Catalyst@Leicester

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University of Leicester and DiRAC Catalyst

- DiRAC provides HPC resources for the UK theory communities in astrophysics, particle physics, cosmology and nuclear physics
- Leicester hosts DiRAC Data Intensive service: Catalyst@Leicester 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 and BeeGFS

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Configuration

- Catalyst Arm cluster currently set up as standalone system
- Access open to selected DiRAC users and Leicester research groups
- IB spine ready to integrate with DiRAC Data Intensive service in due course
  - Will access main DiRAC lustre storage.
- Currently using PBS but working on Moab/Torque
- Currently using NFS but testing BeeGFS

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Utilization

- A key goal of DiRAC/Leicester Catalyst is to assess viability of operating the Arm cluster as part of a national HPC service
  - Early access for external users important
- Open to DiRAC and UoL researchers since 18th Feb
- Majority of system usage has been on real user codes being run by researchers
- Hackathon held in early February
  - Flexible schedule with focus on hands-on work
  - Users had access to system throughout event and subsequently are continuing to use it
  - Support provided by Arm, HPE, Mellanox and Leicester RSE and technical support teams
  - 6 user codes successfully ported over 3 days
  - Majority of codes saw good performance on Arm

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Leicester/DiRAC Catalyst target codes and research areas

- DiRAC codes - astrophysics, particle physics, cosmology:
  - **sphNG** - star formation simulations
  - **Swift** - cosmological N-body+Hydrodynamics simulations of galaxy formation and evolution
  - **TROVE** - molecular line-list calculations for molecules such as methane for interpretation of exoplanet spectra
  - **GRID** - lattice-Quantum ChromoDynamics (QCD) calculations of properties of fundamental particles from first principles
- Codes from across Leicester research community:
  - **Earth Observation Science** - processing and modelling of satellite data, including forest cover mapping
  - **Computational Chemistry** - image processing for Cryo Electron-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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Simulating planetary collisions

Borrows (Durham), Kegerreis (Durham), Schaller (Leiden)

- Saturn's rings and mid-sized moons recently discovered to be significantly younger than previous thought.
- Suggestion that they formed from the debris from collisions between a previous generation of icy moons.
- Key questions:
  - What is the size distribution of the fragments that survive a collision?
  - How fast and in what directions are any fragments ejected?
- These results then feed into models of the whole Saturn system to test formation scenarios.
- Smoothed particle hydrodynamics simulations
  - ~40 million particles (over 100x resolution of previous studies)
  - unprecedented detail in the ejected debris
  - significantly different distribution of fragments than previous, lower-resolution studies.

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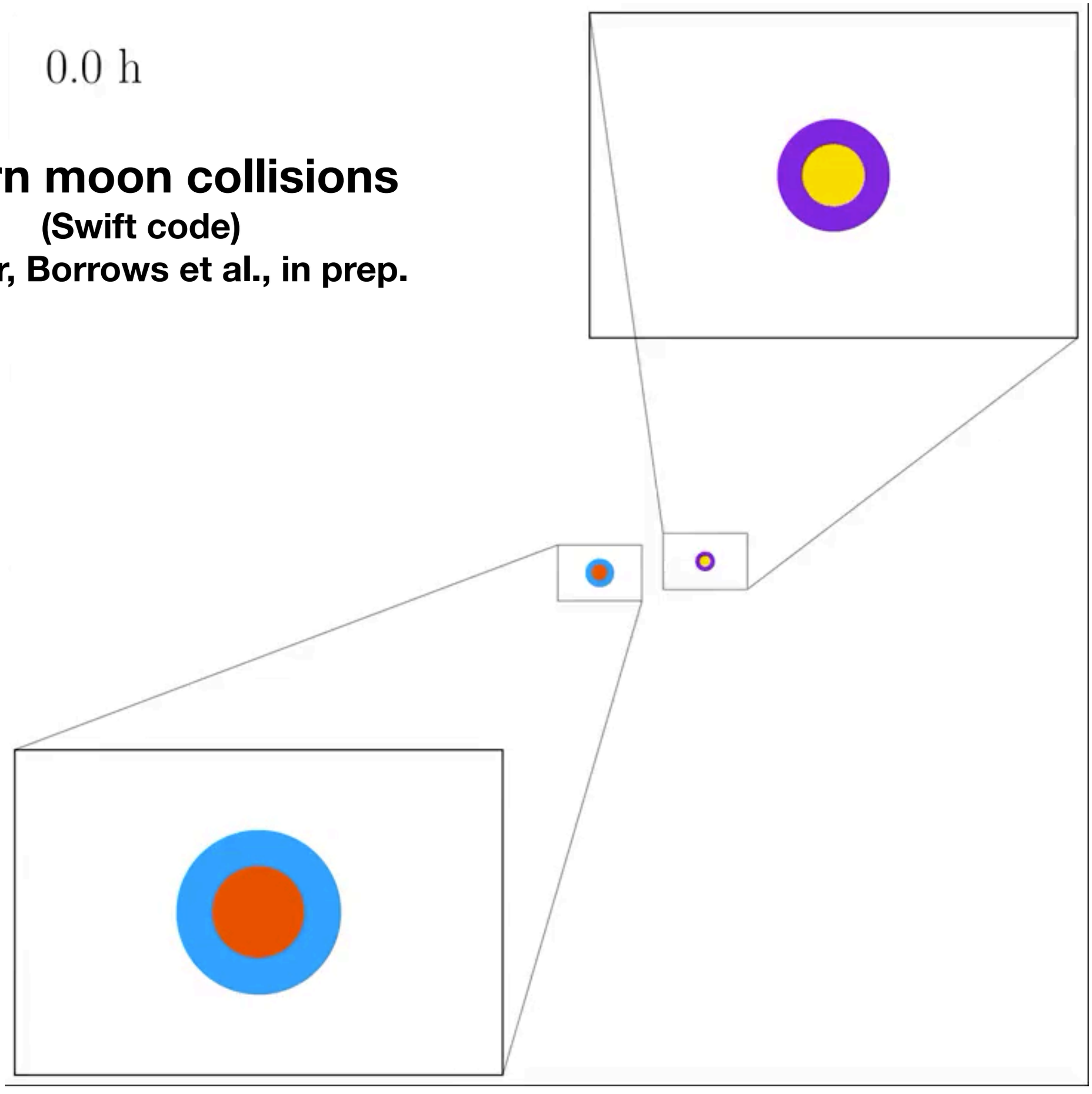
Saturn moon collisions

(Swift code)

Schaller, Borrows et al., in prep.



sphNG

Matthew Bate (Exeter)

- Smooth Particle Hydrodynamics (SPH) code
  - Typically used for star and planet formation, accretion discs
- Multi-physics:
  - Gravity, hydrodynamics, sink particles
  - (non-)ideal MHD
  - Radiative transfer (flux-limited diffusion)
  - Dust/gas fluid mixtures (1-fluid and 2-fluid)
  - Dark matter
- Hybrid MPI/OpenMP code
  - Fortran 77+
  - No other libraries or dependencies

Summary

- Experience of standing up the cluster was no more difficult than standard installations
- User experience of code porting has been very positive in terms of ease of porting and performance obtained
- Further system work and code optimisation on-going
- 2nd Leicester Catalyst hackathon, Sept 9-11
  - Details at **www.dirac.ac.uk** shortly
- For access contact Mark Wilkinson (miw6@leicester.ac.uk)

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