Scientific Computing RTP

Part 1 : Computers, Access, & Support

WARWICK

`warwick.ac.uk/scrtp`
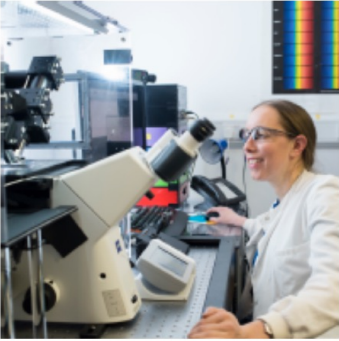
Presenter

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Slides adapted from

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Director, Scientific Computing RTP
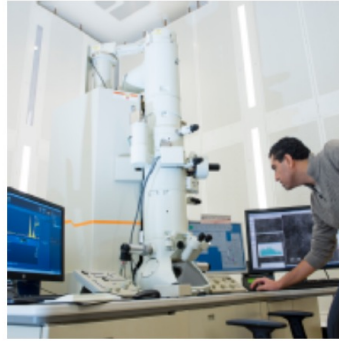
Scientific Computing RTP

▶ What is the Scientific Computing RTP?

▶ SCRTP-managed Linux computers

▶ Support and common problems

▶ High performance computing

▶ Research Software Engineering
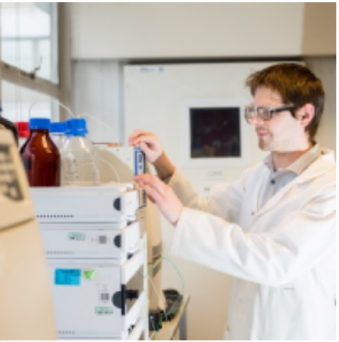
Research Technology Platforms
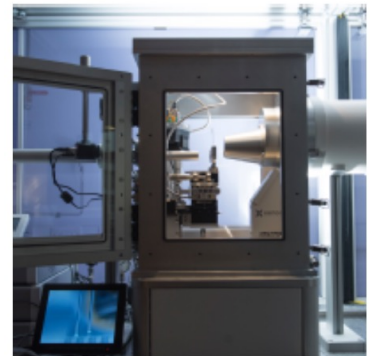
Advanced Bioimaging

Electron Microscopy

Spectroscopy

Polymer Characterisation

Scientific Computing

X-ray Diffraction

SCRTP Equipment and Infrastructure

▶ 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 (all accessible via a Slurm Queue)

– Taskfarm (CPU Compute Nodes 48 Cores)

– Avon (Nodes inc. GPU & high-speed interconnect via a Batch Queue)

– Sulis (Available by application only)

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 RDP 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 (warranty expired July 2017)

bulalo.complexity.warwick.ac.uk
caldereta.complexity.warwick.ac.uk
dinuguan.complexity.warwick.ac.uk
embutido.complexity.warwick.ac.uk   Alive & well as of 11/10/2021
jamon.complexity.warwick.ac.uk
niliga.complexity.warwick.ac.uk
torta.complexity.warwick.ac.uk

kinilaw.complexity.warwick.ac.uk
halabos.complexity.warwick.ac.uk
adobo.complexity.warwick.ac.uk
inihaw.complexity.warwick.ac.uk   Missing in action
rilyeno.complexity.warwick.ac.uk
sinuglaw.complexity.warwick.ac.uk

GPU-equipped workstations

▶ Newer high-end workstations

kumeta.scrtp.warwick.ac.uk

keiko.scrtp.warwick.ac.uk

All up as of 11/10/21

kalocsa.scrtp.warwick.ac.uk

kaluga.scrtp.warwick.ac.uk

▶ 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

Remote interactive servers for CDTs

▶ Shared (with HETSYS CDT) servers for remote interactive work

▶ No batch queue submission necessary. Just log in and run.
  - `hetmathsys[1-4].scrtp.warwick.ac.uk`

▶ 4x servers each with
  - 2x Xeon Processors, 40 cores/processor
  - 384 GB RAM
  - 10Gb/s connection to /home, /storage and the SCRTP HPC clusters

▶ *Shared* resource – be a good citizen.

Software

▶ Packages

– Part of the Linux distribution (CentOS9), 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

Connect to the VPN first to be able to reach your jupyter notebook.

▶ Python notebooks

```
$ module load GCC/11.3.0 OpenMPI/4.1.4 IPython/8.5.0
$ jupyter notebook --no-browser --ip=`hostname -f`
```

▶ Julia notebooks

```
$ module load GCC/11.3.0 OpenMPI/4.1.4 IPython/8.5.0
$ module load julia/1.8.2-linux-x86_64
$ export JULIA_DEPOT_PATH=~/.julia_pkgs/
$ mkdir ~/.julia_pkgs/
$ 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/scrtp/user_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

- 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/8.3.0  OpenMPI/3.1.4 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`
$
```