UCL Research Computing

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Who we are:

- 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

The Problem:

- 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.

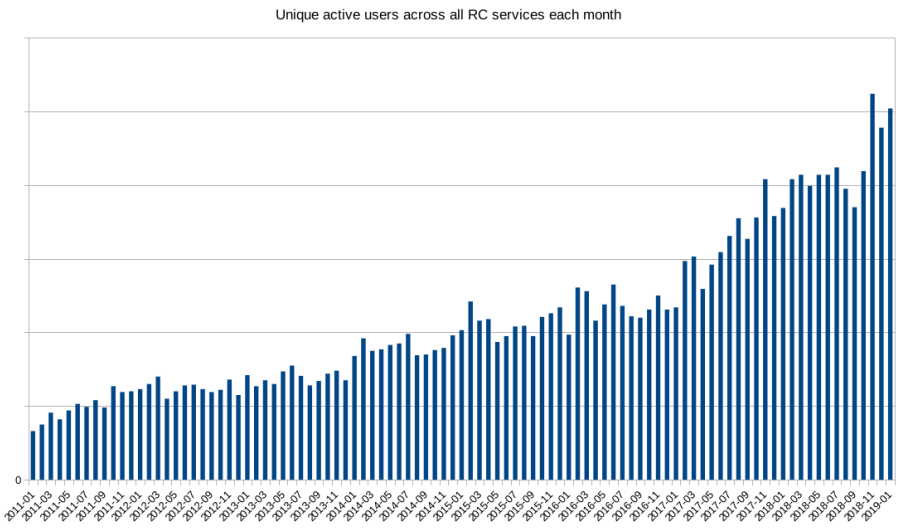
(This is not just true of Research Computing but the whole of ISD!)

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...

Challenges

- 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



What we do:

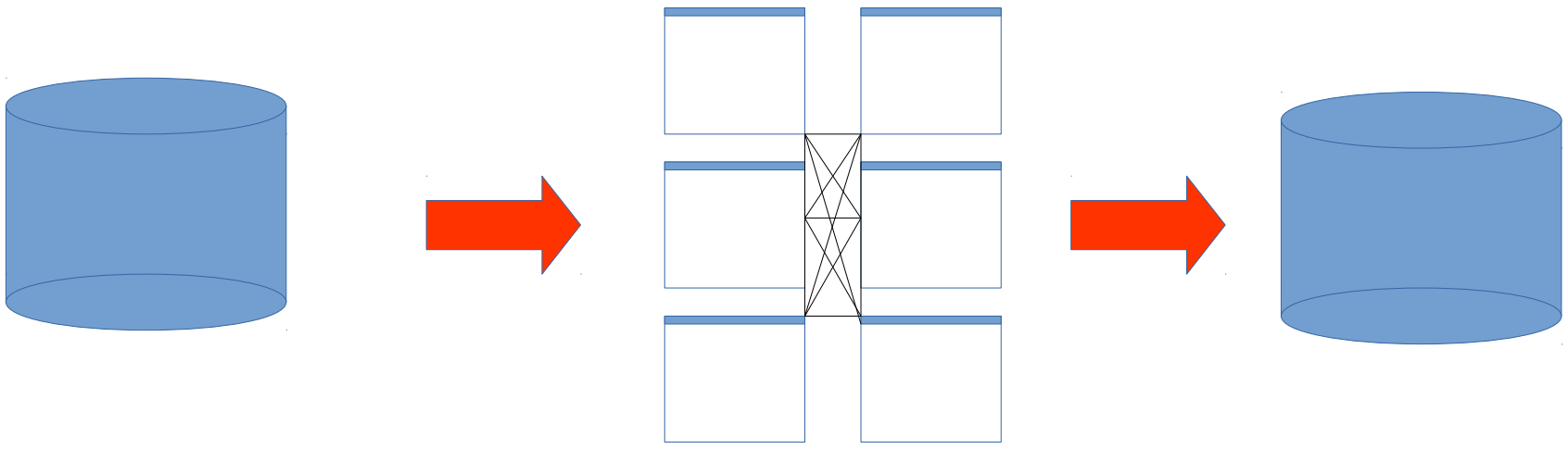
- UCL only services:
  - **Grace,** ~~Replacement~~ → High Performance Computing (HPC)
  - **Myriad**, ~~Legion~~ → High Throughput Computing (HTC)
  - **Aristotle** → Interactive teaching Linux service
  - **DSH** → secure data storage and compute (not currently under RC control)
- National services:
  - **Thomas** (Tier 2 MMM hub)
  - **Michael** (Faraday Institution)

COMMON software stack across RC controlled services

- 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

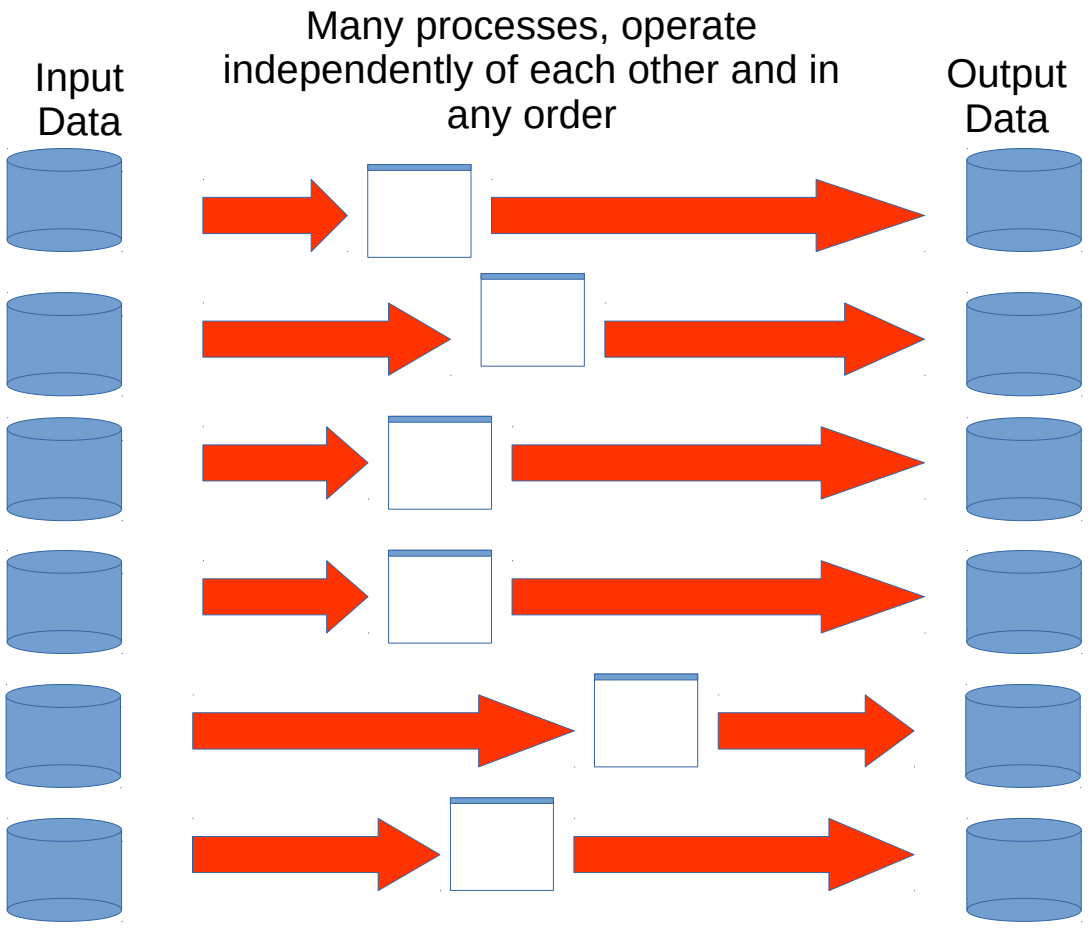
Many processes on many processors work simultaneously + communicate between each other

Input Data



Output Data

HTC


Many processes, operate independently of each other and in any order
Input Data
Output Data

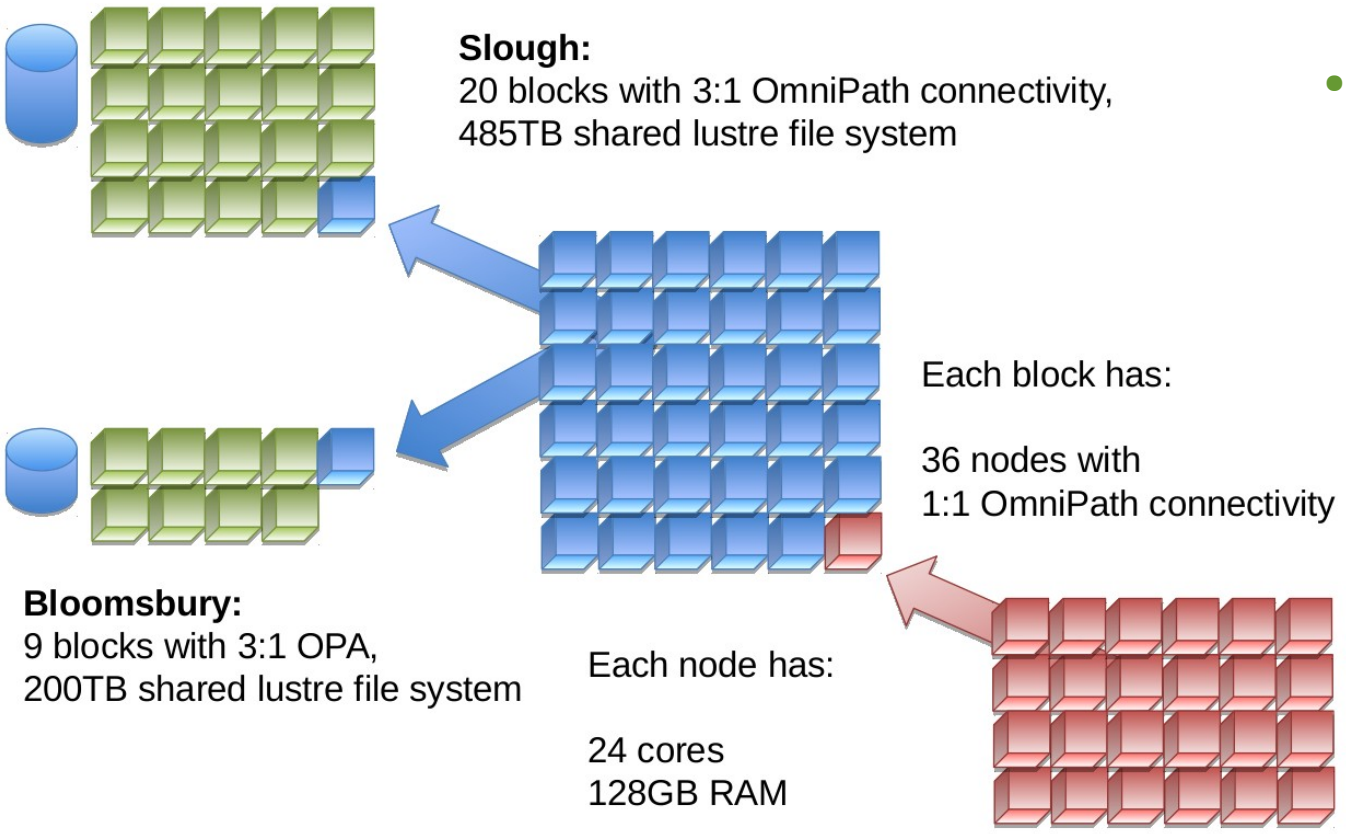
HPC – Grace

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

HTC – Myriad

- 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

National Services



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

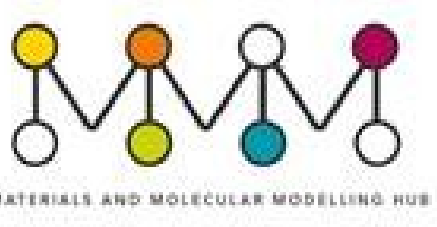
National Services

- 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
  - >2.57×10^8 CPU hours used by user jobs

    → >29,300 years on one core
    → Upper Palaeolithic start!



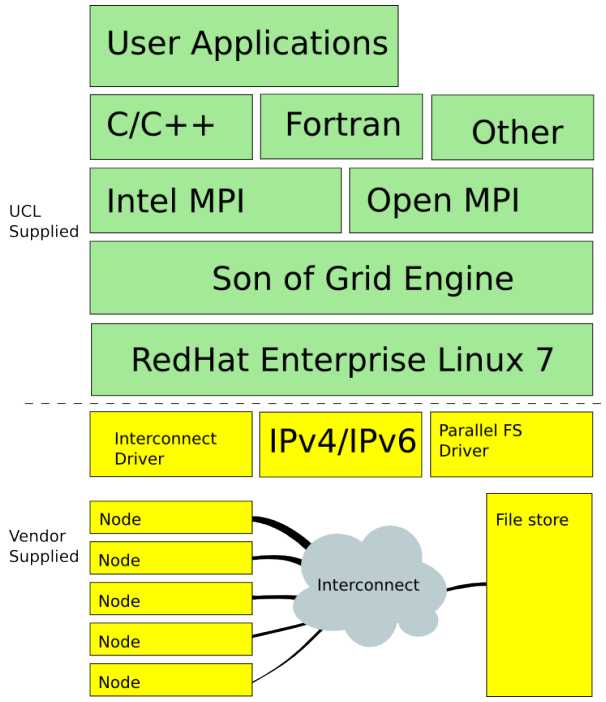
National Services

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

THE FARADAY INSTITUTION

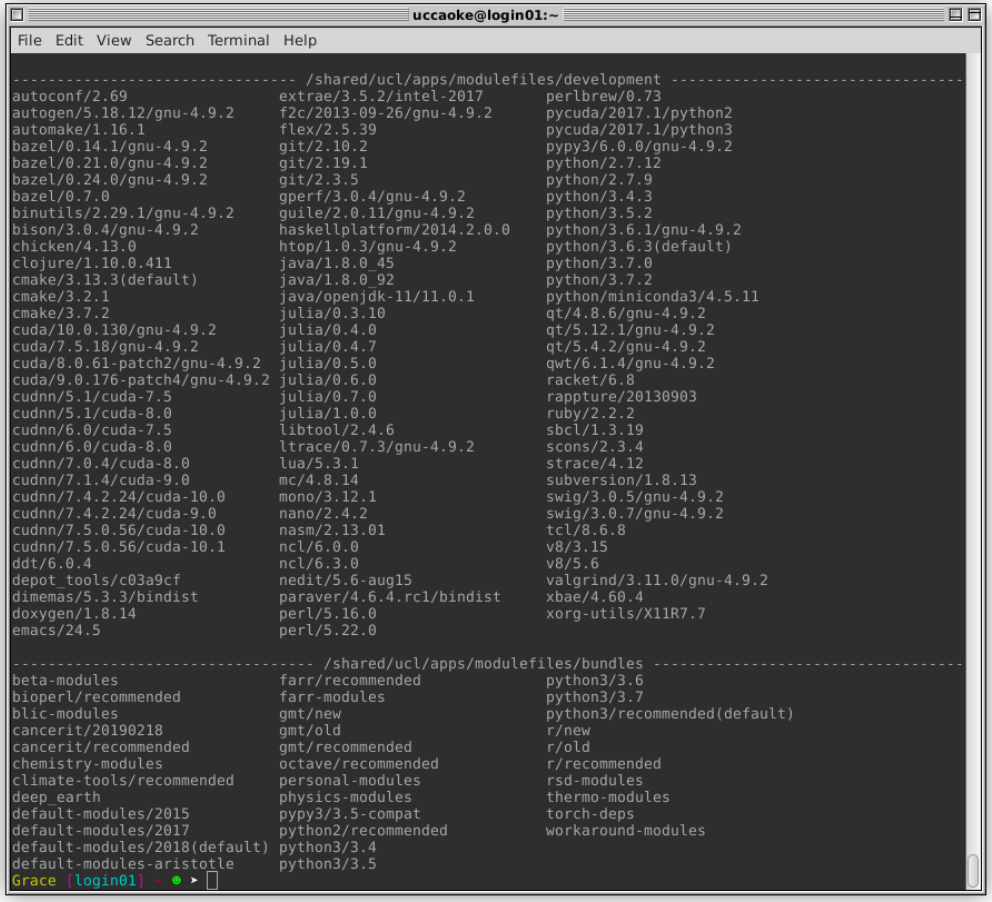
Common software stack

- 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!



Common software stack

- 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.)

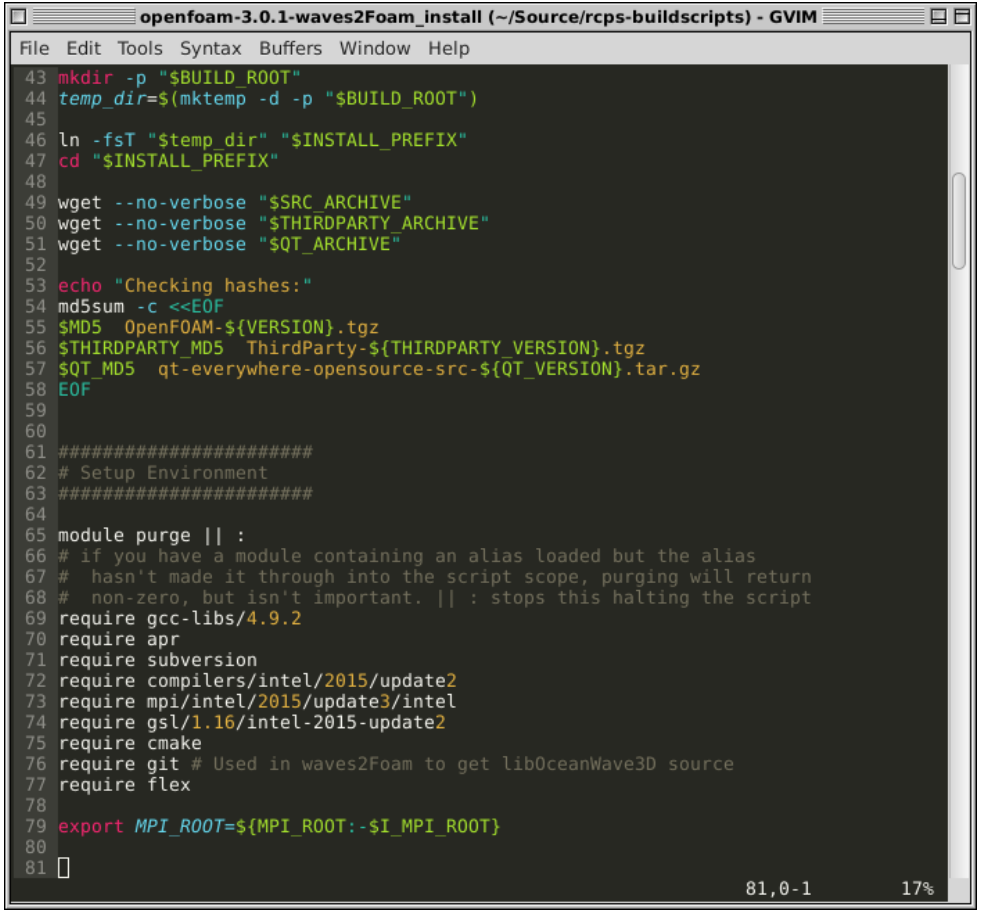
Open an issue to ask for a package to be installed.

We install software...

- From the easy:

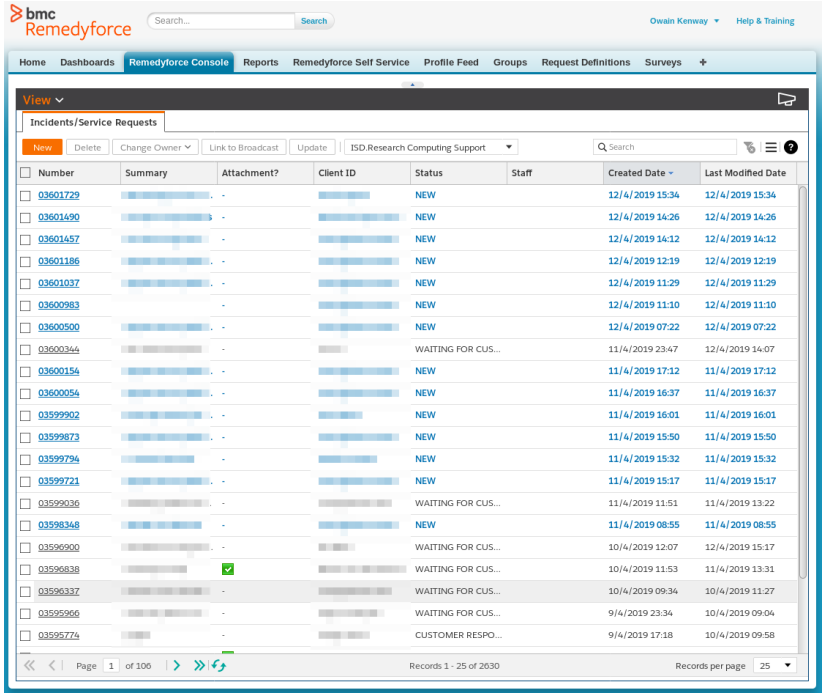
```
$ pip3 install numpy
```

- 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=NSemlYagjIU



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



Future developments: HPC

- 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**

Future developments: User Interface

- 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

Future developments: Collaborations

- 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!

UCL

Questions?