The DiRAC HPC Facility

HPC resources for theoretical astrophysics, particle physics, cosmology and nuclear physics in the UK

Dr Mark Wilkinson, Director
The DiRAC Facility, a brief history

Aggregation, Co-location & Sharing

2009: DiRAC-1 funded
- Systems at 13 host sites

Nov 2011: DiRAC-2 awarded £15M capital by BIS
- 5 systems at 4 sites - architectures set by science needs
- Cambridge, Durham, Edinburgh, Leicester
- Procurement completed in 100 days
- OPEX provided by STFC

Dec 2012: DiRAC-2 operations begin
- Systems full within 1 week - usage >90%
- Access via international peer-review process
- Free to use for STFC researchers

April 2017: DiRAC-2.5 operations begin
- 3 services: Extreme Scaling, Memory Intensive, Data Analytic

April 2018: DiRAC-2.5x
- Interim BEIS funding to support 2018/19 science programme
**DiRAC 2.5**

- November 2016: £1.67M capital funding awarded by STFC
- April 2017: 2x uplift to support 2017/18 science programme

<table>
<thead>
<tr>
<th>Service</th>
<th>Description</th>
<th>Available</th>
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<tbody>
<tr>
<td>BGQ (Extreme Scaling 2.5)</td>
<td>98000 cores, 1.3 Pflop/s</td>
<td>✓</td>
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<tr>
<td>Data Centric 2.5</td>
<td>14000+ cores with 128GB RAM/node</td>
<td>✓</td>
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<tr>
<td>Data Analytic 2.5</td>
<td>• 13% access to 0.5 Pflop/s KNL system</td>
<td>✓</td>
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<tr>
<td></td>
<td>• 13% access to 1.0 Pflop/s GPU system</td>
<td>✓</td>
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<tr>
<td></td>
<td>• 13% access to 25000 core Skylake system</td>
<td>From 10/17</td>
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<tr>
<td></td>
<td>• 50% access to 8000 core Sandybridge system</td>
<td>✓</td>
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<tr>
<td>Complexity 2.5</td>
<td>• 4700 cores for very large jobs</td>
<td>✓</td>
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<td></td>
<td>• 3072 cores for shorter jobs</td>
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<td>SMP</td>
<td>14.8TB, 1856 core system, KNL offload</td>
<td>Until 03/18</td>
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DiRAC 2.5x Announcement

• June 2017: BEIS release £9M capital to maintain DiRAC-2.5
• Planned investment (currently out to tender):
  • Extreme Scaling: 1024-node, 2.5 PFlop/s system
  • Memory Intensive: 144 nodes, ~4600 cores, 110 TB RAM
  • Data Analytic: 128 nodes, ~4000 cores, 256GB/node
    • Hierarchy of fat nodes (1-6TB)
    • I/O-accelerated storage for data intensive workflows
• Additional storage at all DiRAC sites to relieve pressure
• Target date for new hardware full availability: 1st April 2018
• Call for proposals in November 2017
Breadth of DiRAC science

• STFC Science Roadmap:
  - All questions have projects which use DiRAC resources

• Capability calculations:
  - Galaxy formation - most realistic simulations to date
  - QCD - high precision calculation of quark masses

• Data Intensive calculations:
  - Gravitational waves
  - Gaia modelling
  - Precision cosmology using Planck satellite data

<table>
<thead>
<tr>
<th>STFC Science Challenge</th>
<th>DiRAC-3 Project</th>
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<tbody>
<tr>
<td>A: How did the universe begin and how is it evolving?</td>
<td>Unveiling the early Universe; Black holes and gravitational waves; Beyond the Standard Model physics; QCD in extreme environments</td>
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<tr>
<td>A.1. What is the physics of the early universe?</td>
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<td>A.2. How did structure first form?</td>
<td>Science Exploitation of the Cosmic Microwave Background</td>
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<td>A.3. What are the roles of dark matter and dark energy?</td>
<td>Dark Matter Physics; Large Scale Structure; Dark Energy and Tracers of Large-Scale Structure; Scientific data analysis for Cosmological studies with DES, VISTA &amp; LSST</td>
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<tr>
<td>A.4. When were the first stars, black holes and galaxies born?</td>
<td>Black holes and gravitational waves; Simulating galaxy formation; Galactic Archaeology in the Milky Way; Galaxy spectral surveys</td>
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<tr>
<td>A.5. How do galaxies evolve?</td>
<td>Black holes and gravitational waves; Simulating galaxy formation; Galactic Archaeology in the Milky Way; Galaxy spectral surveys</td>
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<tr>
<td>A.6. How are stars born and how do they evolve?</td>
<td>Star formation; ISM and astro-chemistry; Nuclear Physics</td>
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<tr>
<td>B: How do stars and planetary systems develop and is life unique to our planet?</td>
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<tr>
<td>B.1. How common are planetary systems and is ours typical?</td>
<td>Planet formation</td>
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<tr>
<td>B.2. How does the Sun influence the environment of the Earth and the rest of the Solar System?</td>
<td>Planetary MHD modeling; Planetary Modelling; Solar and planetary magnetism – MHD simulations</td>
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<td>B.3. Is there life elsewhere in the universe?</td>
<td>Spectroscopy of large exoplanetary hydrocarbons</td>
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<td>C: What are the fundamental constituents and fabric of the universe and how do they interact?</td>
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<tr>
<td>C.1. What are the fundamental particles?</td>
<td>Beyond the Standard Model physics</td>
</tr>
<tr>
<td>C.2. What is the nature of space - time?</td>
<td>Black holes and gravitational waves</td>
</tr>
<tr>
<td>C.3. Is there a unified framework?</td>
<td>Beyond the Standard Model physics; Lattice QCD and Flavour physics; Black holes and gravitational waves</td>
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<tr>
<td>C.4. What is the nature of dark matter?</td>
<td>Beyond the Standard Model physics</td>
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<tr>
<td>C.5. What is the nature of dark energy?</td>
<td>Dark Energy and Tracers of Large-Scale Structure</td>
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<td>C.6. What is the nature of nuclear and hadronic matter?</td>
<td>Hadron Spectroscopy and Structure; Lattice QCD and Flavour physics; QCD in extreme environments; Nuclear Physics</td>
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<td>C.7. What is the origin of the matter - antimatter asymmetry?</td>
<td>Lattice QCD and Flavour physics</td>
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<td>D: How can we explore and understand the extremes of the universe?</td>
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<tr>
<td>D.1. How do the laws of physics work when driven to the extremes?</td>
<td>High energy astrophysics with CTA; Black holes and gravitational waves; QCD in extreme environments; Nuclear Physics</td>
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<tr>
<td>D.2. How can high energy particles and gravitational waves tell us about the extreme universe?</td>
<td>High energy astrophysics with CTA; Black holes and gravitational waves; Beyond the Standard model physics</td>
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<tr>
<td>D.3. How do ultra-compact objects form, what is their nature and how does extreme gravity impact on their surroundings?</td>
<td>High energy astrophysics with CTA; Black holes and gravitational waves</td>
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Diverse science cases require heterogenous architectures

Complexity

Cosma-5

Darwin/HPCS

COSMOS

BGQ

SMP/Xeon Phi for data-intensive workflows (Planck data analysis; molecular line lists)

3 clusters with variety of interconnect and RAM/core for complex astrophysics and cosmology simulations

Many-core Chips and innovative networking for high-precision lattice QCD
DiRAC Research Output

- DiRAC Services support 2000+ researchers
- Refereed publications 2012-2015: 600+ papers; ~22000 citations
- Most cited paper in all astronomy in 2015
- 250 refereed papers in 2016
Industrial Strategy

• Industrial engagement brings many benefits to DiRAC
  - supports sustainability and improves service provision
  - innovation: early-access to next generation hardware
  - generates impact cases for DiRAC researchers

• Goal: facilitate easier industry collaboration for DiRAC researchers
  - DiRAC-level engagement activities allow majority of users to focus on their science

• Previous successes:
  - Co-design of BGQ chips for DiRAC-2 (Peter Boyle/IBM)
  - 3 INTEL Parallel Computing Centres (IPCC: Cambridge, Durham, Edinburgh)
  - 4 iCASE studentships; support for all STFC Data Intensive Centres for Doctoral Training
  - Co-design of Xeon-Phi box for SMP (with SGI)
  - HPCWire 2015 Readers' Choice Award “Best Use of High Performance Data Analytics”
Software Innovation: COSMOS@DiRAC

• OSPRay XEON PHI Viz - collaboration with Intel
Demonstrator of remote visualisation on Phi
Training

• DiRAC provides **access** to training from wide pool of providers

• Currently offering:
  - **DiRAC Driving Test:** now available online (and compulsory!)
  - **Workshops:** Many-Core programming; Software Design & Optimisation; MPI programming

• Coming soon:
  - Domain-specific workshops
  - Online individual training portal

**Why do we do this?**

- maximise DiRAC science output
- flexibility to adopt most cost-effective technologies
- future-proofing our software and skills
- contributes to increasing skills of wider UK economy
• Science requirements for DiRAC-3 demand 10-40x increases in computing power to stay competitive
  - hardware alone cannot deliver this
• We can no longer rely on “free lunch” from the Xeon era
• Vectorisation and code efficiency now important
• Next generation hardware is more difficult to program efficiently
• RSEs are increasingly important
  - RSEs can help with code profiling, optimisation, porting, etc
• DiRAC now has 3 RSEs: effort allocated via peer review process
DiRAC-3

Many-Core Coding

Extreme Scaling

Data Intensive

Data Analytics Programming

Data Handling Archiving

Maximal computational effort applied to a problem of fixed size

Internet Analytics

Data Management

Tightly coupled compute & storage: confrontation of complex simulations with large data sets

Memory Intensive

Disaster Recovery

Fine Tuning Parallel Management

Multi-threading

Larger memory footprint per node: problem size grows with increasing machine power
All Data Activities contain elements of:
- Collection/generation
- Analysis/discovery
- Modelling/fitting
- Simulation

**Experiment**
Bespoke systems that are directly connected to experiments

**Simulation Only**
Systems generate data from a set of starting assumptions/equations

**Data Analysis & Discovery**
Systems analyze data to discover relationships, structures and meaning within, and between, datasets

**Data Modelling & Fitting**
Systems use a combination of simulations, experimental data and statistical techniques to test theories and estimate parameters from data
DiRAC-GridPP Engagement

• Data Transfer project with DiRAC@Durham:
  - Goal: enable disaster recovery data transfers to RAL
  - Involved work on firewalls, FTS3, GridFTP to create interface between GridPP tools and RAL archive
  - Report written: “Setting up a system for data archiving using FTS3” by Lydia Heck, Jens Jenson, Brian Davies
  - Lessons learned included: file sizes; file ownership & creation dates; issues about incremental changes remain
  - Demonstrated that GridPP-DiRAC collaboration works
  - Now taking this further through DiRAC2.5x Data Transfer pilot study and via Cloud proposal submitted in the summer

• UKTier-0 proposal

• Opportunities for further/deeper collaboration:
  - Training: access to common training programmes
  - Hardware: benchmarking; time-swapping (eg. via UKT0 and NeI)
Summary

- DiRAC is the HPC facility for theoretical astrophysics, particle physics, cosmology and nuclear physics
- Successful demonstration of the cost effectiveness of distributed facility model to deliver a broad science programme
- Already working with GridPP - opportunities to develop this further