

UCL Research Computing

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- A team within Research IT Services (RITS), which is within ISD (UCL's central IT division)
- We (two teams of ~4) look after UCL's central, and UCL-hosted national services
 - RCI → “The systems team” look after the hardware, OS, are `root`
 - RCAS → “The user support team” look after users, user applications, are `ccspapp`
 - **Together** design, deliver + support all the services

- UCL is a world leading research institution :)
 - Research in almost every field :)
 - *All institutions* see IT as a cost area (i.e. minimise funding) :(

aka

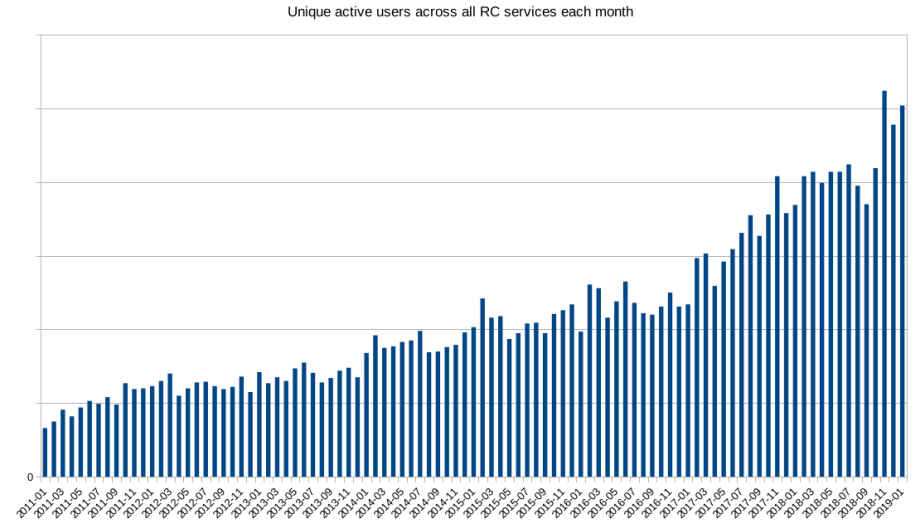
We have limited funding but must support wildly diverse needs.

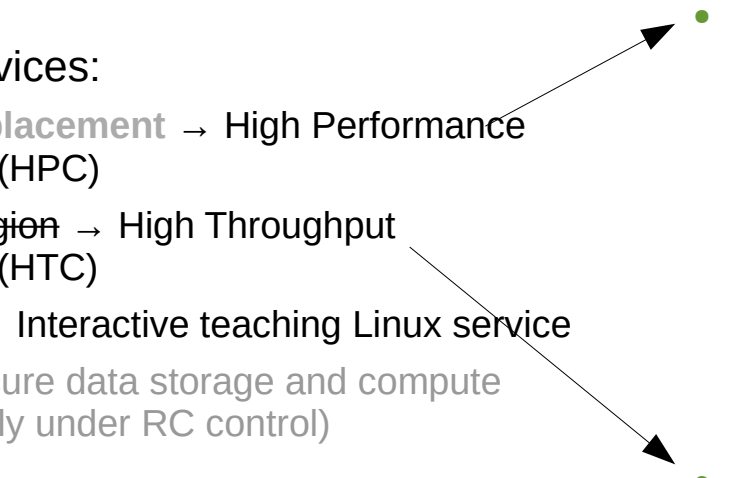
(This is not just true of Research Computing but the whole of ISD!)

The Problem:

- Some users need traditional HPC (massively parallel workloads)
- Some users need HTC (thousands of independent jobs)
- Some users need a mix of the two (High Throughput High Performance Computing?)
- Some users need GPUs
- Some users need terabytes of RAM
- Some users need to use massive amounts of (temporary) storage
- Some users are HPC experts, some are novices
- Some users are developing their own code, some are using centrally installed applications
- Some users...

- Geography
 - There is no space for anything anywhere in central London
 - There is no power for anything anywhere in central London
- Money
 - IT is incredibly underfunded sector-wide
 - HPC is funded worse than that (a national problem, not a UCL one)
 - Not enough money for kit or staff
- Insatiable demand for compute from researchers

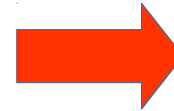
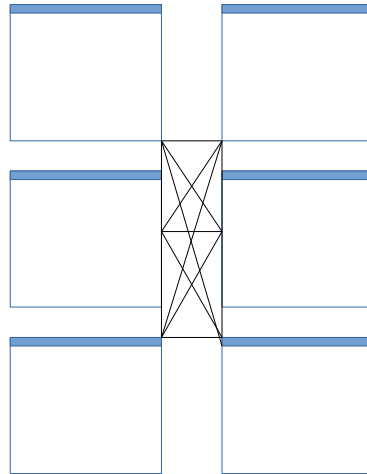
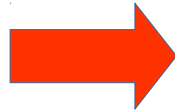
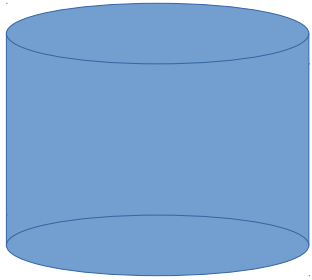


- UCL only services:
 - **Grace, Replacement** → High Performance Computing (HPC)
 - **Myriad, Legion** → High Throughput Computing (HTC)
 - **Aristotle** → Interactive teaching Linux service
 - **DSH** → secure data storage and compute (not currently under RC control)
 - National services:
 - **Thomas** (Tier 2 MMM hub)
 - **Michael** (Faraday Institution)
 - Parallel
 - Single job spans multiple nodes
 - Tightly coupled parallelisation usually in MPI
 - Sensitive to network performance
 - Currently primarily chemistry, physics, engineering
 - High throughput
 - Lots (tens of thousands) of independent jobs on different data
 - High I/O
 - Currently, primarily biosciences, physics, computer science
 - In the future, digital humanities
- 

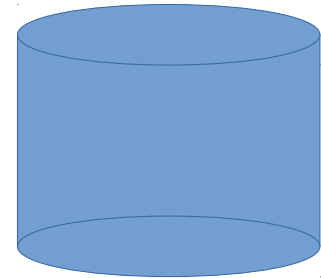
COMMON software stack across RC controlled services

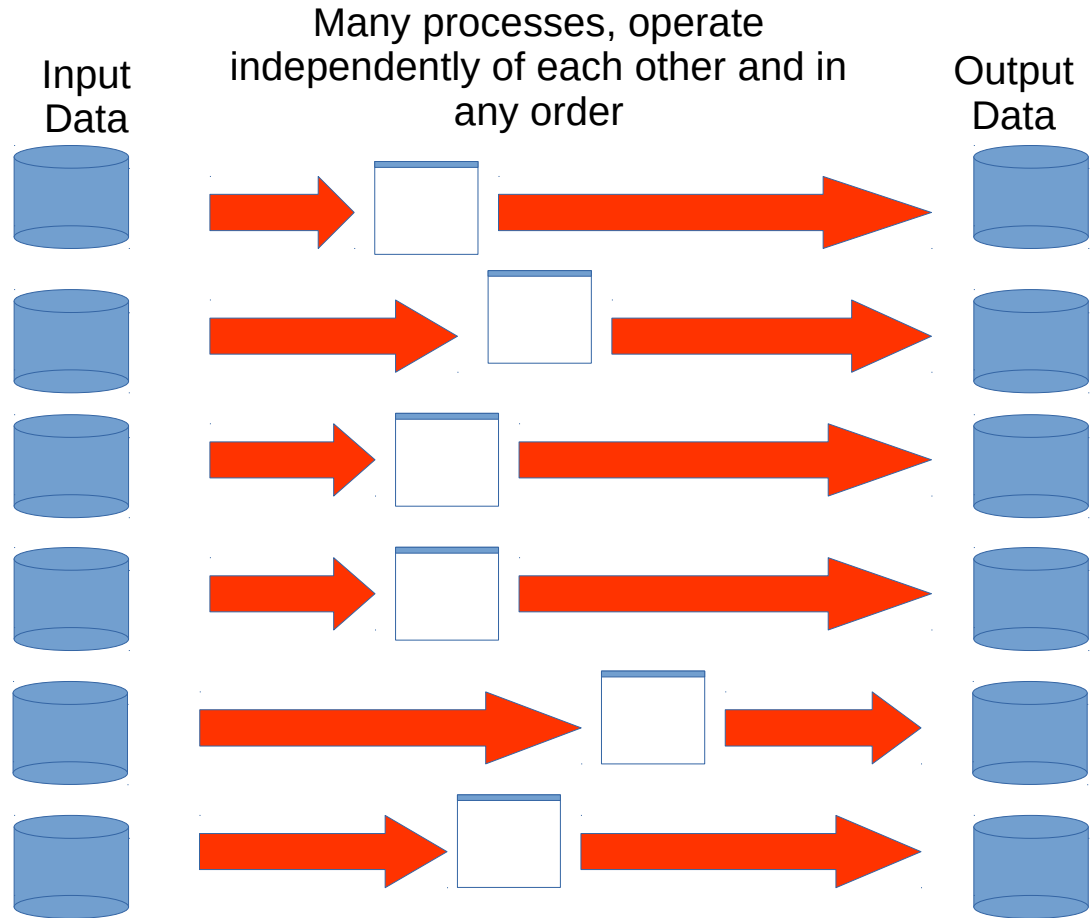
Many processes on many processors
work simultaneously + communicate
between each other

Input Data



Output Data



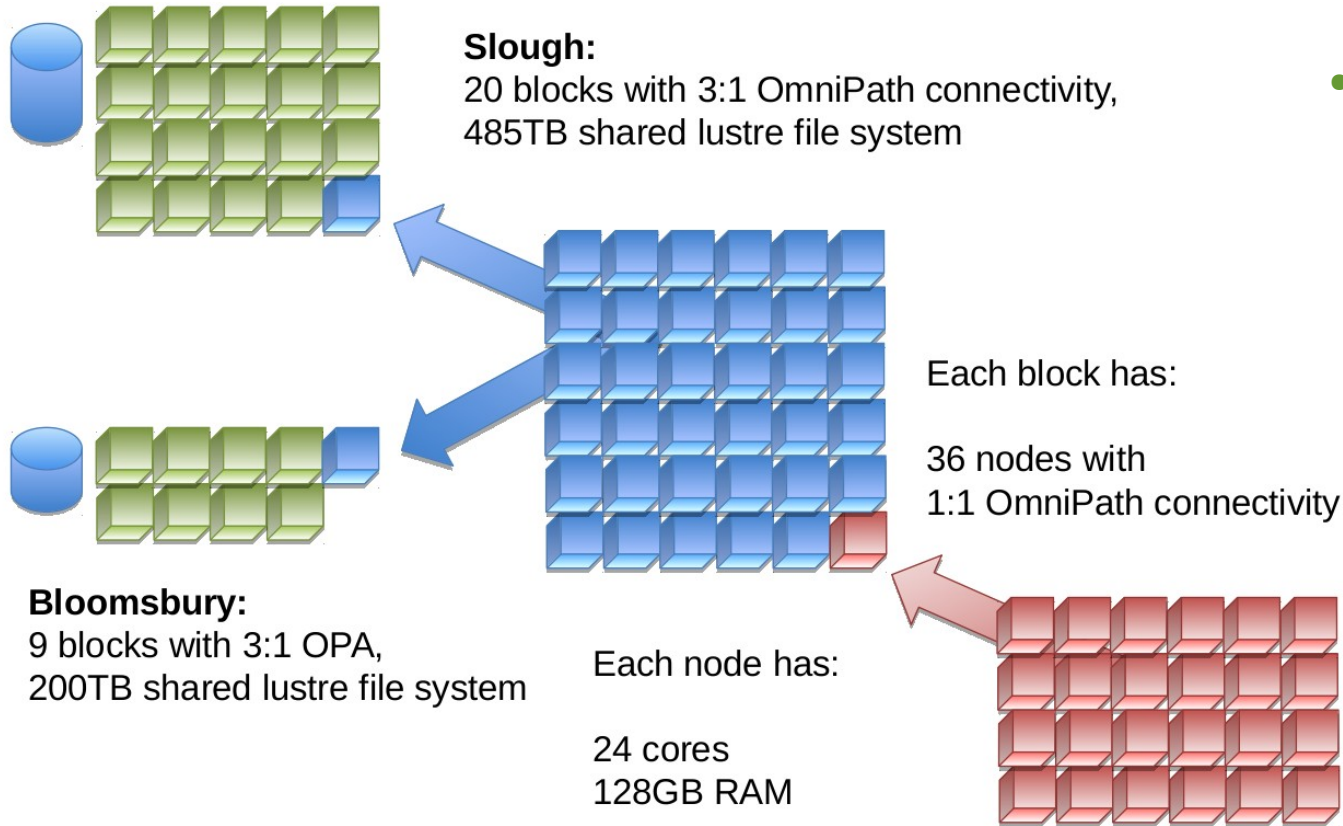


- Grace is UCL's primary HPC service.
 - OCF/Lenovo, QDR IB
 - ~11K cores
 - 16 cores/node
 - 1PB of Lustre storage



- Myriad is UCL's High Throughput/Data intensive service:
 - OCF/Lenovo, EDR IB (storage only)
 - ~3168 cores
 - 8 GPUs
 - 3 high memory nodes
 - 1 PB of Lustre Storage
 - Upgrade project underway (2016 cores, 8 large memory, 16 GPUs, +2PB storage)
- Free and paid access models

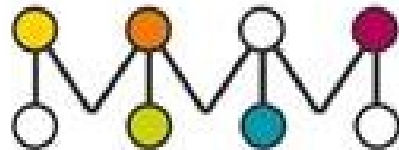




- Two national services,
 - both for specialised research
 - both “High Throughput High Performance Computing”
 - (i.e. arrays of small parallel jobs)

- Thomas (the Tier 2 MMM Hub)
 - Built off of Grace (OPA)
 - 18,000 cores
 - £4M of EPSRC funding
 - Running costs paid for by partner institutions:

Imperial College London, University of Kent, Kings College London, Oxford University, Queen Mary University of London, Queen's University Belfast, University of Southampton and **UCL**
- High Throughput High Performance Computing!
- Running for almost two years.
 - >1,000,000 user jobs to date
 - >2.57x10⁸ CPU hours used by user jobs
 - >29,300 years on one core
 - Upper Palaeolithic start!

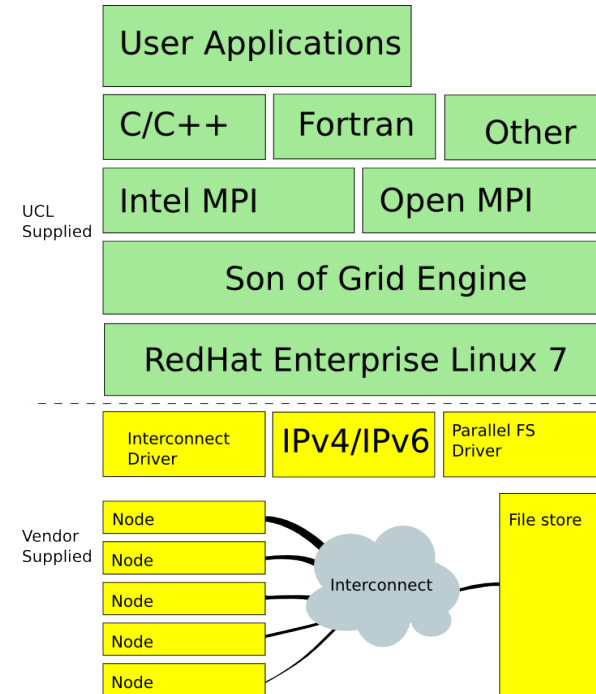


- Michael (the Faraday Institution machine)
 - Built off of Grace (OPA) in summer last year
 - 7,000 cores
 - £1M of external funding



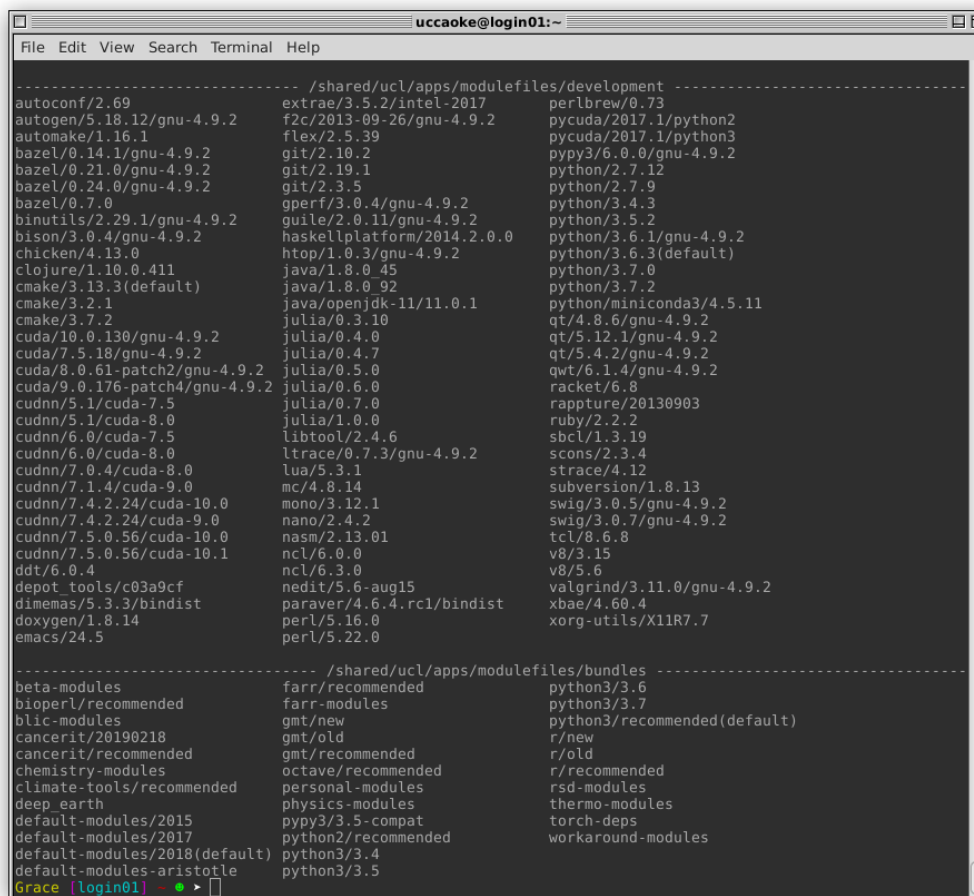
Common software stack

- Deployed across all our resources (inc Thomas + Michael)
 - ~750 user applications + development tools, presented through environment modules
 - Scripts + data from one machine can be run “seamlessly” on another
 - Same interface presented to users
 - **AUTOMATED**



Common software stack

- This is **not** a stack “just for traditional HPC users” (Fortran/C/C++)
- Supports Python (Cpython, Anaconda, PyPy), R, Julia, Perl (+ Bioperl), Java, Clojure, Common Lisp, Scheme, Mono (.Net), Lua, Go, Racket, Ruby, JavaScript, Matlab...
- ML tools like Tensorflow (GPU, MKL variants), Caffe, OpenCV...
- Allow departmental sysadmins access to install specialist applications centrally!



```
ucckoake@login01:~
File Edit View Search Terminal Help
----- /shared/ucl/apps/modulefiles/development -----
autoconf/2.69                extrae/3.5.2/intel-2017      perlbrew/0.73
autogen/5.18.12/gnu-4.9.2    f2c/2013-09-26/gnu-4.9.2    pycuda/2017.1/python2
automake/1.16.1              flex/2.5.39                  pycuda/2017.1/python3
bazel/0.14.1/gnu-4.9.2       git/2.10.2                   pypy3/6.0.0/gnu-4.9.2
bazel/0.21.0/gnu-4.9.2       git/2.19.1                   python/2.7.12
bazel/0.24.0/gnu-4.9.2       git/2.3.5                     python/2.7.9
bazel/0.7.0                  gperf/3.0.4/gnu-4.9.2       python/3.4.3
binutils/2.29.1/gnu-4.9.2    guile/2.0.11/gnu-4.9.2      python/3.5.2
bison/3.0.4/gnu-4.9.2        haskellplatform/2014.2.0.0  python/3.6.1/gnu-4.9.2
chicken/4.13.0               htop/1.0.3/gnu-4.9.2        python/3.6.3(default)
clojure/1.10.0.411           java/1.8.0.45                python/3.7.0
cmake/3.13.3(default)        java/1.8.0.92                python/3.7.2
cmake/3.2.1                  java/openjdk-11/11.0.1      python/miniconda3/4.5.11
cmake/3.7.2                  julia/0.3.10                 qt/4.8.6/gnu-4.9.2
cuda/10.0.130/gnu-4.9.2      julia/0.4.0                  qt/5.12.1/gnu-4.9.2
cuda/7.5.18/gnu-4.9.2         julia/0.4.7                  qt/5.4.2/gnu-4.9.2
cuda/8.0.61-patch2/gnu-4.9.2  julia/0.5.0                  qwt/6.1.4/gnu-4.9.2
cuda/9.0.176-patch4/gnu-4.9.2  julia/0.6.0                  racket/6.8
cudnn/5.1/cuda-7.5           julia/0.7.0                  rapture/20130903
cudnn/5.1/cuda-8.0           julia/1.0.0                  ruby/2.2.2
cudnn/6.0/cuda-7.5           libtool/2.4.6                sbcl/1.3.19
cudnn/6.0/cuda-8.0           ltrace/0.7.3/gnu-4.9.2      scones/2.3.4
cudnn/7.0.4/cuda-8.0         lua/5.3.1                    strace/4.12
cudnn/7.1.4/cuda-9.0         mc/4.8.14                     subversion/1.8.13
cudnn/7.4.2.24/cuda-10.0     mono/3.12.1                   swig/3.0.5/gnu-4.9.2
cudnn/7.4.2.24/cuda-9.0      nano/2.4.2                     swig/3.0.7/gnu-4.9.2
cudnn/7.5.0.56/cuda-10.0     nasm/2.13.01                  tcl/8.6.8
cudnn/7.5.0.56/cuda-10.1     ncl/6.0.0                      v8/3.15
ddt/6.0.4                    ncl/6.3.0                      v8/5.6
depot_tools/c03a9cf          nedit/5.6-aug15               valgrind/3.11.0/gnu-4.9.2
dimemas/5.3.3/bindist        paraver/4.6.4.rc1/bindist     xbae/4.60.4
doxygen/1.8.14               perl/5.16.0                    xorg-utils/X11R7.7
emacs/24.5                    perl/5.22.0

----- /shared/ucl/apps/modulefiles/bundles -----
beta-modules                 farr/recommended              python3/3.6
bioperl/recommended          farr-modules                   python3/3.7
blic-modules                 gmt/new                        python3/recommended(default)
cancerit/20190218            gmt/old                        r/new
cancerit/recommended         gmt/recommended               r/old
chemistry-modules           octave/recommended             r/recommended
climate-tools/recommended   personal-modules               rsd-modules
deep_earth                   physics-modules                 thermo-modules
default-modules/2015         pypy3/3.5-compat               torch-deps
default-modules/2017         python2/recommended            workaround-modules
default-modules/2018(default)  python3/3.4
default-modules-aristotle    python3/3.5

Grace [login01] ~ ● ▶
```

- Most of the code that builds/runs stuff on our clusters is in Github e.g.
 - Build scripts: <https://github.com/UCL-RITS/rcps-buildscripts>
 - GERun: <https://github.com/UCL/GERun>
 - ... and others

METHOD NOT APPLICATION!

- Works on our clusters but maybe no-where else!
- (relies on /shared/ucl/apps existing, not well documented etc.)

Open an issue to ask for a package to be installed.

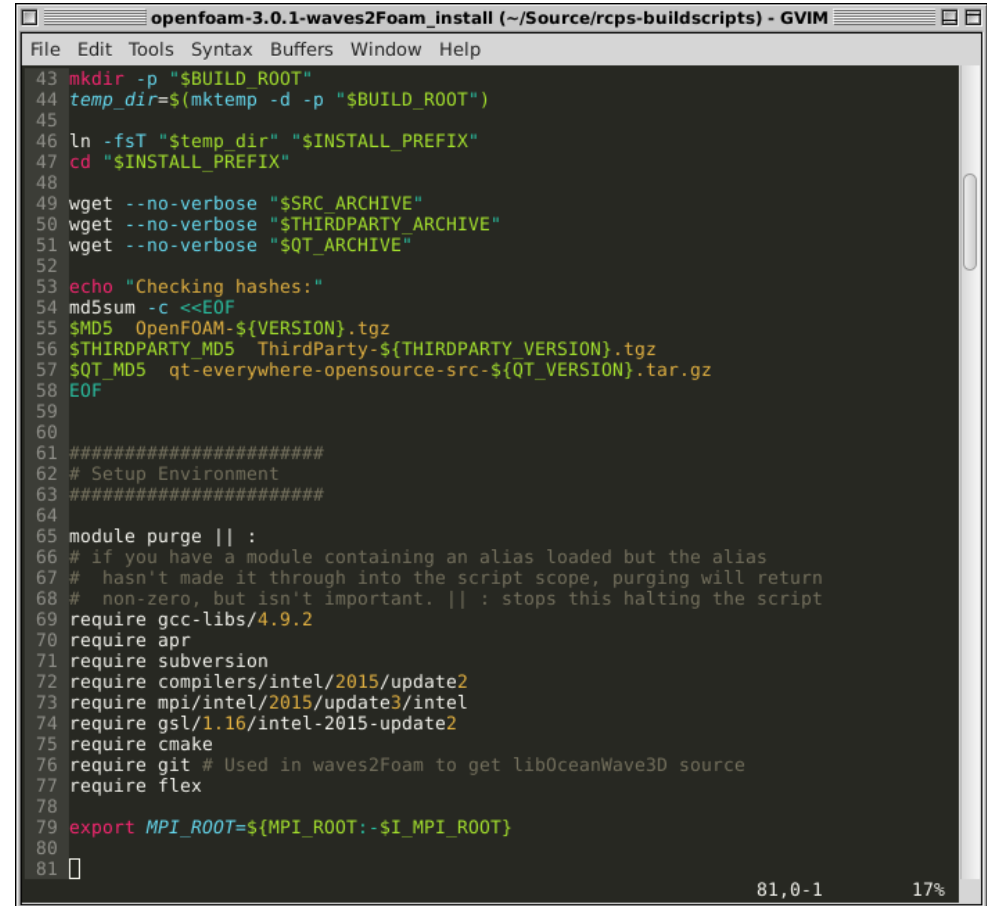
We install software...

- From the easy:

```
$ pip3 install numpy
```

- To the hard:

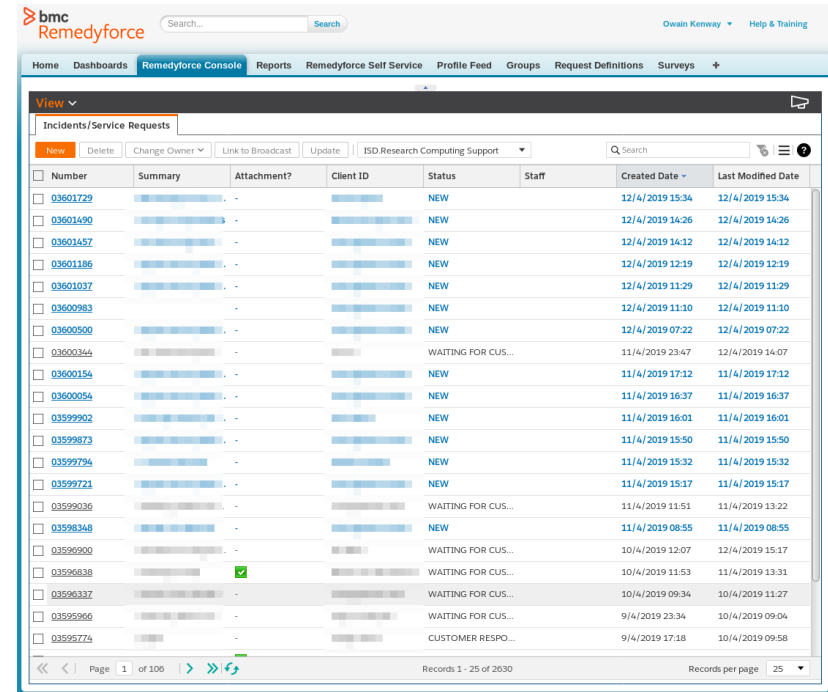
- Multiple incompatible dependencies
- Bazel
- MPI/Cuda builds...
- For more examples, see Kenneth Hoste's excellent FOSDEM talk "How to Make Package Managers Cry" on Youtube
<https://www.youtube.com/watch?v=N5emiYagjIU>



```
openfoam-3.0.1-waves2Foam_install (~/.Source/rcps-buildscripts) - GVIM
File Edit Tools Syntax Buffers Window Help
43 mkdir -p "$BUILD_ROOT"
44 temp_dir=$(mktemp -d -p "$BUILD_ROOT")
45
46 ln -fsT "$temp_dir" "$INSTALL_PREFIX"
47 cd "$INSTALL_PREFIX"
48
49 wget --no-verbose "$SRC_ARCHIVE"
50 wget --no-verbose "$THIRDPARTY_ARCHIVE"
51 wget --no-verbose "$QT_ARCHIVE"
52
53 echo "Checking hashes:"
54 md5sum -c <<EOF
55 $MD5 OpenFOAM-${VERSION}.tgz
56 $THIRDPARTY_MD5 ThirdParty-${THIRDPARTY_VERSION}.tgz
57 $QT_MD5 qt-everywhere-opensource-src-${QT_VERSION}.tar.gz
58 EOF
59
60
61 #####
62 # Setup Environment
63 #####
64
65 module purge || :
66 # if you have a module containing an alias loaded but the alias
67 # hasn't made it through into the script scope, purging will return
68 # non-zero, but isn't important. || : stops this halting the script
69 require gcc-libs/4.9.2
70 require apr
71 require subversion
72 require compilers/intel/2015/update2
73 require mpi/intel/2015/update3/intel
74 require gsl/1.16/intel-2015-update2
75 require cmake
76 require git # Used in waves2Foam to get libOceanWave3D source
77 require flex
78
79 export MPI_ROOT=${MPI_ROOT:-$I_MPI_ROOT}
80
81
```

We answer user tickets...

- E-mail rc-support@ucl.ac.uk for help and advice (**not just for our services!**)
- Manned by the RCAS team on a rota



The screenshot displays the BMC Remedyforce console interface. The main content area shows a table of 'Incidents/Service Requests' for the 'ISD-Research Computing Support' group. The table includes columns for Number, Summary, Attachment?, Client ID, Status, Staff, Created Date, and Last Modified Date. The status of the requests varies, with many marked as 'NEW' and some as 'WAITING FOR CUS...'. A green checkmark is visible in the 'Attachment?' column for one record.

Number	Summary	Attachment?	Client ID	Status	Staff	Created Date	Last Modified Date
03601729		-		NEW		12/4/2019 15:34	12/4/2019 15:34
03601490		-		NEW		12/4/2019 14:26	12/4/2019 14:26
03601457		-		NEW		12/4/2019 14:12	12/4/2019 14:12
03601186		-		NEW		12/4/2019 12:19	12/4/2019 12:19
03601037		-		NEW		12/4/2019 11:29	12/4/2019 11:29
03600983		-		NEW		12/4/2019 11:10	12/4/2019 11:10
03600500		-		NEW		12/4/2019 07:22	12/4/2019 07:22
03600344		-		WAITING FOR CUS...		11/4/2019 23:47	12/4/2019 14:07
03600154		-		NEW		11/4/2019 17:12	11/4/2019 17:12
03600054		-		NEW		11/4/2019 16:37	11/4/2019 16:37
03599902		-		NEW		11/4/2019 16:01	11/4/2019 16:01
03599873		-		NEW		11/4/2019 15:50	11/4/2019 15:50
03599794		-		NEW		11/4/2019 15:32	11/4/2019 15:32
03599721		-		NEW		11/4/2019 15:17	11/4/2019 15:17
03599036		-		WAITING FOR CUS...		11/4/2019 11:51	11/4/2019 13:22
03598348		-		NEW		11/4/2019 08:55	11/4/2019 08:55
03596900		-		WAITING FOR CUS...		10/4/2019 12:07	12/4/2019 15:17
03596638		✓		WAITING FOR CUS...		10/4/2019 11:53	11/4/2019 13:31
03590337		-		WAITING FOR CUS...		10/4/2019 09:34	10/4/2019 11:27
03595966		-		WAITING FOR CUS...		9/4/2019 23:34	10/4/2019 09:04
03595774		-		CUSTOMER RESPO...		9/4/2019 17:18	10/4/2019 09:58

- Grace is now more than three years old!



- Time to design and procure a replacement!

- Design project in 2017/18
- Procurement in 2018/19

Procurement Completed

- **Awarded to HPE**
- **New Machine called “Kathleen”**
- **Into Service in January**

- File system access:
 - Presenting home directories via CIFS → people **not** using Linux will **also** be able to mount their home directories on their desktop!
(Linux users can already do this with FUSE/SSHFS)
 - Mounting Research Data Storage on login nodes
(all sorts of exciting authentication challenges!)
- Usability:
 - Work with CS to present VDI front-end
 - Other ways of accessing resource?
 - Booking system for training courses on Aristotle

- From mid 2019 we will be *collaborating with CS* in running a centrally funded R&D activity.
- Collaboration is tentatively called RCNIC (Research Computing & Networking Innovation Centre).
- Early access to technologies for researchers e.g. FPGAs, Arm etc outside of a defined service.
 - Successful technologies will be adopted in *future* ISD service offerings
- Software collaborations (e.g. Linux VDI, our software stack, service reporting...)
- **Not just CS** – we're keen to bring in other departments that do HPC (Physics, Engineering etc.).

Thanks!

Questions?