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Viper

High Performance Computing

TNA Facility

University of Hull

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What is High Performance Computing?

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What is High Performance Computing?

> *"High performance computing (HPC) refers to the use of leading-edge computers for simulation and modelling and for advanced data analysis."*

A Strategic Vision for UK e-Infrastructure, 2011

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Introducing Viper

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Introducing Viper

- 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
- Since coming online:
  - More than 300 researchers have made use of Viper
  - Over 3.2 million jobs have been run
  - A total of nearly 138 million core hours, or about 16,000 years of processing time

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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 110 publications in over 50 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/)

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What is Viper

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What is Viper – Compute Nodes

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

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What is Viper – GPU Nodes

	 Nvidia Tesla K40M	 Nvidia Tesla P100	 Nvidia Ampere A40	Visualisation Nodes  Nvidia GTX-980 Ti
Nodes	3	1	1	2
Cards per Node	4	2	1	2
Single Precision Performance	4.29 TFLOPS	9.3 TFLOPS	38.7 TFLOPS	6.4 TFLOPS
RAM	12GB	16GB	48GB	6GB
CUDA Cores	2880	3584	10752	2816

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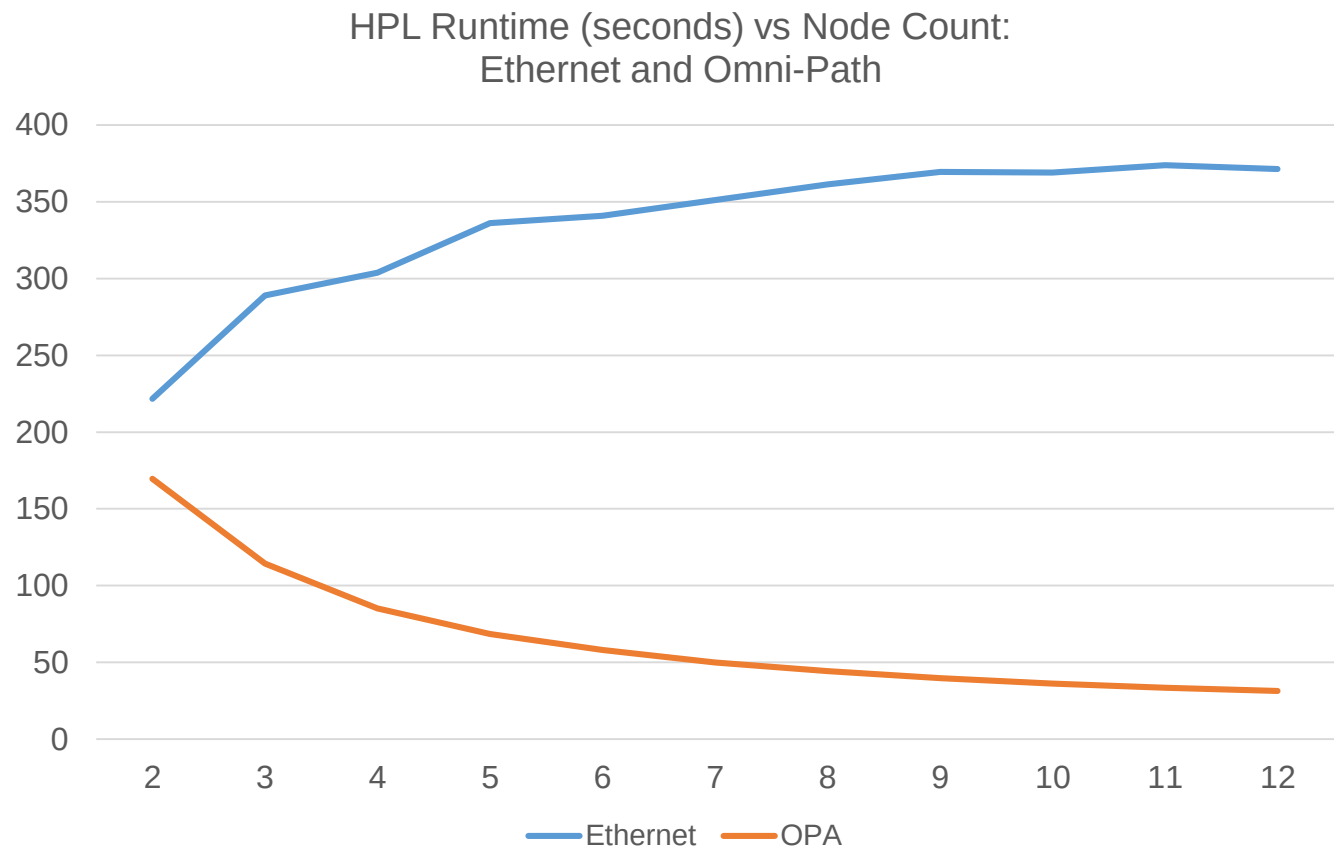
What is Viper – High Performance Interconnect

	Gigabit Ethernet	Intel Omni-Path
Bandwidth	1 Gbit/s (125 MB/s)	100 Gbit/s (12.5 GB/s)
Latency	125ms	100ns



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What is Viper

- Parallel High-Availability 500TB + 200TB BeeGFS user storage
- Running CentOS 7 Linux
- Slurm Scheduler
- Hundreds of software applications, tools and libraries
- Accessed completed remotely via SSH

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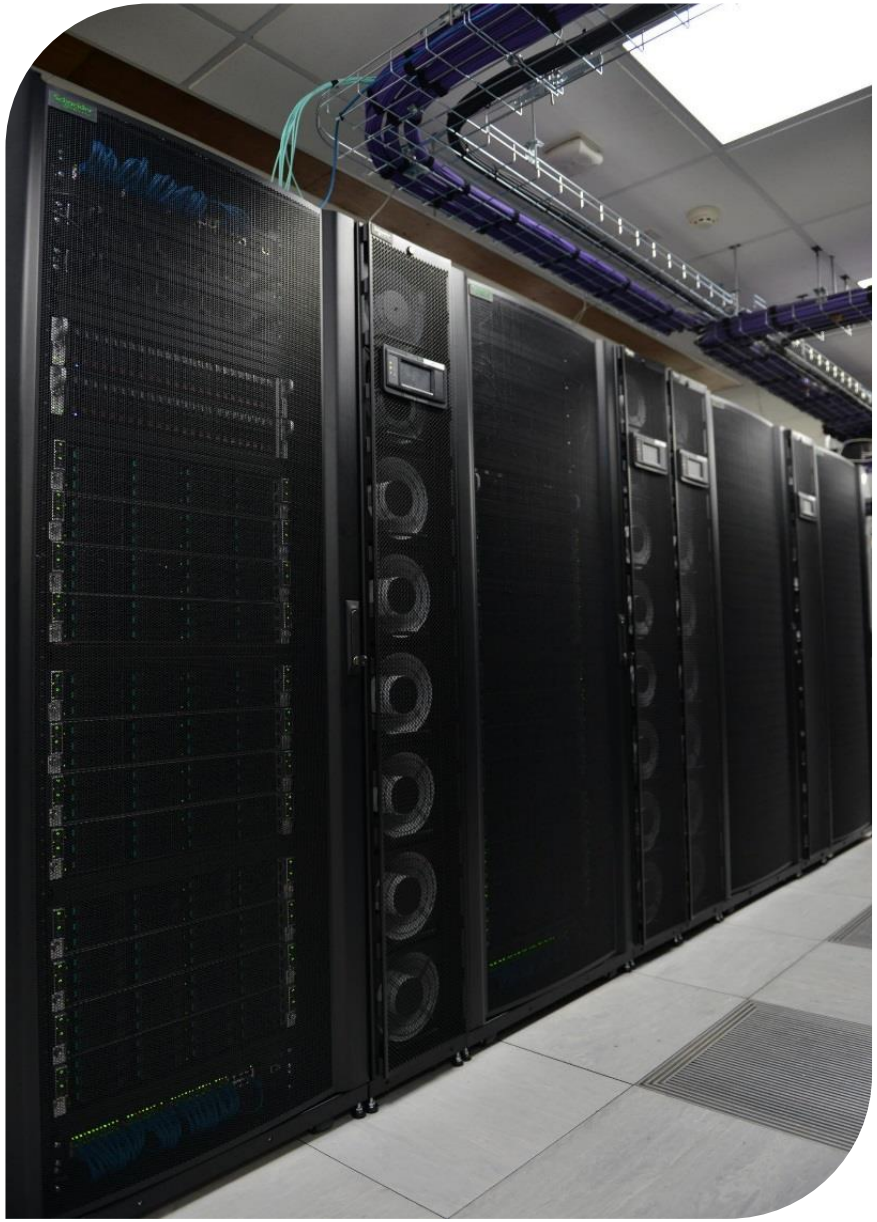
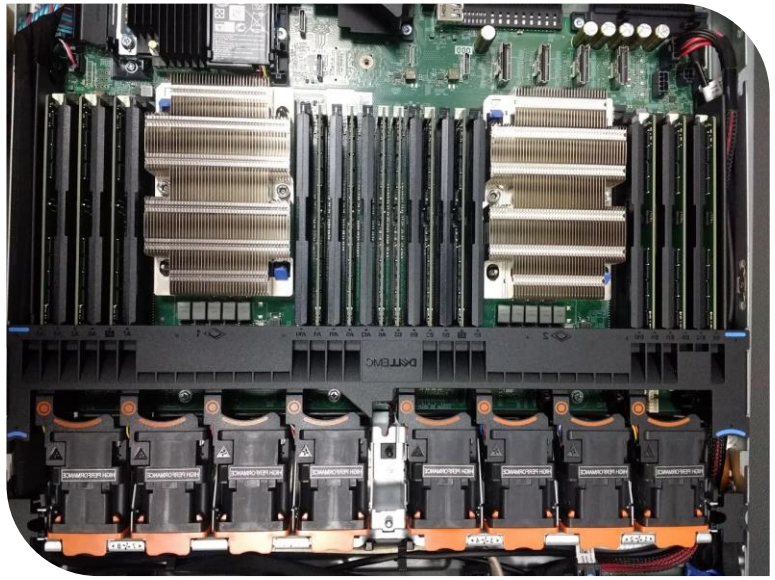
What is Viper





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What is Viper

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How Can Viper Benefit Research

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How Can Viper Benefit Research

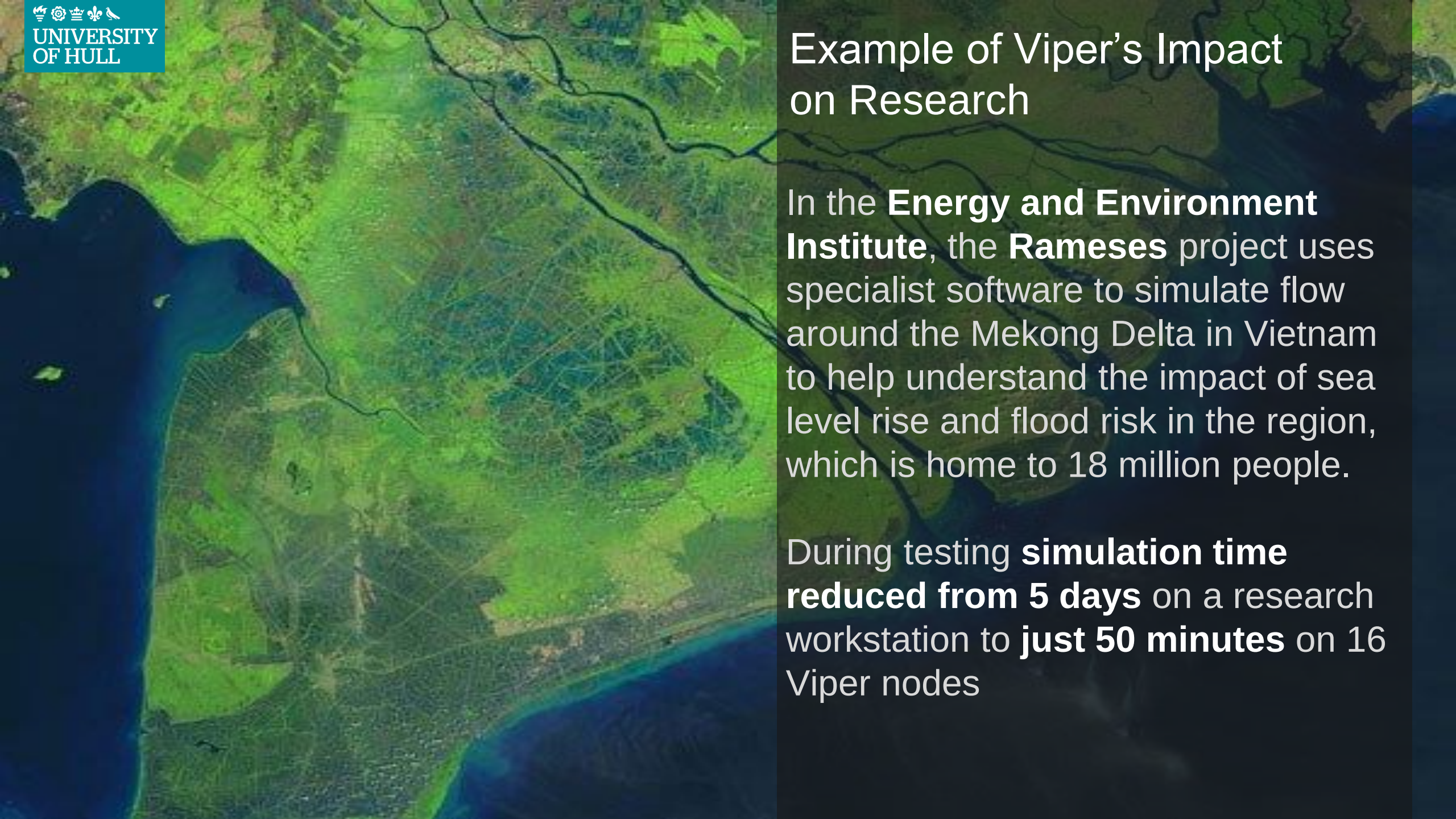
"The use of Viper allows simultaneous calculations of CO_2 with solid materials to be carried out in real time. ***What would have taken hours to days using conventional computer systems has now been reduced to minutes****.*

This level of high speed performance is essential in providing an in-depth study of a chemical reaction"

Matthew Bennett, PhD student

HPC Case Study: Direct Reaction of Anion-Deficient Solids with CO_2

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



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Example of Viper's Impact on Research

In the **Energy and Environment Institute**, the **Rameses** project uses specialist software to simulate flow around the Mekong Delta in Vietnam to help understand the impact of sea level rise and flood risk in the region, which is home to 18 million people.

During testing **simulation time reduced from 5 days** on a research workstation to **just 50 minutes** on 16 Viper nodes

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How Can Viper Benefit Research

"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, E.A. Milne Centre for Astrophysics

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

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Example of Viper's Impact on Research

Astrophysicists from the E.A. Milne Centre rely on Viper for modelling and simulation using FLASH mesh refinement hydrodynamics code.

Large parallel tasks run over between 1540 cores (55 nodes) and 2800 cores (100 nodes). Across the nodes of each job between 4.5TB and 12TB of RAM used.

Tasks can produce tens of TB of output per run.

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Applying For Access

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Applying For Access

Applications Details

Example Task

Job Details

Storage Details

User Experience

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Applications Details

Example Task

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User Experience

What are the main application or codes you will be using?

- Name
- Description
- Download URL
- Required version (if not latest)
- License / Permission details

So we can assess if the required application or code will actually run.

Existing application list:
https://hpc.hull.ac.uk/upload/module.html

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Applications Details

Example Task

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User Experience

Is there a sample task we can run on Viper?

A sample task along with information such as the following helps us check both if and how an application will work on Viper:

- How to configure and compile the code
- Sample driving or configuration data
- How to run the application / command options
- Expected output file for deterministic task or expected/acceptable range for non-deterministic task
- How the sample task compares to production job (e.g. lower core count, shorter runtime, smaller dataset)

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Applications Details

Example Task

Job Details

Storage Details

User Experience

Additional details about the job, in particular regarding any previous runs such as:

- For single node tasks, a description of the single node performance.
- If run on other HPC or multi-node facility, please provide a table of runtime (or performance) against number of nodes or a plot of the performance against number of nodes (a plot of runtime is not acceptable).

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Applications Details

Example Task

Job Details

Storage Details

User Experience

Information about storage requirements of the task helps us judge if we can accommodate the task.

- How much data is read and written by each job?
- What percentage of the produced data do you expect to transfer off Viper on a) each task completion and b) at end of call?

Also includes important information about the type of data that can be stored on Viper

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Applications Details

Example Task

Job Details

Storage Details

User Experience

Some information about your previous HPC experience – this doesn't impact the assessment process but is just to help us identify any training requirements:

- Have you previous experience of running tasks on HPC systems?
- Do you require training relating to HPC scheduler?

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HPC Support

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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

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HPC Support

Introduction to High Performance Computing Video Tutorials

HPC Video Tutorials: Linux Fundamentals

HPC Video Tutorials: Linux Key Commands

HPC Video Tutorials: Linux Command Line Tips

HPC Video Tutorials: Linux Data and Data Commands

HPC Video Tutorials: Introduction to HPC

HPC Video Tutorials: HPC Scheduler I

HPC Video Tutorials: Software Modules

HPC Video Tutorials: Batch Jobs

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Questions?

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Questions?

For more information:

https://hpc.wordpress.hull.ac.uk/chetec-infra-information-page/

Email:

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Follow us on Twitter:

@HULL_HPC_VIPER

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Thank You