Viper
High Performance Computing at the University of Hull

- The University of Hull's first institutional High Performance Computing (HPC) cluster.

- At 'go live' in June 2016, Viper was the fastest HEI HPC facility in the north of England, and the 6th ranked HEI in the country. It remains a significant computing resource for researchers across the university.

- Additional resource is being added in 2021.

Introducing Viper

- Used by researchers across the University of Hull

  - Department of Computing and Technology
  - Department of Engineering
  - Department of Chemical Engineering
  - Energy and Environment Institute
  - Department of Geography, Geology and Environment
  - Department of Maths and Physics

  - Department of Chemistry and Biochemistry
  - Department of Biological and Marine Sciences
  - Department of Psychology
  - Department of Biomedical Sciences
  - Hull York Medical School
  - Hull University Business School
  - School of Arts

- More than 80 publications in 52 journals or conference proceedings across fields such as:

  Physics and Astrophysics, Materials Science and Engineering, Health and Biomedical Sciences, Computing Science, Machine Learning and Big Data, Environmental Science, Biology and Bioinformatics, Chemistry and Marine Science

  (https://hpc.wordpress.hull.ac.uk/research-outputs/)

University of Hull

@Brad Gibson: Director
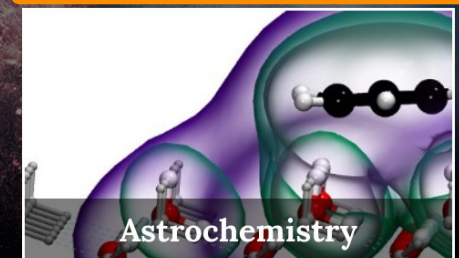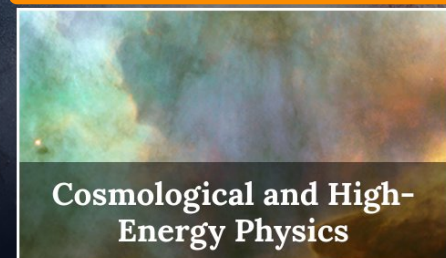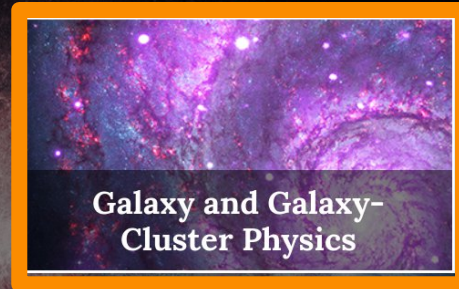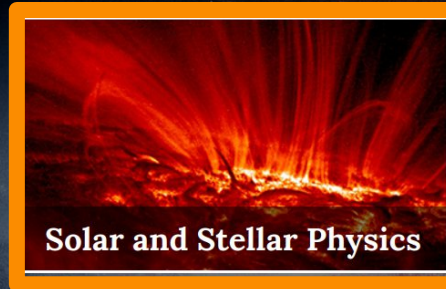ChETEC-INFRA WP6, WP4, ...

E.A. Milne Centre
for Astrophysics

Research Centre @Hull:
EA Milne Centre for Astrophysics
Ongoing HPC in ChETEC-INFRA research areas:
Stellar nucleosynthesis and galaxy evolution
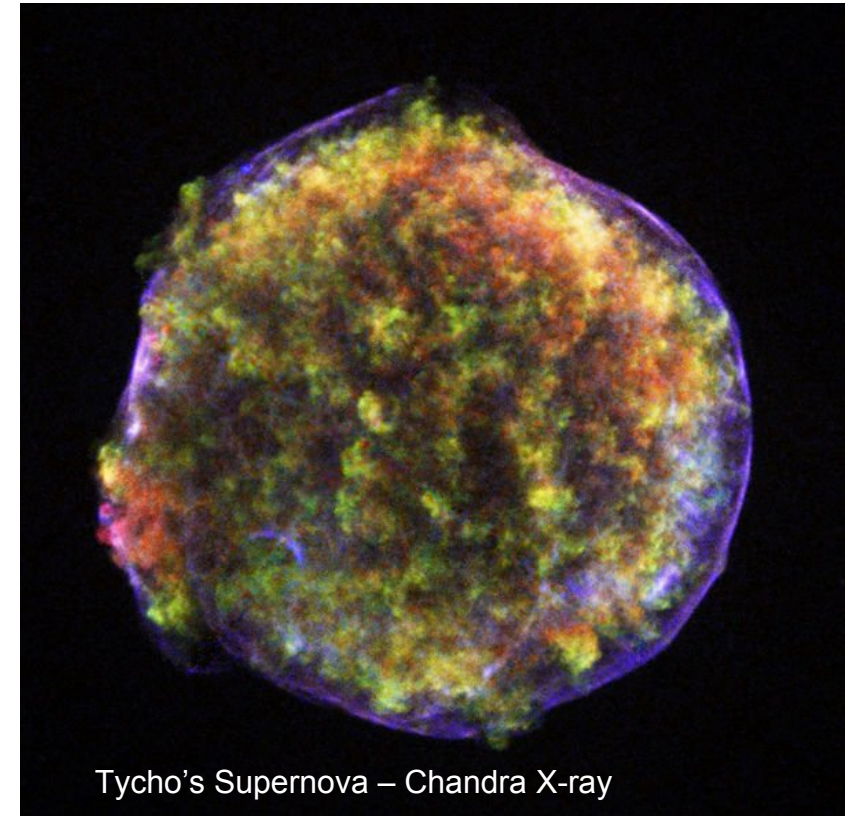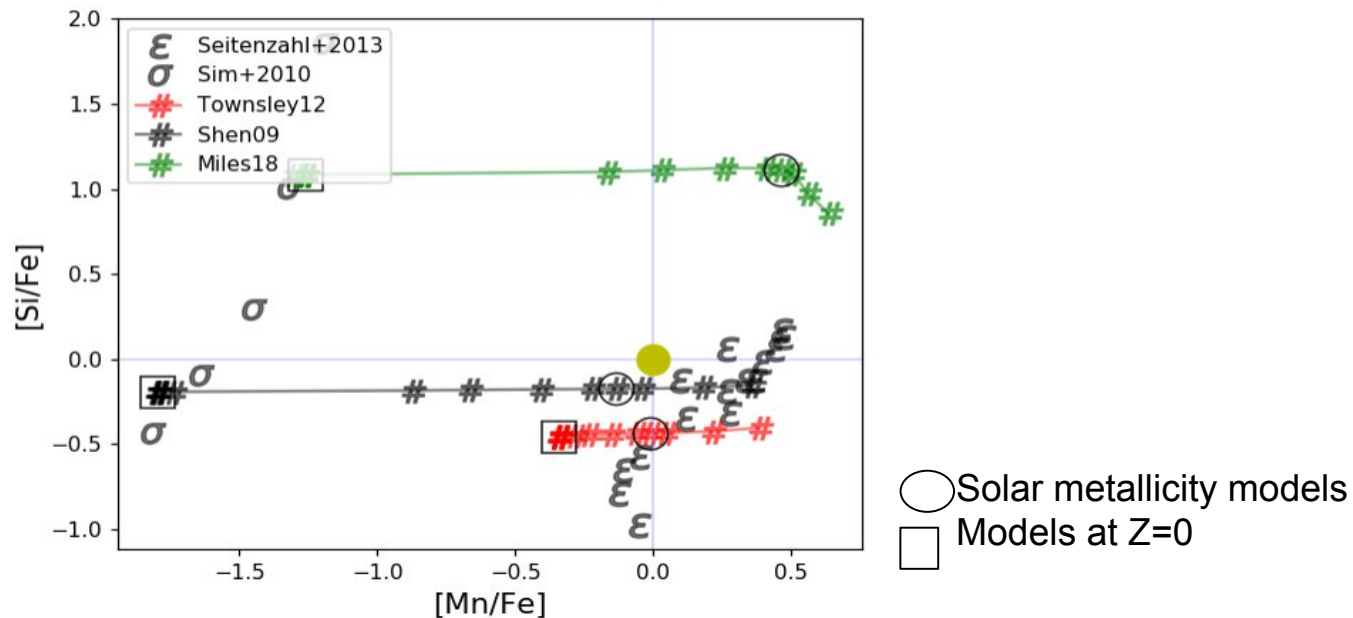
Research areas

Publications ›
External Research Talks ›

Solar and Stellar Physics

Galaxy and Galaxy-Cluster Physics

Cosmological and High-Energy Physics

Astrochemistry

Example of HPC and nucleosynthesis in stars: SNIa and impact on GCE

- Production of the elements in SNIa:
  PhD project: J. Keegans. Thesis submitted this week
  – yields for models by Townsley et al. 2012,
  Shen et al. 2009 and Miles et al. 2018);
- Production of Si, Mn and Fe shown below;
- Impact of different progenitors and metallicities
- Comparison with SNIa models made by

  other groups (HESMA).

Plot legend:
- ε Seitenzahl+2013
- σ Sim+2010
- Townsley12 (red)
- Shen09 (black)
- Miles18 (green)

Axes: [Si/Fe] vs [Mn/Fe]

◯ Solar metallicity models
▢ Models at Z=0

Tycho's Supernova – Chandra X-ray

Viper Compute Resource

	Standard Compute Nodes (180 nodes)	Enhanced Compute Nodes (10 nodes coming soon)	High Memory Nodes (4 nodes)	Standard GPU Nodes (4 nodes)
CPU	Broadwell E5-2680 v4	Cascade Lake 6528R Gold	Haswell E5-4620 v3	Broadwell E5-2680 v4
Cores	28	56	40	28
Speed	2.40GHz (3.30GHz Turbo)	2.70GHz (4.0GHz Turbo)	2.00GHz (2.60GHz Turbo)	2.40GHz (3.30GHz Turbo)
RAM	128GB (2400MHz)	384GB (2933MHz)	1TB (2400MHz)	128GB (2400MHz)
GPU	-	-	-	4x Nvidia K40M

Viper High Performance Interconnect

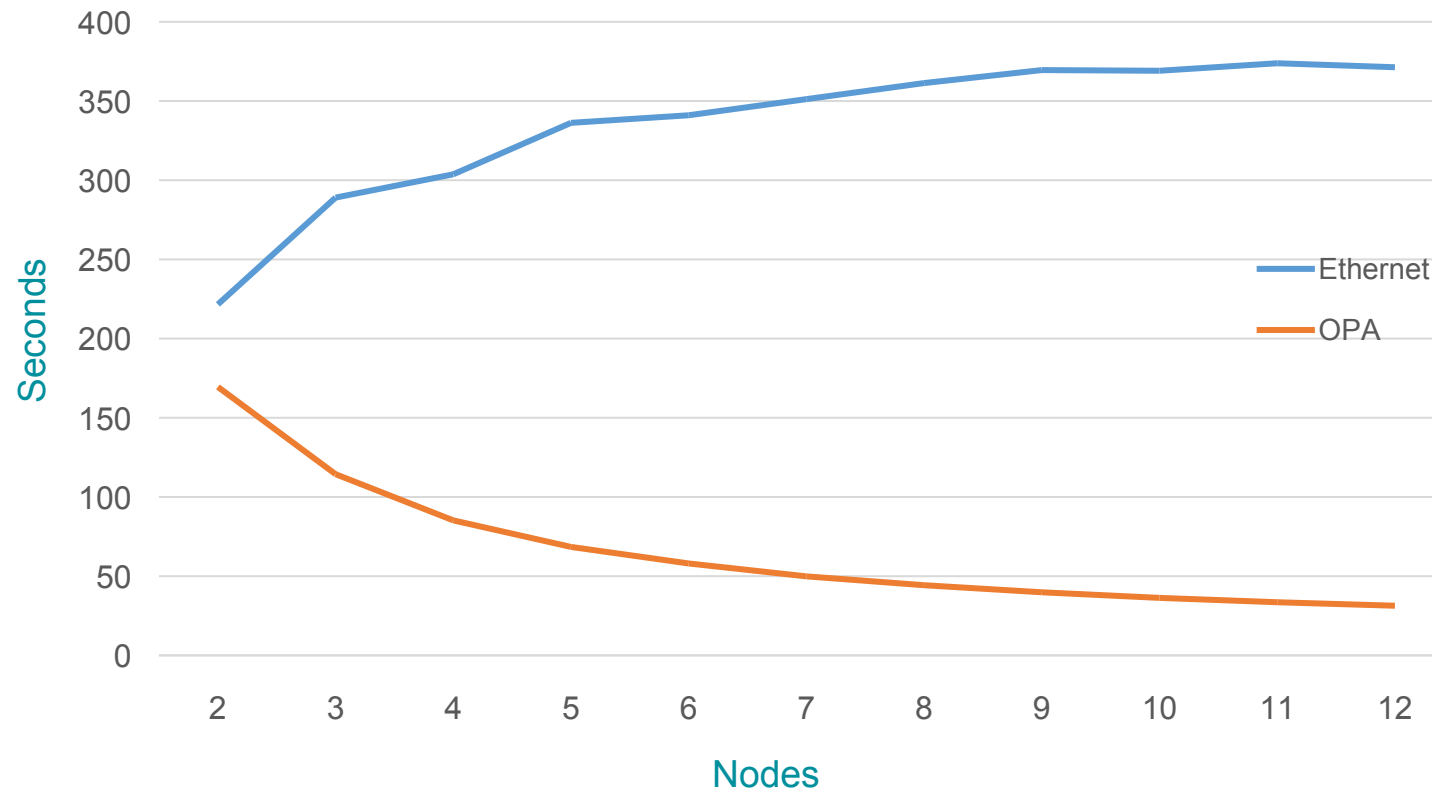| Interconnect	Bandwidth	Latency
Gigabit Ethernet	1 Gbit/s (125 MB/s)	125ms
Omni-Path	**100 Gbit/s (12.5 GB/s)** (observed 11.82 GB/s)	**100ns**

HPL Runtime (seconds) vs Node Count: Ethernet and Omni-Path

> 2 x Visualisation nodes 2 x Nvidia GTX-980 Ti in each

> 500 TB of BeeGFS user storage

> Running CentOS 7 Linux

Using Viper

"Without access to a HPC facility, and Viper in particular, this work would simply not be possible. The large number of particles to process, the time involved and the data storage requirements of this and related projects would simply be too great. Without HPC, these problems in nuclear astrophysics would remain unanswered"
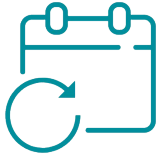
HPC Case Study: The Effect of Progenitor Metallicity on Nucleosynthesis in Multidimensional Type Ia Supernova Models
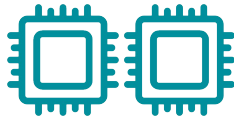James Keegans

(https://hpc.wordpress.hull.ac.uk/phd-case-studies-spring-2018/)

Surface Evolver
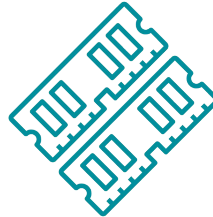
Software to model liquid surfaces shaped by various forces and constraints. Finite Element Analysis to study adsorption dynamics.

|				
Single user expected to run over 2¼ million jobs over the course of PhD	**Single core (up to 28 jobs per node)**	**Less then 2GB of RAM per task**	**Input data less than 1MB, output files approximately 50MB**	**Tasks complete with 20-60 minutes**

Examples of Viper use - Parallel

Water modelling platform used to simulate flow around key areas of the Mekong Delta in Vietnam to investigate changing flood risk with climate.
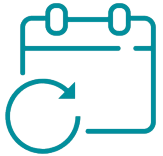
One hundred jobs run over 5 month period
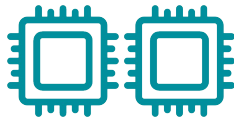
Between 140 cores (5 nodes) and 560 cores (20 nodes) depending on model size
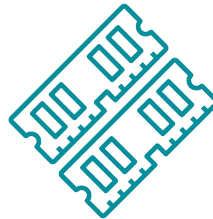
Uses most of the memory on the nodes running the model

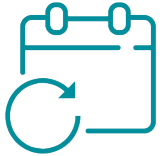**Input data around 500MB, output files around 3GB depending on run length**
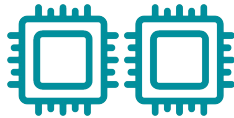
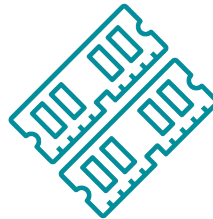**Typical jobs run between 4 and 30 hours**

Astrophysics – FLASH mesh refinement hydrodynamics code.

Multiple users running 40+ large scale parallel jobs in last year

Large parallel tasks between 1540 cores (55 nodes) and 2800 cores (100 nodes)

Across the nodes of each job between 4.5TB and 12TB of RAM used

Input data < 10MB, output files of 50GB. Multiple TB of output per task

Jobs typically run for up to 5 days

HPC Support

- Supported by a dedicated HPC administration team, including Research Software Engineering support

- Wiki site providing documentation, training material and example jobs

- Virtual user drop-in session held weekly via MS Teams

- Range of Linux and HPC tutorials videos available from introductory topics to more advanced and specialist videos

For more information:
https://hpc.wordpress.hull.ac.uk/home/