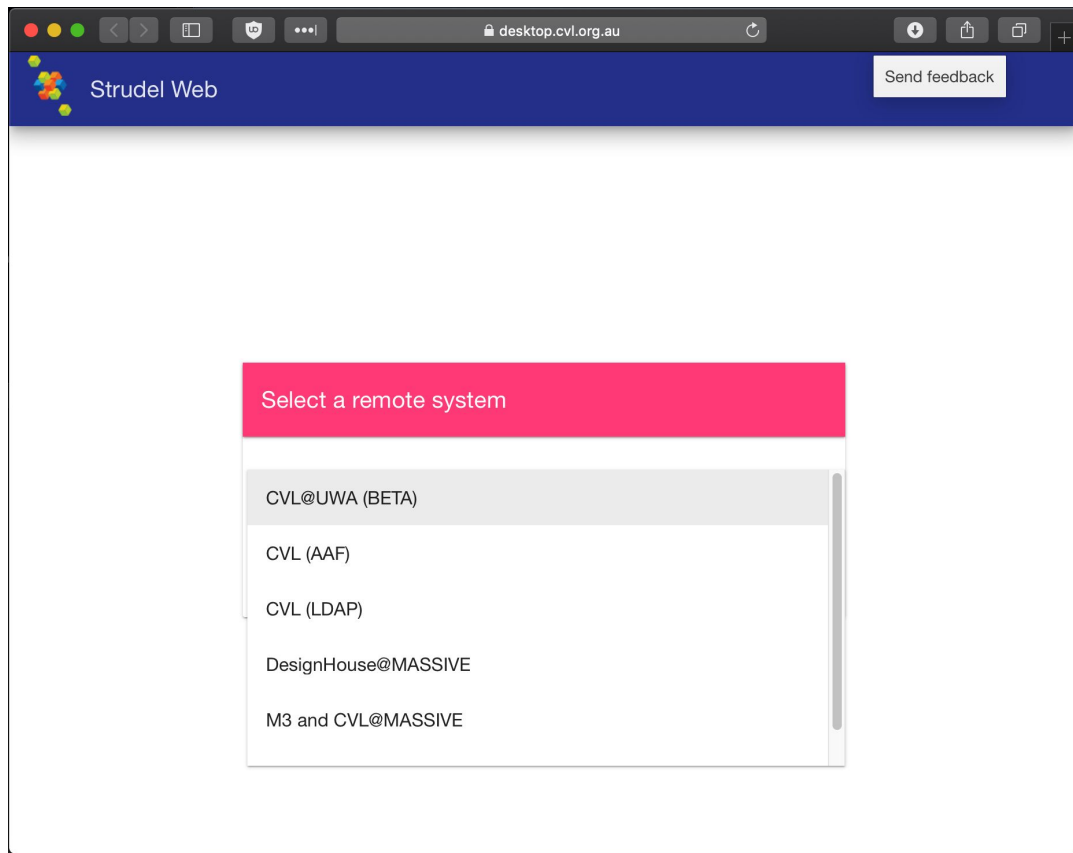
Intel E5-2680 v3, 3 cores

NVIDIA GRID K1, 1 x GK107

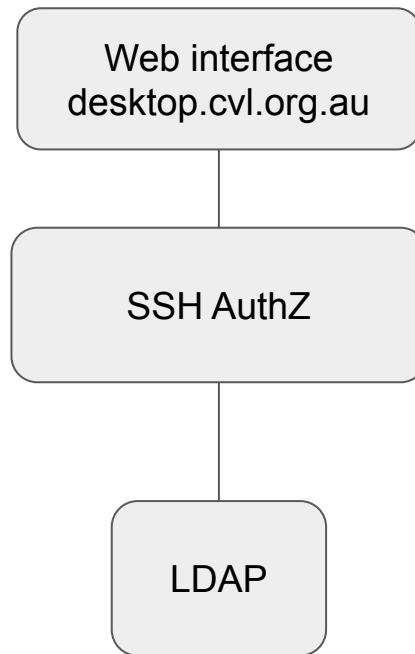
13GB RAM

help@massive.org.au

CVL | Characterisation Virtual Laboratory



Strudel Web & Desktop



Strudel Web

Lance.Wilson@monash.edu

M3 Standard Desktop

SIGN OUT

MASSIVE M3

M3 STANDARD DESKTOP

M3 LARGE DESKTOP

Launch a desktop

Nodes: 1, Processors per node: 3, Memory (gb): 13, Time (hours): 4, Project: br76

LAUNCH

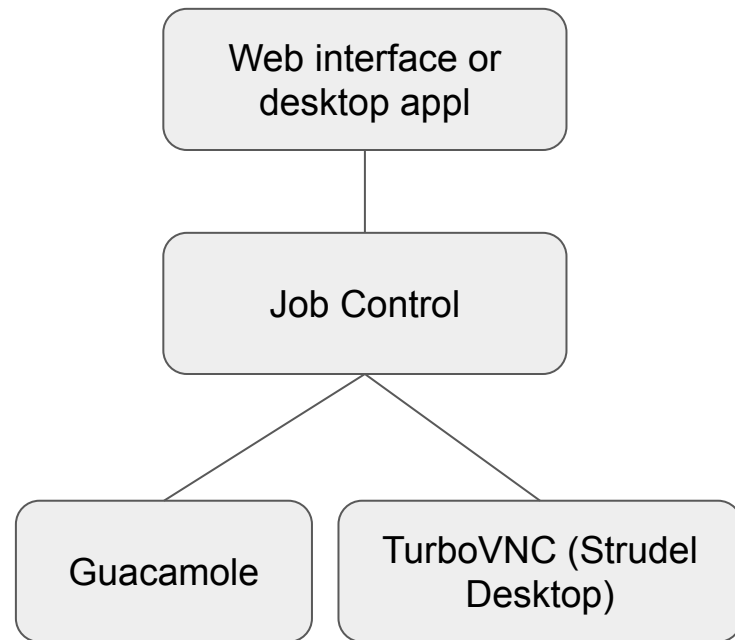
Running desktops

You currently have no running desktops.

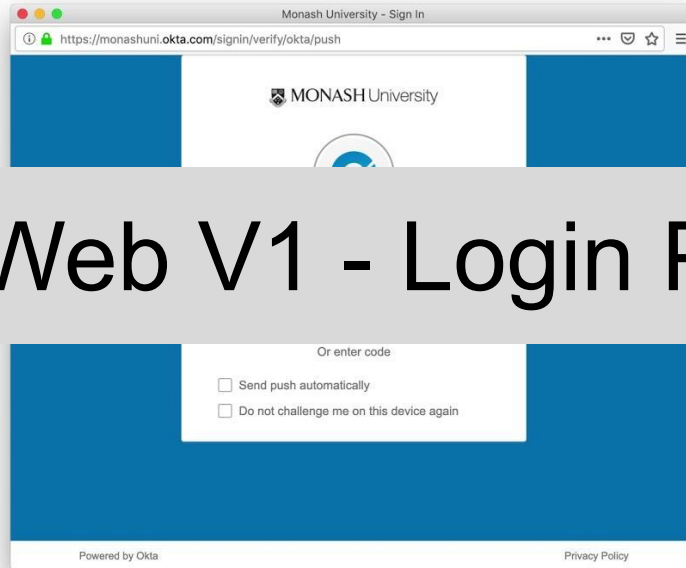
Server messages

Any messages from the server will be displayed here

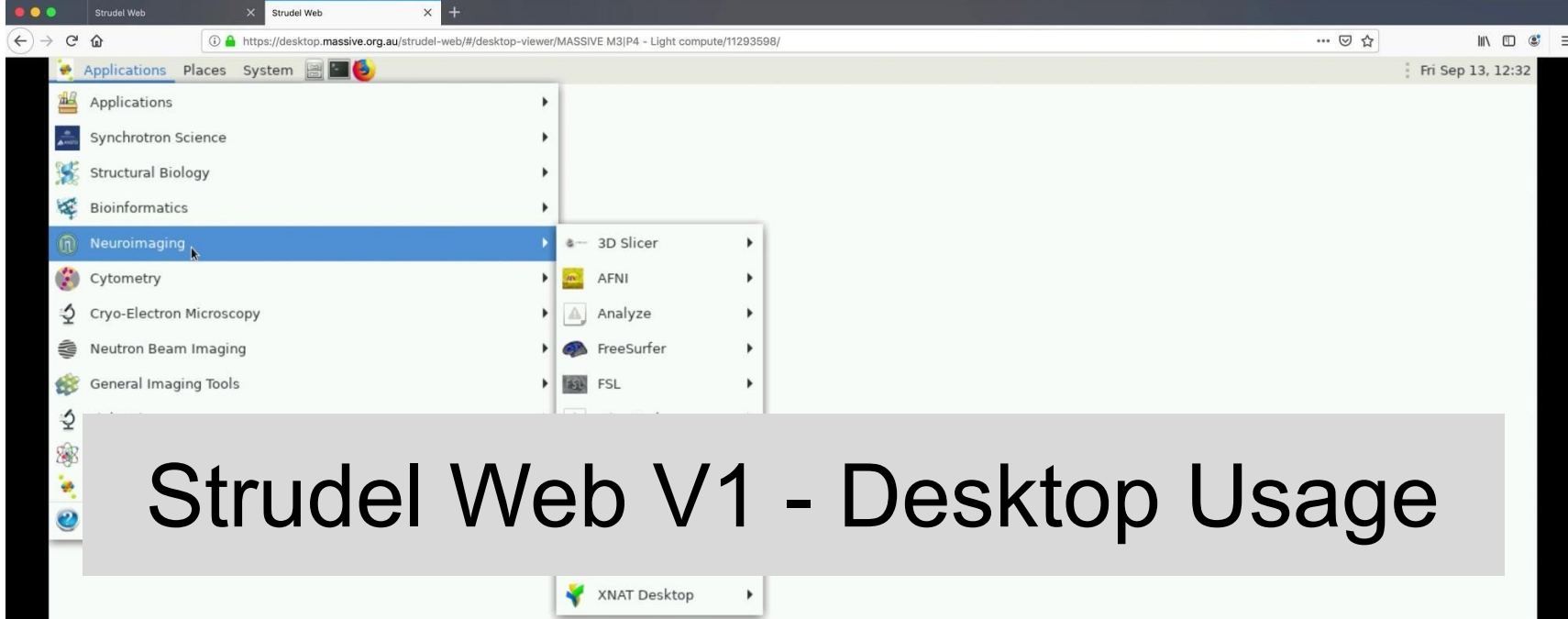
Strudel Web & Desktop



Live Demo of Strudel Web V1



Strudel Web V1 - Login Process



Strudel Web V1 - Desktop Usage

CVL

Characterisation
Virtual Laboratory

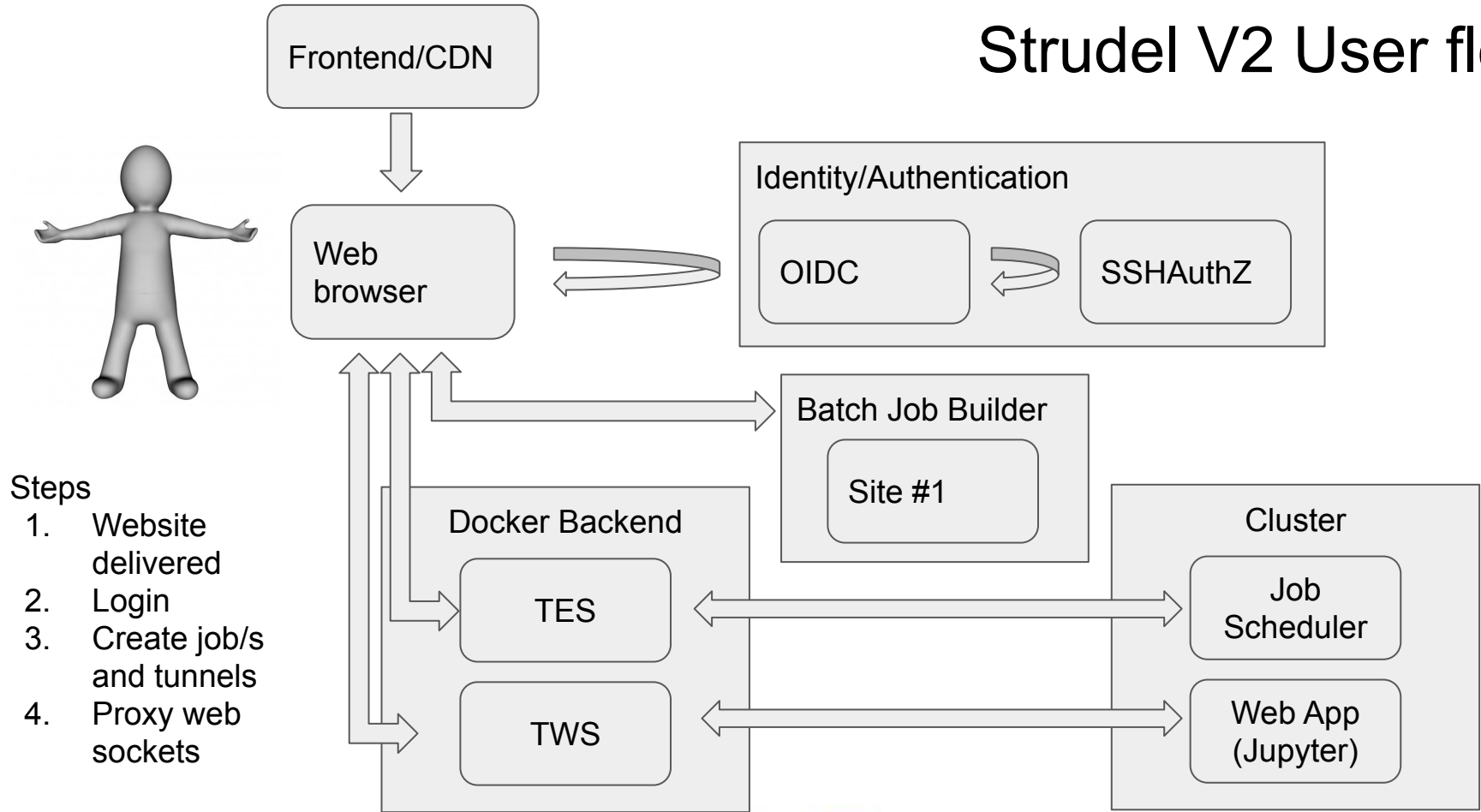
Running at
MASSIVE M3

P4 - Light compute (CUDA enabled)

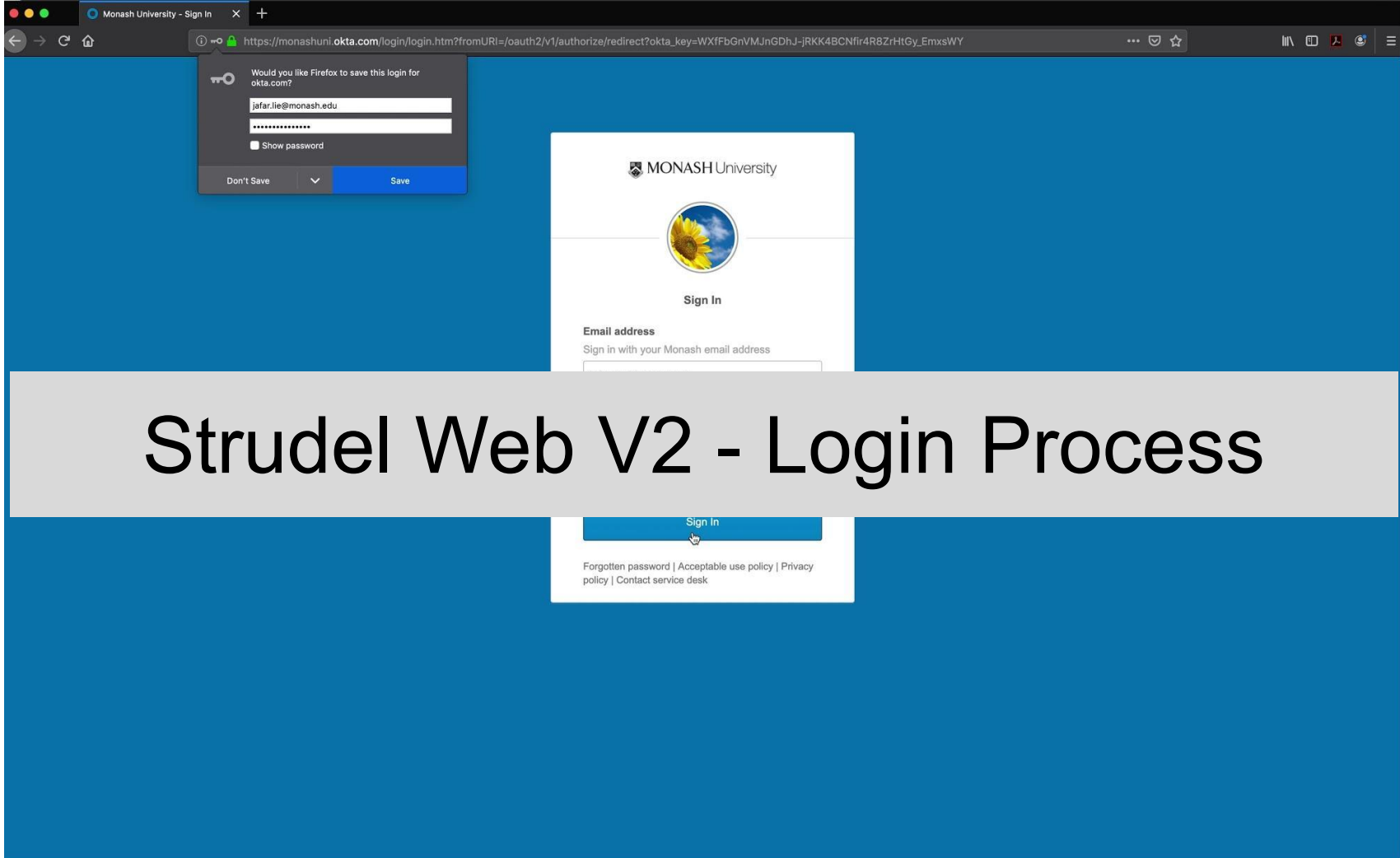
Full Cuda Support
Intel Xeon Gold 6150, 6 cores
NVIDIA GRID P4, 1 x GP104
55GB RAM
help@massive.org.au

What are tools we have developed?

Strudel V2 User flow



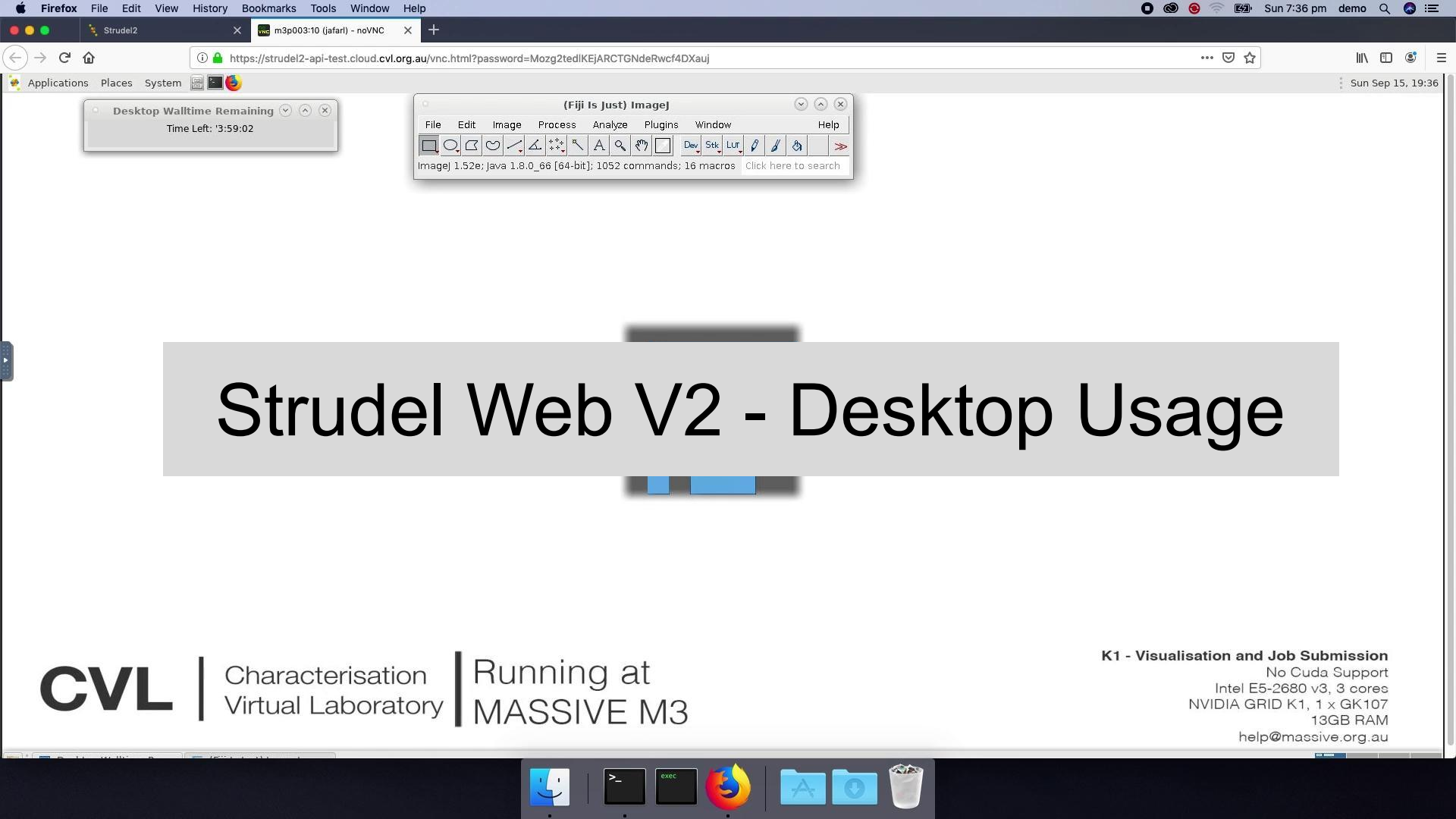
Live Demo of Strudel Web V2



Strudel Web V2 - Login Process

Sign In

[Forgotten password](#) | [Acceptable use policy](#) | [Privacy policy](#) | [Contact service desk](#)



Strudel Web V2 - Desktop Usage

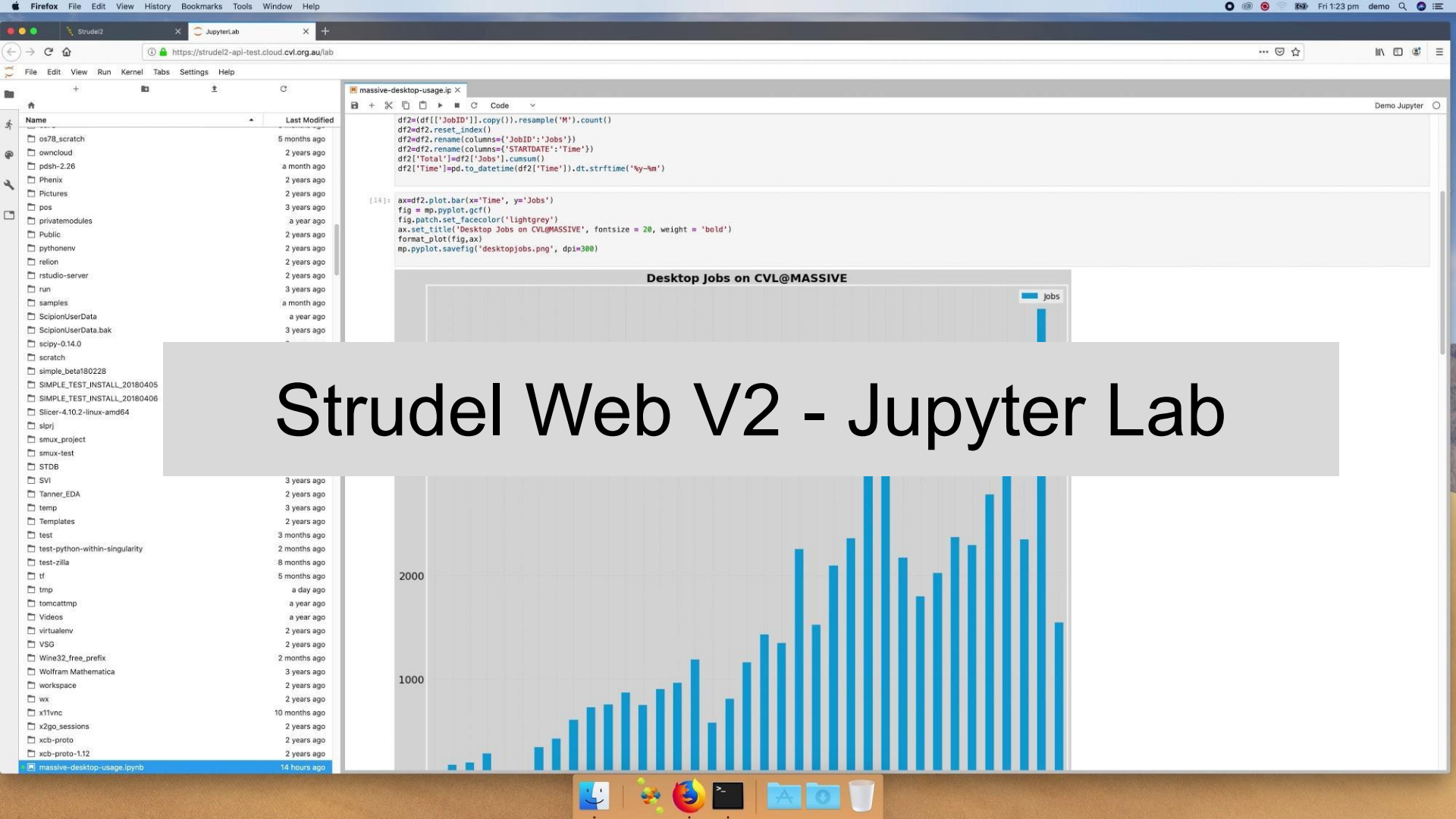
CVL

Characterisation
Virtual Laboratory

Running at
MASSIVE M3

K1 - Visualisation and Job Submission

No Cuda Support
Intel E5-2680 v3, 3 cores
NVIDIA GRID K1, 1 x GK107
13GB RAM
help@massive.org.au



Strudel Web V2 - Jupyter Lab

How do we manage research software? (How do we get contributions from the community?)

Federated Research Software Stacks

- Procedures for contributions have been developed ([link](#))
- A public repository is now available for container build scripts

<https://github.com/Characterisation-Virtual-Laboratory/CharacterisationVL-Software>

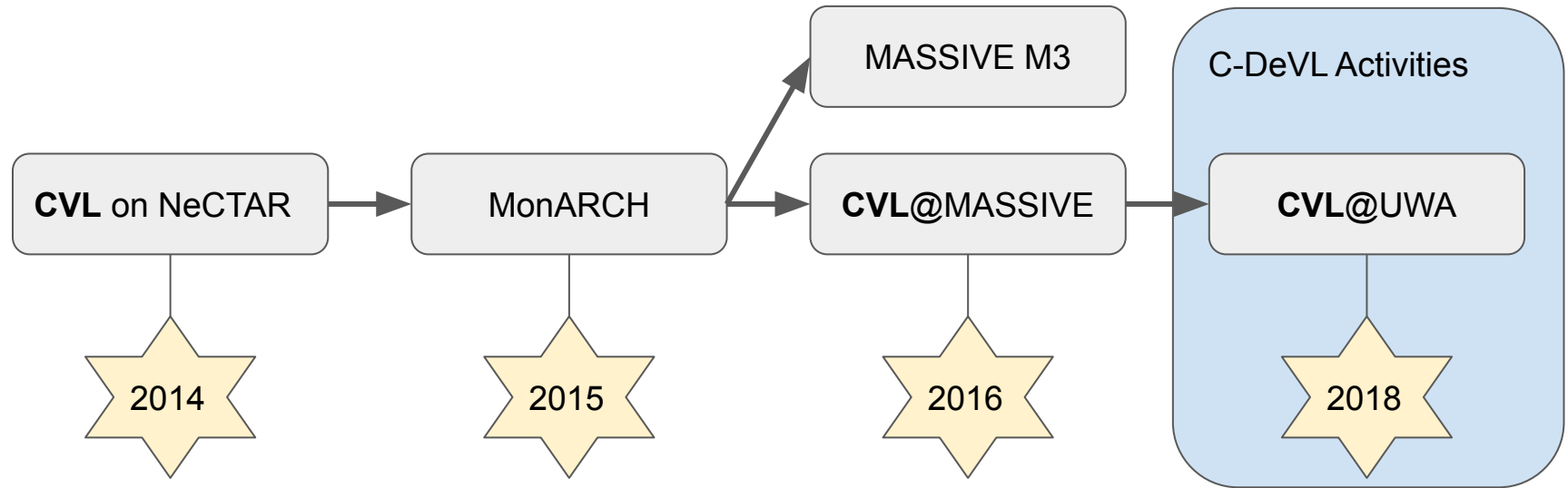
- 40 Packages have been committed to the repositories (and growing)
- Pre-built containers are available from a public repository (Singularity Hub)
- Ongoing work to accommodate disparate clusters

What communities (new and/or existing) are important to you?

How are we making CVL sustainable (Federation of nodes nationally)

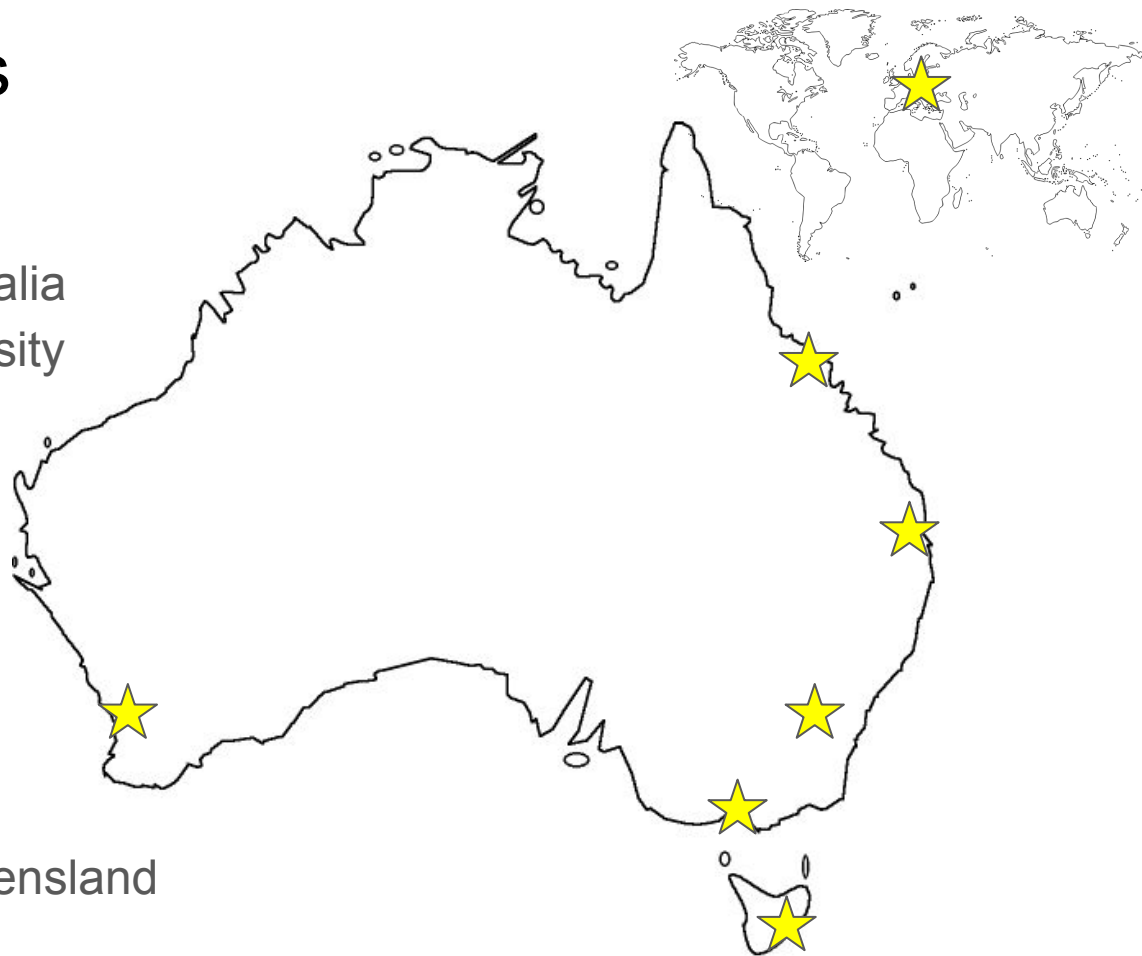
CVL “Cluster in a Box” Deployment Technology

Timeline of development and reuse



Strudel Deployments

- University of Queensland
- University of Western Australia
- Central Queensland University
- NCI
- Pawsey
- Julich
- TERN
- TPAC
- Swinburne University
- University of Melbourne
- University of Southern Queensland



Reusable Software and Infrastructure

- Strudel and Strudel Web
- MyTardis (www.mytardis.org)
- AuthZ (authentication certificates)
- Ansible scripts for all services/applications
- Data repatriation scripts from ANSTO Australian Synchrotron
- Software containers

Demo

Strudel Web V1

How do we manage research data?

MyTardis Ecosystem

<https://store.synchrotron.org.au/dataset/54331>

<https://store.erc.monash.edu/dataset/13>



Live Demo

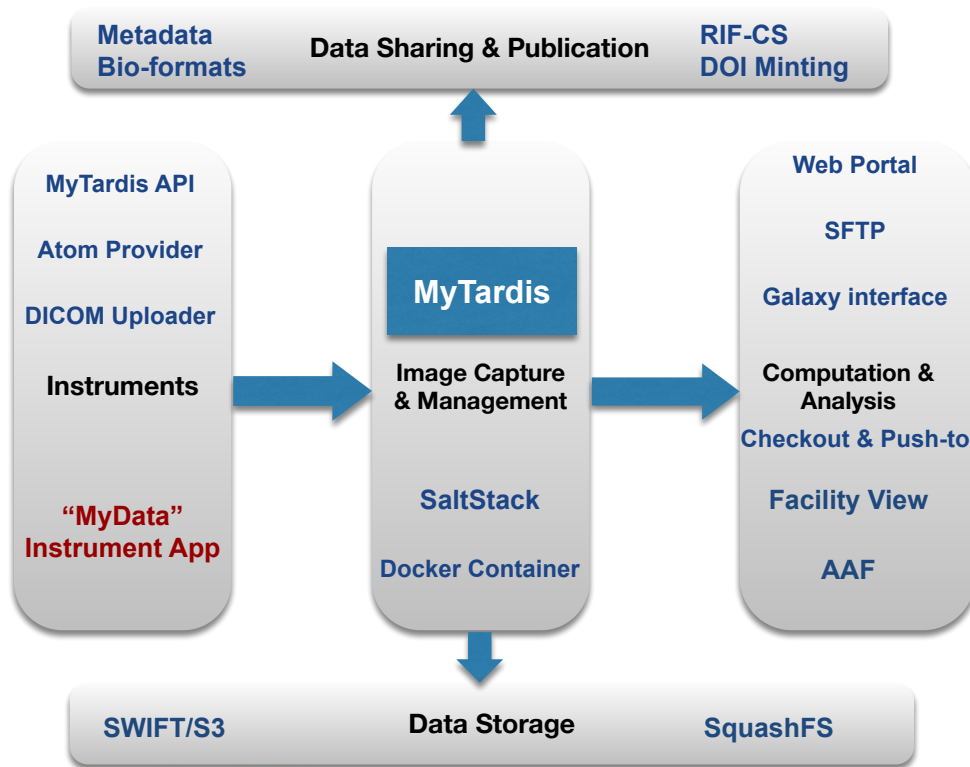
[MyTardis - Monash University](#)

What is MyTardis?

A data management system for instruments - <http://mytardis.org/>

MyTardis is a data management system, developed by Monash, for instrument data.

The Monash instance of the MyTardis service is called Store.Monash



Store.Monash

Monash University instance of the
MyTardis



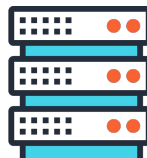
94

Instruments



12 Million

Data Files



0.75 PB

Managed Storage



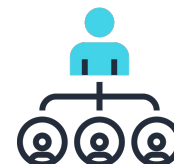
1974

Users



68,189

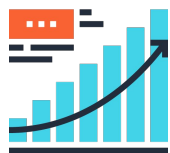
Datasets



1023

Groups

My Tardis Version 4.1 : New Features



Scalable Platform



Dynamic Priority Queue



Sustainable / Scalable Data Storage



Monolithic to Microservices



Easier to Operate and Maintain



Automated Provisioning, Deployment, and Configuration Management



Automatic Scaling



Better Monitoring & Log Aggregation



Better User Experience



Search Improvements



User Interface Improvements



React

Client-side interaction Improvements

Acknowledgments



<http://www.cvl.org.au/>



<https://github.com/Characterisation-Virtual-Laboratory>



<https://docs.cvl.org.au>



help@cvl.org.au



<http://www.mytardis.org/>



<https://github.com/mytardis/mytardis>



<https://mytardis.readthedocs.io>



store.star.help@monash.edu

CVL and MyTardis has been supported by:



Australian Research Data Commons



Summary

- **Reusable Components**

- Strudel Desktop and Strudel Web (desktop.cvl.org.au)
- MyTardis (www.mytardis.org)
- AuthZ (<https://github.com/monash-merc/ssh-authz>)
- Software containers -
<https://github.com/Characterisation-Virtual-Laboratory/CharacterisationVL-Software>

- **Federation**

- www.cvl.org.au
- <https://github.com/Characterisation-Virtual-Laboratory>