# High Performance Computing Newsletter

December 2016 Edition 1

## Pro-Vice-Chancellor for Research and Enterprise: Dr David Richards

Welcome to the first edition of this newsletter, highlighting the fantastic work that has been done with the University's new High Performance Computer (HPC), Viper. We are now a leading university for computing power in the North of England and our researchers are already reaping the rewards of this superb equipment. A lot of hard work has gone into the success of Viper and the project team has done a brilliant job.

I very much enjoyed the launch event where we saw real examples of how the HPC is already influencing both how we do research and the outcomes. I am really looking forward to more researchers having the opportunity to see how their work can be influenced by the superb computing capability we now have. I want the HPC community to grow and, based on demand from our researchers, I look forward to seeing Viper II in a couple of years.

Viper is not only having a real impact on our researchers, but also attracting the attention of the HPC community, which has hailed the University's 'impressive procurement and implementation process' and I was particularly pleased to see comments from people like Robert Maskell, Intel's Director of High Performance Computing, who wrote: "I've always wondered why Hull came out of nowhere in relation to HPC and got up to speed so quick. You've certainly made a positive impact."

A huge well done to everyone involved and let's see what more we can do.

# INTRODUCING VIPER

On Friday October 7th the University hosted a formal launch event for Viper, the University's first centrally supported High Performance Computing (HPC) facility. Having gone live as a pilot service in June, the formal launch event saw researchers and senior managers from across the university being joined by external guests to learn more about Viper and how it is already contributing to research outcomes. External guests on the day included representatives from other regional universities, the N8 and partners who helped deliver Viper such as Red Oak Consulting and Intel.

Speeches from Dr David Richards, PVC for Research and Enterprise and Graeme Murphy Head of Research and Enterprise ICT Services highlighted the university's strategy and ambitions for the HPC service and detailed Viper's journey into live service.

Members of the HPC Steering Group then showcased some of the research that has already been carried out on Viper in the first few months of pilot service. Dr Dave Lunt explained how the EvoHull group are using Viper to look at environmental genomics and bioinformatics and how access to the sig-

nificant computational resource has provided the opportunity to develop new and novel approaches to research; to truly experiment and push boundaries.


Dr Dave Lunt presenting the work of EvoHull

Dr Nina Dethlefs described how utilising Viper has transformed her research in deep learning and natural language processing almost halving computation time. This has already resulted in the submission of two papers and an invitation for her to present at external events.

Professor Brad Gibson presented some of the work of the E.A. Milne Centre for Astrophysics that Viper has contributed to whilst highlighting some of the larger questions Viper will help answer. Prof. Gibson made it clear that the university's HPC could contribute to game changing science.

Dr David Benoit showed some of the research that he and his colleagues have carried out on Viper. This has resulted in Dr Benoit being the heaviest user of Viper since go live date. Dr Benoit also revealed that the first paper attributable to work carried out on Viper had recently been accepted. '*Amine catalysis for the organocatalytic diboration of challenging alkenes* to be published in Chemistry – A European Journal (2016)[1]' is the first of a number of papers submitted by Viper users to be been accepted for publication.

Darren Bird from the Viper support team providing a tour of Viper

The afternoon concluded with tours of Viper and discussions with potential new Viper users.

[1] *A. Farre, K. Soares, R.A. Briggs, A. Balanta, D.M. Benoit and A. Bonet, "Amine catalysis for the organocatalytic diboration of challenging alkenes"'* 'Chemistry - A European Journal (2016)'

## Research Outputs June - November 2016

- Dr Elke Roediger, presentation titled "**Fluid dynamics in the ICM Presentation**" at Physics of the Intracluster Medium: Theory and Computation 2016, University of Minnesota, August 2016
- Dr Nina Dethlefs, presentation titled "**Deep natural language learning on Viper**", at Network on Computational Statistics and Machine Learning Workshop, Edinburgh University, August 2016
- Dr Angela Dyson, presentation titled "**The effects of non-equilibrium phonons on electron transport in GaN & AlN**", at the High Efficiency Materials for Photovoltaics (HEMP), Imperial College London, September 2016
- Dr Angela Dyson, presentation titled "**Monte-Carlo simulation of a GaN Gunn diode**" at the International Workshop on Nitride Semiconductors, Orlando Florida, October 2016
- Albert Farre, Kaline Soares, Rachel.Briggs, Dr Angelica Balanta, Dr David Benoit and Dr Amadeu Bonet, paper titled "**Amine catalysis for the organocatalytic diboration of challenging alkenes Publication**" in Chemistry - A European Journal, October 2016 (10.1002/chem.201603979)
- Christina Roggatz, presentation titled "**How quantum chemical methods help to unravel the effects of pH on marine communication**" at Molecular Graphics and Modelling Society Young Modellers' Forum 2016, The Old Naval College London, November 2016

If you have presented or published work carried out on Viper, please let us know at viper@hull.ac.uk

# HPC STEERING GROUP

The HPC Steering Group has been formed to provide governance of the HPC service. Comprising of researchers from across the university who are amongst the most experienced users, the steering group were involved in the procurement and acceptance testing phases of Viper and continue to provide a level of independent governance for the HPC service. The HPC Steering Group consists of:

- Dr David Benoit, School of Mathematics and Physical Sciences
- Dr Nina Dethlefs, School of Engineering and Computer Science
- Professor Michael Fagan, School of Engineering and Computer Science
- Professor Brad Gibson, School of Mathematics & Physical Sciences
- Dr Dave Lunt, School of Biological, Biomedical and Environmental Sciences
- Dr Jason Wood, School of Engineering and Computer Science

In Focus: Dr David Benoit, Senior Lecturer in Physical Chemistry, is a computational chemist who has over 15 years experience in high-performance computing. His research focusses on the development of novel high-performance computational techniques to understand dynamics and properties of large molecular systems. He also has a particular interest in hardware-accelerated computing, vibrational theory, astrochemistry, biological signalling and molecule-surface interactions. Dr Benoit also chairs the HPC user forum.

In Focus: Dr Nina Dethlefs is a lecturer in Computer Science carrying out research on natural language processing. For the latter, Dr Dethlefs investigates machine learning models that can automatically extract linguistic patterns from data, and then use them to understand and generate language in new contexts. Recently, Dr Dethlefs has become interested in deep learning and big data research. These require the use of HPC to run experiments on larger and 'more interesting' datasets.

# Viper HPC Support Team

The HPC Support team manage the day to day administration of the HPC service, and are available to provide training and assistance for those wanting to use HPC in their research. The team consists of:

Chris Collins
HPC Systems Manager

Darren Bird
HPC Software Support Engineer

Ahmed Seif
HPC Systems Support Engineer

Craig Johnson
HPC Software Support Engineer

David Coulson
HPC Support Specialist Intern

Matthew Summerbell
HPC Support Specialist Intern

CASE STUDY

# THE LARGEST COSMIC STRUCTURES SIMULATED ON VIPER

Dr Elke Roediger
Milne Centre's Galaxy Cluster Team

Between Viper going live on June 28th 2016 and November 28th 2016, Elke and her research group ran nearly 900 jobs on Viper, using over 715,000 CPU hours

Researchers at the E. A. Milne Centre for Astrophysics at the University of Hull study the universe on all scales, ranging from solar physics to cosmology, using techniques of both observational and computational astrophysics. Within the Milne Centre, I lead a research group studying clusters of galaxies. One of our recent numerical simulations of galaxy cluster growth run on Viper is shown in Fig. 1. Our simulations are part of local, national and international collaborations with astrophysicists observing galaxy clusters across the electromagnetic spectrum at the world's best facilities. By directly comparing our simulations to our collaborators' observations, we study the formation of structure in the universe to understand why the present universe looks the way that it does. Our work focusses on three main topics: the growth of galaxy clusters, the plasma properties of the cluster atmospheres, and the evolution of galaxies in clusters.

In the early universe, matter was distributed almost homogeneously. The cosmic structures we observe today grew out of tiny inhomogeneities as gravity led to the contraction and collapse of matter in regions of slightly higher density. This in turn led the formation of the first stars, galaxies, and groups, and eventually the formation of clusters of galaxies, the largest gravitationally bound structures in the universe. Clusters of galaxies are still growing by accreting more galaxies and by colliding and merging with each other. Thus they give us the opportunity to observe cosmic structure formation in action, which is a focus of our research.

The cluster galaxies constitute only a small fraction of the total cluster mass. The majority of the baryonic mass, i.e. normal matter in clusters is found as a hot gas in the space between galaxies. However, the largest part of a galaxy cluster's mass is found in dark matter, which dominates the motion of the cluster's galaxies and binds the cluster atmosphere.

At temperatures of tens of millions of degrees the hot cluster, or atmosphere is a fully ionised plasma which is threaded with weak magnetic fields. Despite being a plasma, the cluster atmosphere can be modelled by hydrodynamics, i.e., similar to air. However, due to the complex interactions of the charged plasma particles with each other and the magnetic fields, properties of the cluster "gas" such as thermal conductivity and viscosity are still uncertain, and are a focus of our studies.

Galaxies inside and outside of clusters evolve differently. Figure 1 shows that galaxies can easily lose their own gas by moving through the cluster atmosphere. This gas loss is particularly important for spiral galaxies. This type of galaxy usually continuously forms new stars out of the galaxy's supply of cold

gas. Thus, the loss of gas leads to star formation shutting down, changing many characteristics of the galaxy. Observations show that this can happen both quietly or in a last spectacular burst of star formation. Determining the conditions for the mode of shutdown is another area of our research.

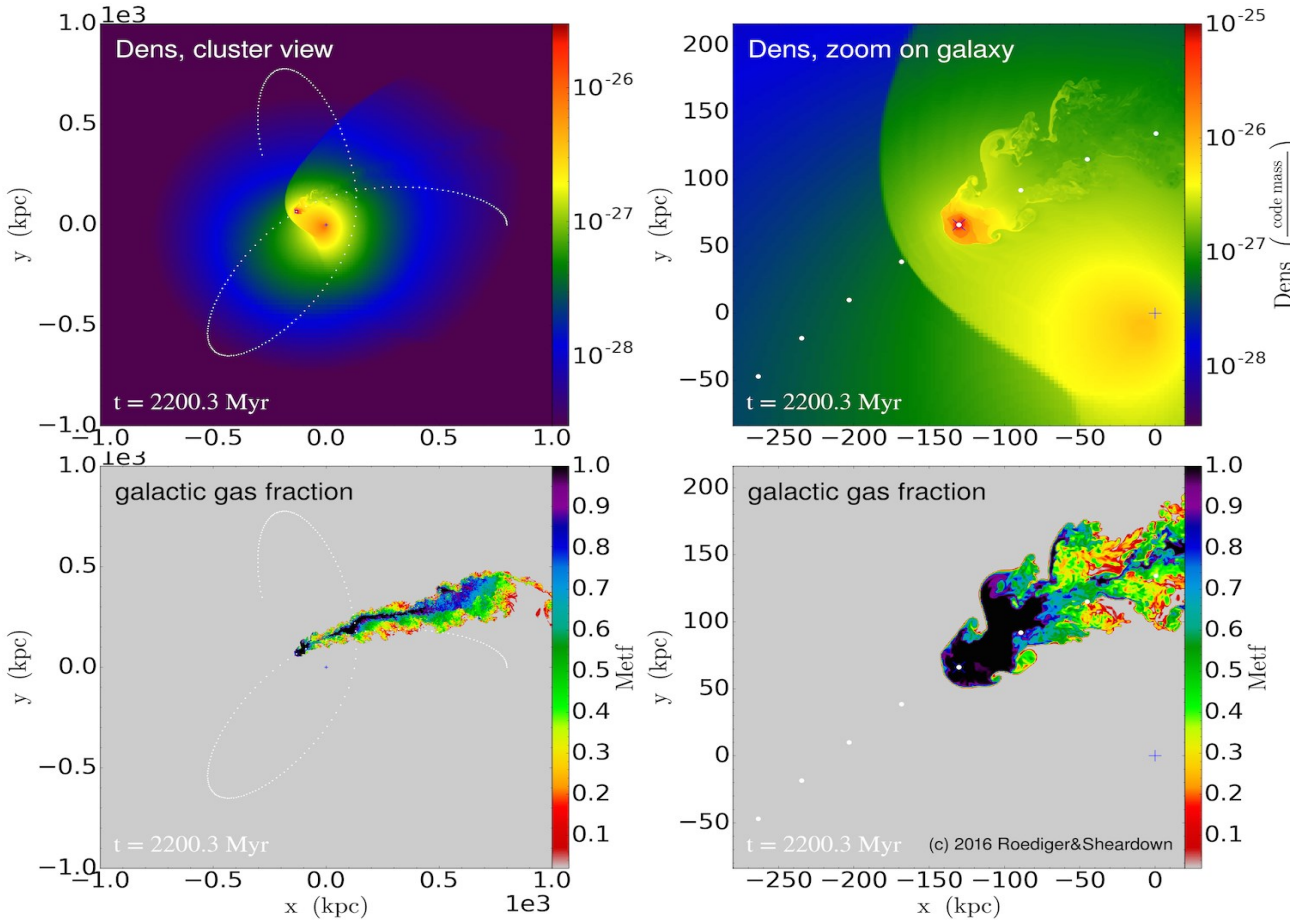


*Figure 1: Simulation of a massive galaxy falling into a galaxy cluster. The galaxy moves through the cluster atmosphere and thus experiences a head wind which strips off the galaxy's gaseous atmosphere. The movie shows slices in the orbital plane of the galaxy. The panels on the right zoom in on the galaxy, the panels on the left show the cluster-scale view. The top panels colour-code the gas density, the bottom panels colour-code the fraction of galactic gas and thus highlight the mixing of the galactic and cluster gas. The presence of turbulent mixing or its suppression by, e.g., viscosity, can now be observed in real clusters. Our simulations provide the reference point to interpret the observations and thus measure the cluster gas properties. The full simulation box spans 12 Mpc (40 million light years). The peak resolution in the galaxy and its wake is 0.36 kpc (about 1000 light years). Thus, the simulation covers a dynamic range of $3x10^5$ in spatial scales. Full movie can be downloaded from http://hpc.hull.ac.uk/media/MinorMerger_or_GasStrippingInGalaxyCluster.mov (25Mb)*

The current members of the Milne Centre galaxy cluster team are PhD students Alexander Sheardown and Matthew Hunt, final year MPhys student Matthew Chan and final year BSc students Alexandra Doherty, Emily Wilcox, and Thomas Fish. Viper provides for us an ideal in-house access to HPC where we can develop new simulations and do production runs. Simulations are led by Alexander, Matthew and Matthew; Alexandra, Emily and Thomas analyse the simulation data to answer a variety of scientific questions.

Our main tool is FLASH (http://flash.uchicago.edu/site/), an adaptive mesh refinement hydrodynamics code. Its adaptive refinement capability is vital to our work because it allows us to cover the large dynamic range of scales involved. For example, the simulation in Fig. 1 uses a simulation box of 40 million light years along a side with smallest grid cells resolving scales of 1000 light years, spanning a dynamic range of a factor of $3x10^5$. However, a large amount of that dynamic range is invested in capturing the cluster environment of the galaxy, and the galaxy's atmosphere is resolved by only 120 grid cells across (at cluster core passage). The high resolution is maintained along a good part of the galaxy's wake which allows us to study mixing of the stripped galactic gas with the ambient cluster gas. This simulation consumed 60,000 core hours, somewhat less than 24 hours on 100 nodes.

To showcase the potential of adaptive mesh simulations on FLASH, Alexander Sheardown and Matthew Hunt simulated a zoom-in on the galaxy in 2D, resolving the galaxy's atmosphere with 8000 grid cells across its diameter. A snapshot and zoom-ins into the mixing regions are shown in Fig. 2. At this high resolution, even the 2D simulation consumes 24 hours on 128 nodes.

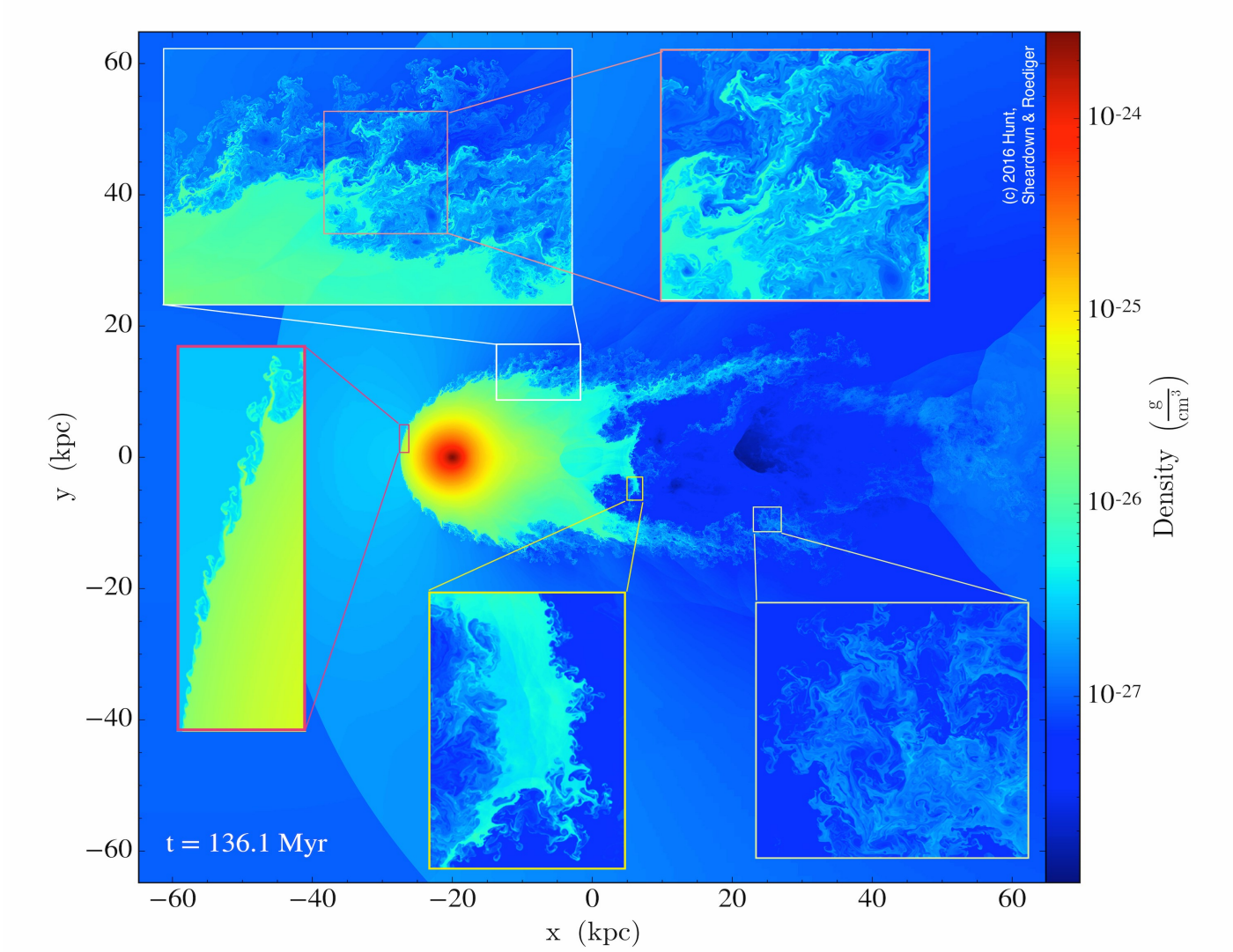


*Figure 2: 2D high dynamic range simulation of galaxy gas stripping and mixing of the stripped gas with the ambient cluster gas. The image shows a density slice through the galaxy and zoom-ins on several regions. The simulation captures mixing features less than 1000 times smaller than the galactic atmosphere.*

3D high dynamic range is essential for our simulations of gas mixing in cluster mergers and in galaxies' wakes. 3D high dynamic range will be even more important to resolve star formation in a galaxy while following the galaxy's motion through its host cluster, which requires improving resolution by about a factor of 10. The adaptive mesh capability of FLASH and the access to Viper computing time of the order of millions of core hours will enable us to do so.

We presented our first Viper results at an international conference (Physics of the Intracluster Medium: Theory and Computation, http://www.ftpi.umn.edu/workshops/2016-2017/ICM2016/) and have supported several submitted observational papers. Our current simulations on Viper will result in a series of papers lead by the Hull Milne Centre galaxy cluster researchers.

For more information on Dr Roediger's work, please contact: e.roediger@hull.ac.uk

If you wish to contribute a case study based on your HPC work, please contact: viper@hull.ac.uk

## Since "Go Live" June 28th - Nov 28th

# Nearly 150,000 jobs were run on Viper

**5.6** million CPU hours were used on Viper (the equivalent of nearly 650 years!)

78% of Viper jobs started running within 1 minute of submission

Viper registered over 90 users from across the university

97 support tickets raised via help@hull.ac.uk, with 81% resolved within 8 hours

## Using Viper

Viper has 180 compute nodes connected via Intel's latest Omni-Path technology. These compute nodes have 28 Intel Broadwell CPU cores and 128GB of RAM. There are also four high memory nodes with 1TB of RAM, four GPU nodes with multiple NVIDIA K40 GPU cards, and two nodes designed specifically for visualisation. For the researchers at Hull this means that whatever the computational requirements, Viper should have the resources to meet their needs.

### Support, Training and Documentation

For more information on Viper please visit our website at http://www.hpc.hull.ac.uk. From there you can find links to additional support on our wiki at http://www.hpc.hull.ac.uk/wiki/ and our user forum at http://www.hpc.hull.ac.uk/forum/. Further documentation for Viper, including introductory Linux and HPC, application specific material and guidance on programming in a HPC environment is currently being developed.

To apply for an account on Viper please follow the link on the main website "Apply for an Account".

For help and support please email help@hull.ac.uk. For other enquiries please email viper@hull.ac.uk

Please contact us if you have any queries regarding Linux or HPC training. We would be happy to discuss how we can meet your requirements with either informal or formal, individual or group sessions.

You can learn more about what we are doing on the HPC service blog at http://www.hpc.hull.ac.uk/blog/ or by following us on Twitter at @HULL_HPC_VIPER.

### Upcoming Events

HPC Drop in session, Nidd Mezzanine Friday 16th December 2pm-4pm - Please pop by to see us with any questions relating to HPC, to find out more about Viper and what we can do for you and your research, or just to say hello!

HPC User Forum, Derwent Seminar Room 4/4A Wednesday 11th January afternoon - The first HPC User Forum meeting. More details to follow.

UNIVERSITY OF Hull

INAUGURAL LECTURE

# BUILDING A UNIVERSE INSIDE A SUPERCOMPUTER

**Professor Brad Gibson**
Director of the E.A. Milne Centre for Astrophysics

**Monday**
**12 December 2016**

**6 pm**

**Allam Lecture Theatre**
**Esk Building**
**University of Hull**

**www.milne.hull.ac.uk**

ADMISSION
FREE
ALL WELCOME