DiRAC UK Update

HPC User Forum fall 23

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UK research HPC Ecosystem

- UKRI – funds most academic UK research
  https://www.ukri.org
- Comprised of 7 Research Councils : EPSRC, NERC, STFC, BBSRC, MRC, ESRC, AHRC plus Innovate UK and Research England
  who choose how to spend the money
- EPSRC, NERC and STFC fund most of the big HPC.

UK HPC Centres

- Tier 1
  - Archer – the national supercomputer for EPSRC, NERC
  - DiRAC – national distributed supercomputing facility for STFC theory
- Tier 2 – large and/or specialist systems eg. GPU, materials science
- Tier 3 – Local University systems, some of which can be quite large
- Others – eg Hartree, Met Office, AWE, Secret Squirrel

DiRAC

- Distributed Research Utilising Advanced Computing https://dirac.ac.uk
- Funded by STFC, UKRI and BEIS (now DSIT)
- Supports research in the STFC theory community (particle physics, astrophysics and cosmology, solar system physics, particle astrophysics and nuclear physics) and the STFC science challenges https://www.ukri.org/publications/stfc-science-challenges/

DiRAC Federated Facilities

- 3 compute services hosted by 4 centres
- Hosted by partner Universities which have their own facilities too
- Universities of Durham, Cambridge, Leicester, Edinburgh
- Each has a different system targeted for specific workloads such as data intensive; memory intensive; extreme scaling, GPU-enabled
- Users bid annually for resources and get awarded time at the most appropriate centre
- Common shared training and consultation and co-ordination and expertise

The DiRAC HPC Facility

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

Memory Intensive
"COSMA 8" (Durham)

DELL EMC

528 TB RAM
Large-scale cosmological simulations

Extreme Scaling "Tursa" (Edinburgh)

Atos

GPU-based system

Large lattice-QCD simulations

Data Intensive "DiaL" (Leicester)

Heterogeneous architecture for complex simulation and modelling workflows

Hewlett Packard Enterprise

Data Intensive "CSD3" (Cambridge)

DELL EMC

Heterogeneous architecture for complex simulation and modelling workflows

Project Office (UCL)

4 machines

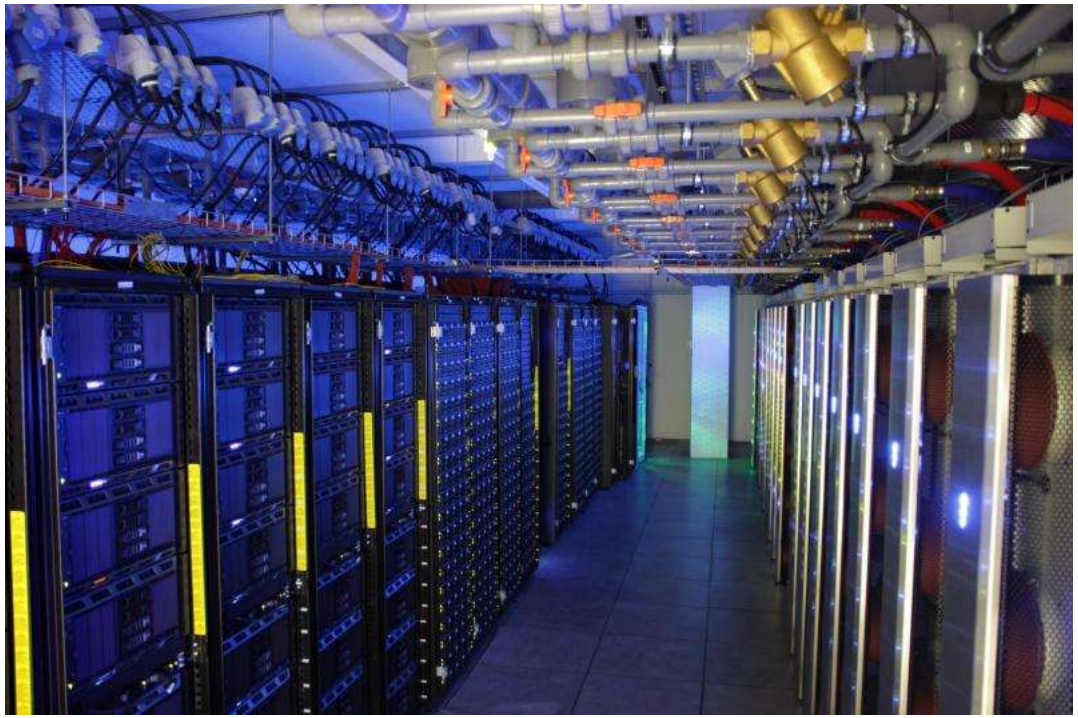
- Each machine is tailored to support a different type of workload, according to the science need
- Machines are periodically upgraded or replaced
- Usually 2 generations of system are run alongside each other to allow for convenient migration of projects and workload

Durham COSMA 8 – memory intensive

- 512 nodes
- 128 cores 1TB RAM
- 4 fat nodes (4TB)
- Some GPU nodes
- Dell

Data Intensive @ Cambridge (DIaC)

- Part of CSD3 system
- Heterogeneous:
  - Intel CPU nodes
    544 icelake, 672 cascade lake
  - Nvidia A100-80GB nodes
- Dell



Data Intensive @ Leicester (DIaL)

- 200 nodes 128 cores (AMD)
- nearly 4GB per core
- 10 large memory 1.5TB
- 1 extra large memory 6TB
- HPE

Edinburgh TURSA – extreme scaling

- 176 nodes each with
  128 AMD CPU cores
  4 A100 GPUs
- Eviden (formerly Atos)

User workload

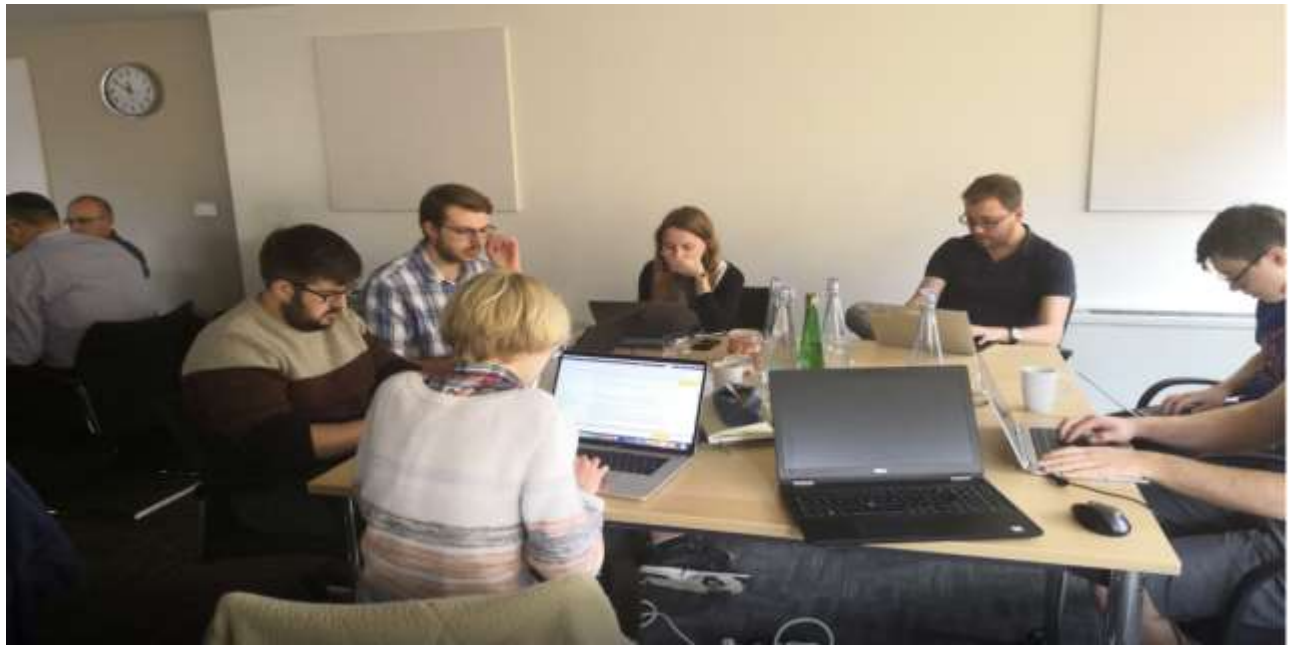
- A few applications use most of the resources on the Memory Intensive and Extreme Scaling services; greater diversity of applications on the Data Intensive service
- Many codes are research/community codes, many of our researchers write their own code
- Targeted efforts to optimize the codes and squeeze out more performance and to improve scalability (exascale), also to improve code maintenance and software sustainability
- Improvements to one code generally benefit many users
- Most are CPU codes, push to implement GPU versions if possible

Software

- Software is equally important as hardware
- Promote community shared applications and their development
- RSE team of programmers give support and training
- RSEs available to work on long term projects with researchers to improve and enhance the code. Collaboration with research groups on code development and evolution.
- Users can bid for RSE time as well as computer time

Training

- Core Skills Programme
  - Foundation HPC Skills
  - Advanced Developer Course
  - AI/ML Techniques for Science
- Partnerships Programme
  - Code-Camps
  - Hackathons
  - Exotic computing (new processors, Quantum)
  - Innovation Placements
- RSE and Technical Teams Training
  - Vendor specific training for new hardware and software



Innovation Programme

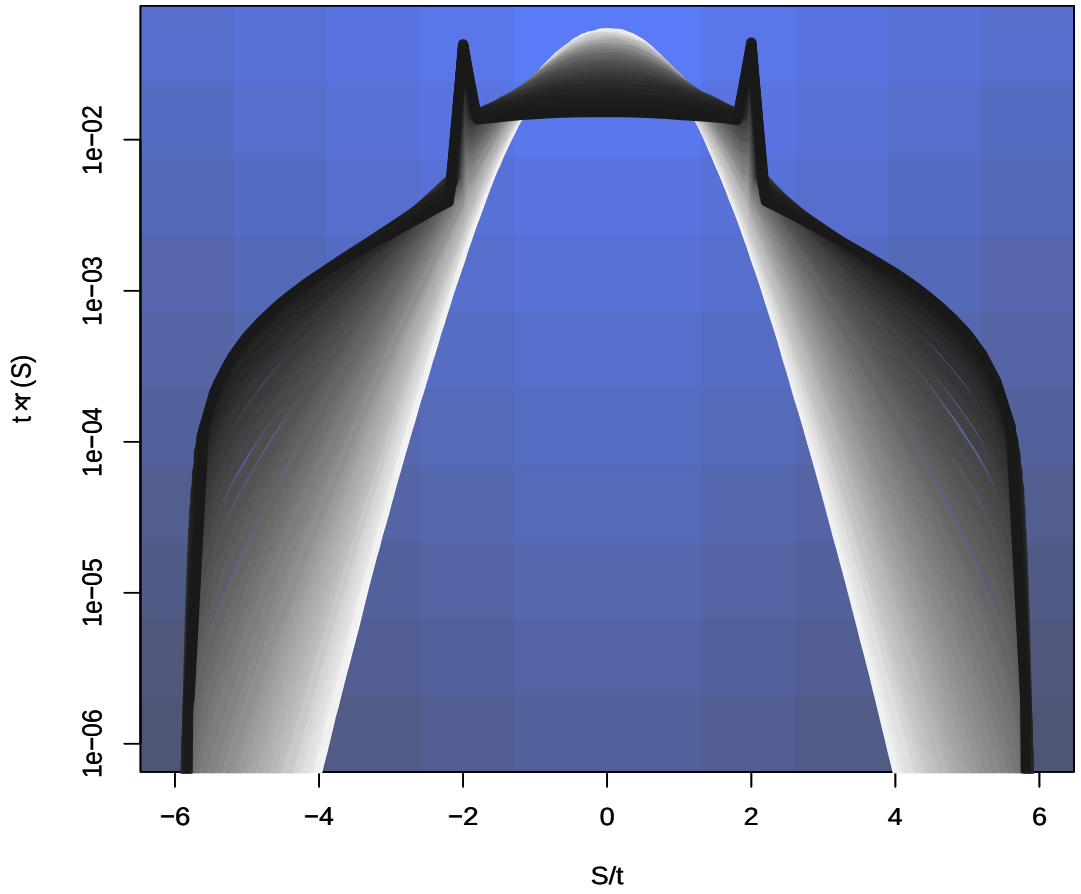
- Benefits Research programmes for STFC/UKRI and external partners Bringing impact and demonstrating the value of capital investment
- Includes co-design activities, deployment of test beds, innovation placements, software development collaborations, application of new algorithms to a field
- Supports future high level plans and new methods
- Collaborative in nature with two way knowledge transfer and skills exchange

Some applications

- Results from some projects run on DiRAC systems, chosen purely for the amazing imagery, but which portrays leading science

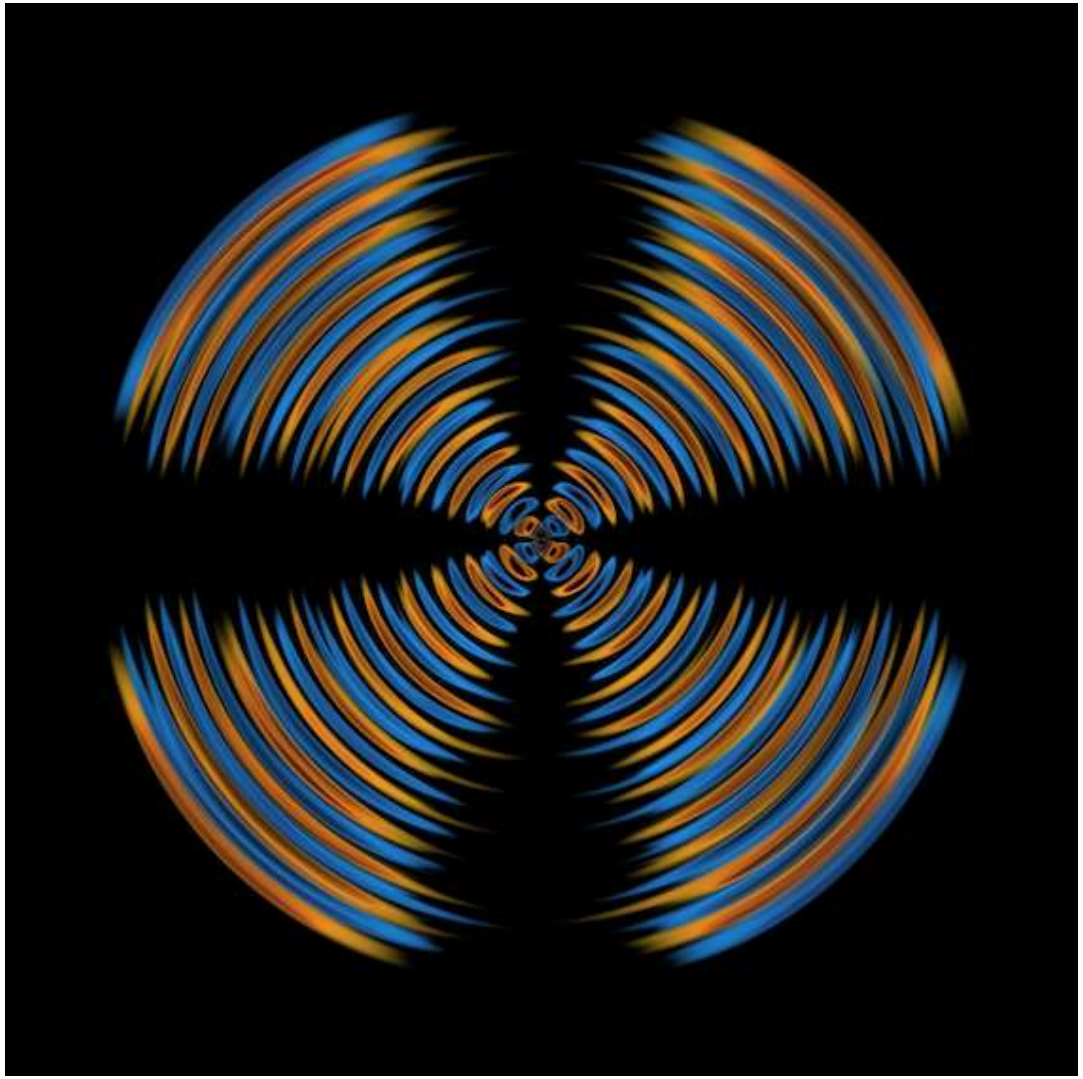
Batman

- BATMAN'S DENSITY OF STATES With this image we aim to provide an intuition for the sign problem of real time evolutions. The depicted density of states of a quantum spin chain smears out with time, starting with black and evolving to white, and thus the sign problem worsens. The image is a visually enhanced version of figure 4 in [arXiv:2209.13970] based on data from the DiRAC-3 Data Intensive service (Cambridge). Credit: Johann Ostmeyer and Pavel Buividovich



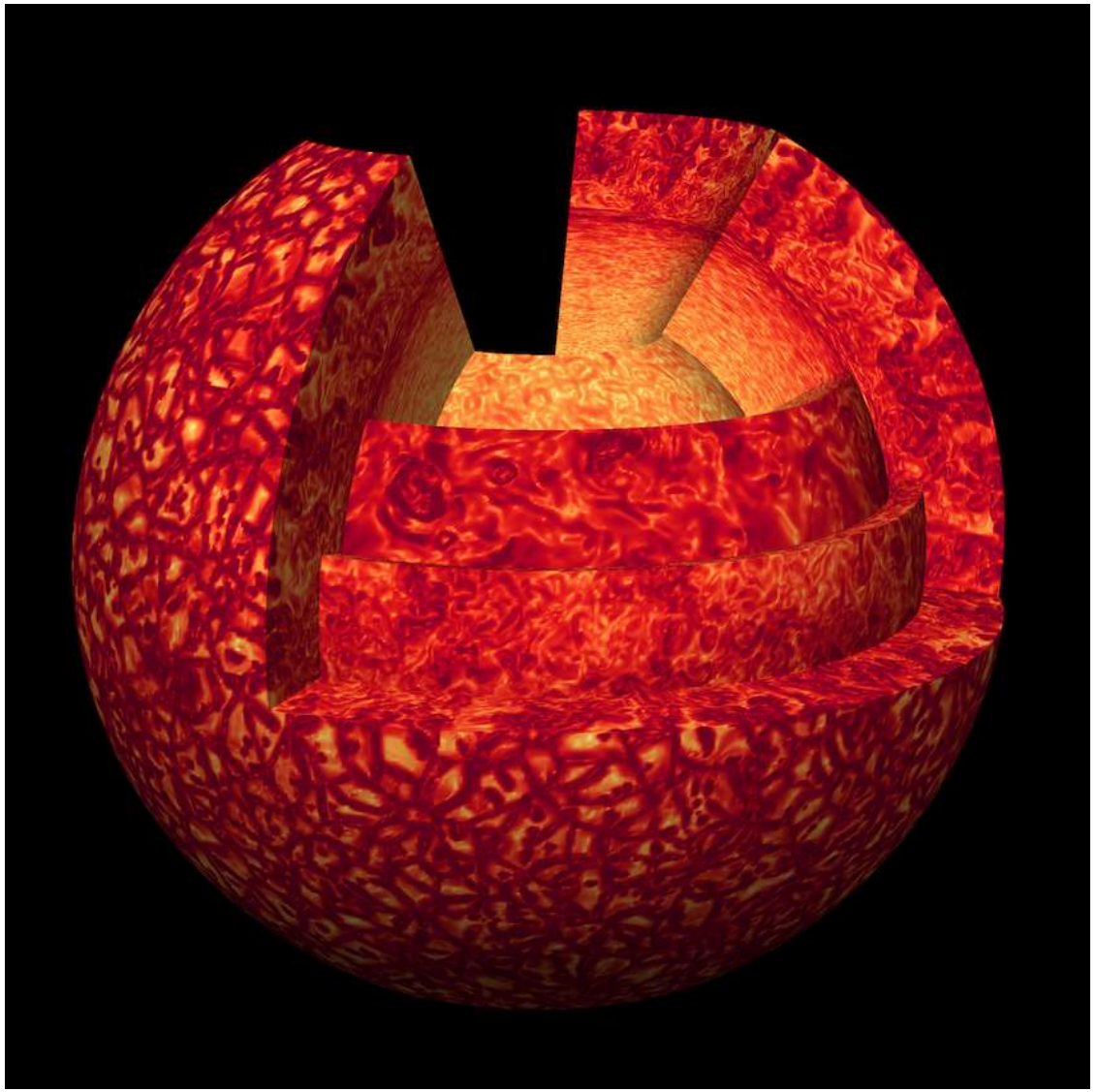
Axion Radiation

- MASSLESS RADIATION FROM AN AXION STRING Volume rendering of axion radiation emitted from a sinusoidally-displaced global cosmic string. The line of sight is parallel to the string axis, and the blue and yellow represent the primarily quadrupole radiation propagating outwards from the oscillating string. This simulation was run using the adaptive mesh refinement code, GRChombo, on the DiRAC-2 ‘Cosmos’ machine and the DiRAC-3 Data Intensive service (Cambridge). The volume rendering and visualisation was performed using Paraview and Intel’s OSPRay ray tracing engine. Credit: Amelia Drew and Carson Brownlee



Stellar Hydrodynamics

- STELLAR HYDRODYNAMICS WITH MUSIC Sun-like stars contain outer layers which are turbulent and convective, and inner stable layers where internal gravity waves can propagate. Different small-scale structures in these layers are captured by the magnitude of the vorticity (darker colour means larger magnitude). The visualisations are based on a simulation of a rotating star with the MUSIC code on the DiRAC-3 Data Intensive Service (Leicester). Credit: Dimitar G. Vlaykov, Thomas Goffrey, Isabelle Baraffe, Thomas Guillet, Adrian Morrison, Arthur Le Saux, Jane Pratt, Thomas Constantino



Questions?

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