Scientific Computing RTP

Part 1: Interactive computing

warwick.ac.uk/srtp

Prof. David Quigley
Director, Centre and RTP for Scientific Computing
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
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/](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
  - 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
  
  Alive & well as of 25/09/2019

- 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**
  
  ```bash
  $ 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**
  
  ```bash
  $ 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**
  
  ```bash
  $ singularity pull docker://ubuntu
  $ singularity shell ubuntu_latest.sif
  ```
Getting help

warwick.ac.uk/scrtp/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
  - 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

- 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

```bash
$ module load GCC/7.3.0-2.30 OpenMPI/3.1.1 FFTW/3.3.8
$ gcc gaussian_fft3.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_fft3.c `pkg-config --libs fftw3`
$ 
```