Leicester and DiRAC plans for Catalyst

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University of Leicester and DiRAC Catalyst plans

- DiRAC provides HPC resources for the STFC theory communities in astrophysics, particle physics, cosmology and nuclear physics
  - established track record of designing HPC systems based on science requirements (dirac.ac.uk)
- Leicester hosts DiRAC Data Intensive service: Catalyst plans focus on data intensive workflows
- Main goals:
  - Port set of key DiRAC community codes to Thunder X2 and provide guidance to other users/communities
  - Provide feedback on performance of Catalyst systems as a national-scale HPC resource, including integration with other DiRAC resources (high-performance file system, etc)
  - Explore use of MOAB/Torque scheduler
- To request access: e-mail Mark Wilkinson (miw6@leicester.ac.uk)

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Leicester/DiRAC Catalyst target codes and research areas

- DiRAC codes from STFC astrophysics, particle physics and cosmology communities:
  - TROVE - molecular line-list calculations for molecules such as methane for interpretation of exoplanet spectra
  - GRID - lattice-Quantum ChromoDynamics calculations of properties of fundamental particle from first principles
  - PRIMAL - made-to-measure N-body simulations of the Milky Way galaxy
  - Swift - cosmological N-body+Hydrodyamics simulations of galaxy formation and evolution
- Codes from across Leicester research community:
  - **Earth Observation Science** - processing and modelling of satellite data, including forest cover mapping
  - **Computational Chemistry** - image processing for Electron Cryo-microscopy with *EMAN2* and *Relion* codes; extraction of information from biological NMR data using Relax code
  - **Engineering** - Detached Eddy Simulations of bandwidth-limited, compressible, turbulent flows to model aircraft noise with *Cosmic* code; post-processing of CFD simulations with *Antares* code

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