



# Scientific Computing RTP



## Part 1 : Interactive computing

`warwick.ac.uk/scrtp`

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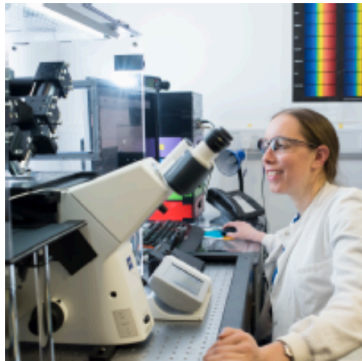
Director, Centre and RTP for Scientific Computing

# Scientific Computing RTP

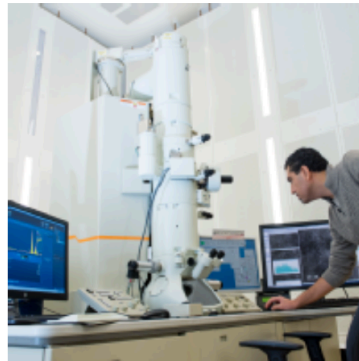
- ▶ What is the Scientific Computing RTP?
- ▶ SC RTP-managed Linux computers
- ▶ Support and common problems
- ▶ High performance computing
- ▶ Research Software Engineering



# Research Technology Platforms



Advanced Bioimaging



Electron Microscopy



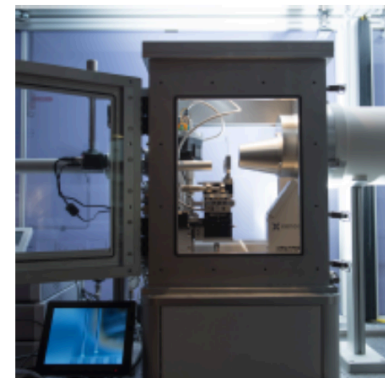
Spectroscopy



Polymer Characterisation



Scientific Computing



X-ray Diffraction



# Scientific Computing RTP

- ▶ Shared infrastructure
  - Managed Linux desktop environment
  - Home & Group storage (separate to ITS H: and M: drives)
  - Hosting of servers owned by groups/departments
  
- ▶ Shared equipment
  - Taskfarm
  - Tinis
  - Orac
  - Athena (HPC Midlands Plus)



# Some statistics (25/09/2019)

## ▶ Managed Linux machines

- 153 Linux desktops
- 70 dedicated compute nodes
- 727 unique users since August 2018 (new desktop software release)

## ▶ HPC clusters

- Orac : 198 unique users since 2017
- Tinis : 677 " " " 2015

## ▶ Storage

- 271TB allocated in /home, 950TB in /storage



# SCRTP Desktop Linux

`warwick.ac.uk/scrtp/desktop/`

# Getting access

- ▶ <https://warwick.ac.uk/scrtp/desktop/gettingstarted/>
- ▶ You need to identify an academic supervisor
  - For modules using our facilities, pick the module leader
  - For research projects, pick your research supervisor
- ▶ DO read the Acceptable Use Policy (AUP)
- ▶ DO subscribe to `scrtp-linux-user` mailing list



# Remote desktop

- ▶ Access from your laptop is available using standard `ssh` terminal, free X2Go software, standard RTP or via the web (`avocado.csc.warwick.ac.uk`)
- ▶ *Shared* remote desktop hosted by `godzilla.csc.warwick.ac.uk`



- This is a *shared resource*, there may be dozens of people logged in at any time
- To be used for editing files, compiling code, plotting simple graphs or submitting computational jobs to the taskfarm *only*
- You must **NOT** run significant computations of any kind on godzilla. This includes calculations within Matlab / Mathematica
- Very strict ‘three strikes’ policy on this





# Machines in the complexity complex

► Older Dell OptiPlex 9010 machines

bulalo.complexity.warwick.ac.uk  
caldereta.complexity.warwick.ac.uk  
lechon.complexity.warwick.ac.uk  
niliga.complexity.warwick.ac.uk  
okoy.complexity.warwick.ac.uk  
rilyeno.complexity.warwick.ac.uk  
torta.complexity.warwick.ac.uk

Alive & well as of 25/09/2019

sinuglaw.complexity.warwick.ac.uk  
kinilaw.complexity.warwick.ac.uk  
jamon.complexity.warwick.ac.uk  
inihaw.complexity.warwick.ac.uk  
halabos.complexity.warwick.ac.uk  
embutido.complexity.warwick.ac.uk  
adobo.complexity.warwick.ac.uk

Missing in action



# GPU-equipped workstations

- ▶ Newer high-end workstations

`kumeta.scrtp.warwick.ac.uk`

`keiko.scrtp.warwick.ac.uk`

`kalocsa.scrtp.warwick.ac.uk`

(+ one more TBA this week)

- ▶ 6 core / 12 thread Xeon processors, 64GB RAM
- ▶ Quadro RTX 6000 workstation class GPU
- ▶ Ideal for GPU-accelerated analytics, machine learning etc.

Available for MathSys students to use remotely and interactively



# Software



## ▶ Packages

- Part of the Linux distribution ([CentOS 7](#)), or distributed via managed repositories ([EPEL](#), [CernVM-FS](#))
- Available via the MATE software menu or in the default terminal environment

## ▶ Environment modules

- Additional software imported into your terminal environment with `module load` commands
- Allows multiple software environments on one system
- Use `module spider` to search



# Containers & remote notebooks

## ▶ Python notebooks

```
$ module load GCC/7.3.0-2.30 OpenMPI/3.1.1 IPython/7.2.0-Python-3.6.6  
$ jupyter notebook --no-browser --ip=`hostname -f`
```

## ▶ Julia notebooks

```
$ module load GCC/7.3.0-2.30 OpenMPI/3.1.1 IPython/7.2.0-Python-3.6.6  
$ module load julia/1.0.0  
$ julia -e 'using Pkg ; pkg"add IJulia" '  
$ jupyter notebook --no-browser --ip=`hostname -f`
```

## ▶ Containers

```
$ singularity pull docker://ubuntu  
$ singularity shell ubuntu_latest.sif
```



# Getting help

`warwick.ac.uk/scrip/support/`

# Top 3 common problems

- ▶ I need admin privileges to “install” software in my account
  - No you don’t, even if some random guy/developer says you do
  - [warwick.ac.uk/scrtp/support/support\\_faq/#software](http://warwick.ac.uk/scrtp/support/support_faq/#software)
  - Or load the Anaconda module and go nuts!
- ▶ I can’t log in
  - Have you mucked about with your `.bashrc`, `.profile` or similar?
  - Read the desktop documentation on startup scripts
- ▶ My managed computer won’t boot
  - Have you moved it to a different network port without telling us?



# Pro Tip : Software in user space

## ► Software distributed as source code

```
$ ./configure  
$ make  
$ sudo make install
```



```
$ ./configure --prefix=$HOME  
$ make  
$ make install
```



```
$ cmake .  
$ sudo make install
```



```
$ cmake --DCMAKE_INSTALL_PREFIX=$HOME .  
$ make install
```



## ► Python packages via pip

```
$ pip install somepackage
```



```
$ pip install --user somepackage
```



```
$ pip install --prefix=$HOME somepackage
```



# Pro Tip : Environment variables

## ▶ `command not found`

- executable file not in `$PATH`
- `export PATH=$PATH:$HOME/bin:$HOME/.local/bin`

## ▶ `error while loading shared libraries`

- Shared object (`.so`) not in `$LD_LIBRARY_PATH`
- `export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$HOME/lib`

## ▶ (Python) `ImportError: No module named ...`

- Python package directory not in `$PYTHONPATH`
- `export PYTHONPATH=$PYTHONPATH:$HOME/lib/python3.6/site-packages`





# Pro Tip : Using libraries

- ▶ `pkg-config` is your friend

```
$ module load GCC/7.3.0-2.30 OpenMPI/3.1.1 FFTW/3.3.8
$ gcc gaussian_fftw3.c
error: undefined reference to 'fftw_create_plan'

$ pkg-config --libs fftw3
-L/warwick/desktop/2018/software/./FFTW/3.3.8/lib -lfftw3

$ gcc gaussian_fftw3.c `pkg-config --libs fftw3`
$
```

