DiRAC thoughts on STFC eInfrastructure development

DiRAC: HPC facility providing resources for theoretical astrophysics, particle physics, cosmology and nuclear physics in the UK

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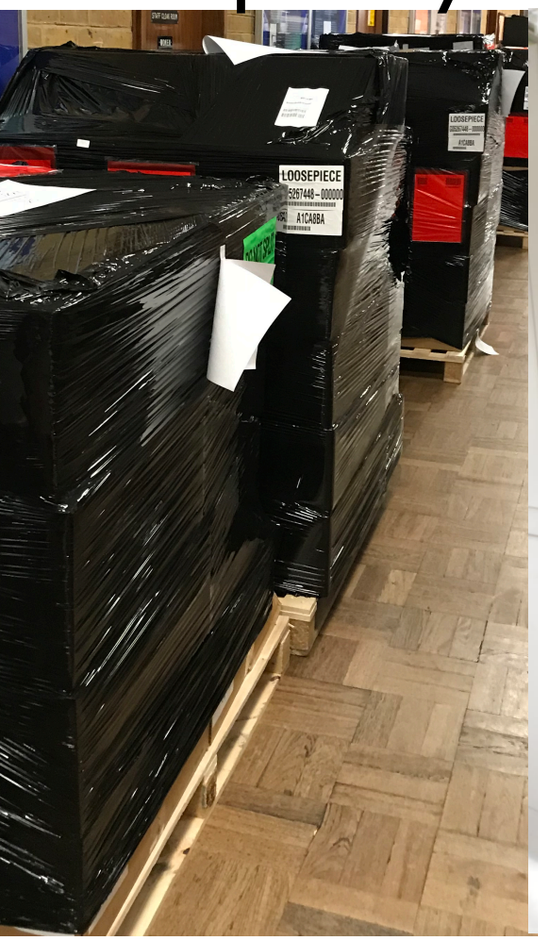
Breadth of DiRAC science

- 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

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

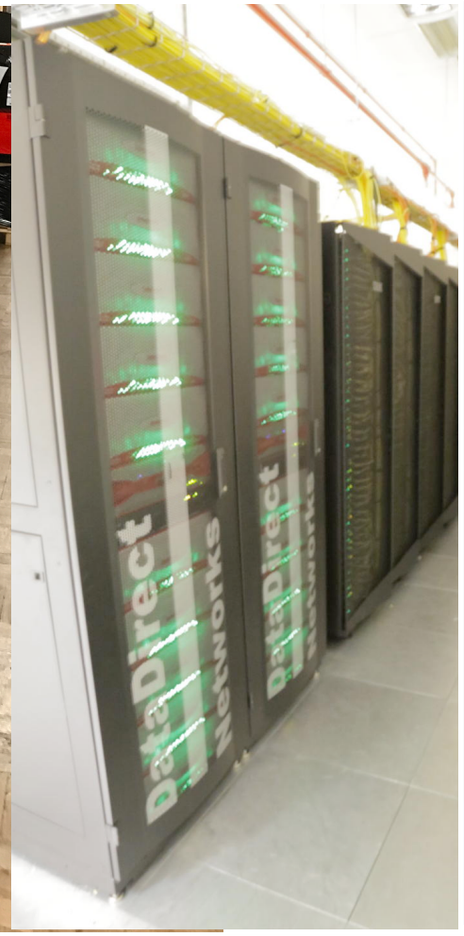
Diverse science workflows require heterogenous architectures

Complexity



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

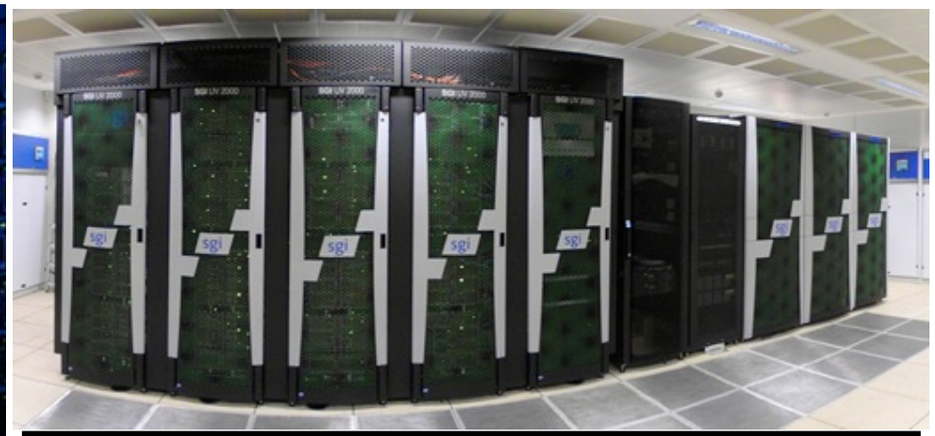
Cosma5 & 6



CSD3

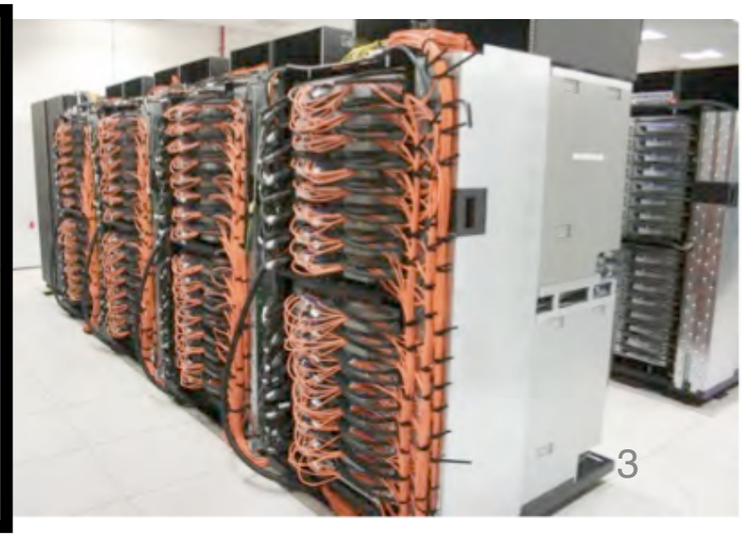
Many-core Chips and innovative networking for high-precision lattice QCD

COSMOS



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

BGQ



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 and STFC

- 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

May 2018: DiRAC-2.5x operations begin

- Interim BEIS funding to support 2018/19 science programme

DiRAC Resource Allocation

- Peer reviewed application process run by STFC
- Resource Allocation Committee (RAC):
  - includes scientists from outside DiRAC consortia.
  - manages the peer review and scientific tensioning of proposals.
- First call for proposals in 2012
- Allocations for 10th Call currently being finalised
  - Oversubscription factors of 1.3 to 5 in current round
  - Pressure on all services
  - Demand increasing significantly faster than resource provision
- Rigorous process covering scientific merit and technical mapping of proposals to DiRAC resources
- DiRAC allocation model now being considered by other national services.

DiRAC-3

Many-Core Coding

Maximal computational effort applied to a problem of fixed size

Extreme Scaling

Data Intensive

Data Analytics Programming

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

Data Handling Archiving

Data Management

Internet Analytics

Memory Intensive

Disaster Recovery

Janet Light Paths (JLP)

External Connections

Fine Tuning Parallel Management Multi-threading

Larger memory footprint per node: problem size grows with increasing machine power

DiRAC thoughts on STFC eInfrastructure development

- Explicit science drivers for all activities are key
  - Doesn't need to be a new UKT0 science case, but we need to be clear about science motivations for UKT0 activities
  - it may be obvious, but worth writing it down
- Common set of approaches - interoperability, not necessarily homogeneity
- Draw on reservoir of experience across UKT0
- Policies/processes are also important:
  - Resource Allocation
  - Time swapping
  - Acknowledgments - capturing impact
- Above will help to bring diverse communities together and build trust and confidence
- Opportunities for shared activities - training; cloud pilots; access to wider range of hardware for benchmarking