Celebrating 12 months of Viper

On the morning of June 28th 2016 Viper, the University of Hull's first institutional High Performance Computer (HPC), went live with Dr Helen Wright from Computer Science submitting the first real research task to the newly installed HPC cluster. The launch into live operation was the culmination of several years' work by a large team of staff from across the institution and has delivered a system that the University can truly be proud of, providing an environment that will stimulate innovation and support world class research.

As we celebrate the end of the first year of service, Viper now has over 120 registered users from across the university, and has run nearly 390,000 jobs. From this, Viper is approaching 14 million core hours of work, research that would have taken a single computer processor nearly 1600 years to complete. This past 12 months has seen work carried out on Viper published in papers, presented at conferences and submitted in theses. Examples of the research outputs from work carried out on Viper can be found later in this newsletter.

Not only does Viper help reduce time to publication, but it is also changing the way research is conducted. Researchers are able to make step changes in their methods and practices with hugely beneficial results by looking at new and novel approaches.

Dr Dave Lunt explains "Viper has changed the way we do bioinformatics research. Analyses that took hours previously are now so fast they are part of a new, continuous analysis framework, allowing us to tackle problems in truly novel ways".

While much of the work carried on Viper is from traditional HPC disciplines in the Faculty of Science and Engineering (computer science, bioinformatics, engineering, computational chemistry or astrophysics) Viper is also attracting interest from more non-traditional areas. The Viper team are speaking with researchers from the Faculty of Arts, Cultures and Education about the application of HPC to their research and, looking forward, Digital Humanities may be the next exciting direction for Viper.

Viper is available to all research staff and postgraduates at the University of Hull and could potentially benefit anyone with a computational element to their research, no matter the size.

The university is already looking to the future, with the HPC-2 project getting recent approval for a phase of requirements gathering and an investigation on the return on investment that HPC provides. Viper users and other stakeholders will be approached in the coming months as ICTD work with HPC partners Red Oak Consulting to look at how the future research requirements for HPC at the University of Hull can be met.

In this edition:

In April the Hull Science Festival showcased the role of science, maths and engineering within our culture. The festival was well attended with all tickets for the discovery zone being taken! Numerous events showcased the wide variety science, research and engineering undertaken at the university such as the Planetarium and the Universities Formula Student entry.

The Viper team provided the answer while our researchers spoke about the impact supercomputers can have on research

The Viper team were present in the Discovery Zone displaying the ground-breaking research performed on Viper. The team answered numerous questions from adults and children regarding usage of Viper, it's specification and performance, HPC in general and lots more. The team displayed two different activities aimed at highlighting the benefits of HPC, with our 'mini Viper' Raspberry Pi Cluster attracting a lot of attention.
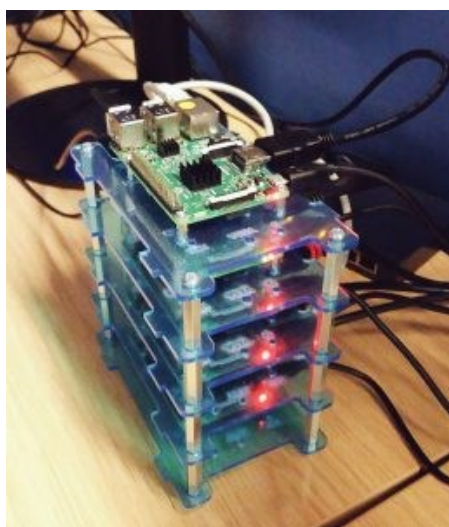
The 'mini Viper' cluster, made from 4 Raspberry Pi computers

The Pi Cluster consisted of 4 Raspberry Pi render-

ing a CGI image, compared to 1 Pi completing the same task. The 4 machines working together complete the render roughly 2 to 3 times faster than the machine working on its own. The basic principle of the Pi cluster applies to Viper providing a great example highlighting the benefits of HPC to researchers.

The Pi cluster in action rendering CGI images, with state of the art desk fan cooling!

Throughout the day we were fortunate to have numerous of our researchers answering questions regarding the research that they are undertaking using Viper.

The festival provided a fantastic opportunity to display the work going on at the university, to inform people of the ground breaking research being undertaken and to answer the many questions on Viper that people asked.

More information on the teams experience can be found at:

hpc.wordpress.hull.ac.uk/2017/04/11/science-festival-and-itil/

More information on the setup of the Raspberry Pi cluster can be found at

hpc.wordpress.hull.ac.uk/2017/03/31/hull-science-festival-2017-parallel-rendering-with-4-raspberry-pis

Viper in UCISA Video Case Study

In March of 2017, the ICT Department (ICTD) submitted a video highlighting the Viper supercomputer for the 17 conference. This three day annual conference, held this year at the 5* Celtic Manor Hotel in Newport, is the go to event for Information Services leaders and professionals from the Higher Education sector and is a great platform to showcase the University's achievements.

UCISA (Universities and Colleges Information Systems Association) is an association in the UK that represents the whole of higher education in the provision and development of academic, management and administrative information systems.

John Hemingway, Director of ICT, thought the UCISA17 video case study was the perfect opportunity to showcase Viper as this has been a huge success story for the University of Hull. Viper's cutting edge infrastructure and technology is helping to transform the University's research capabilities and is now one of the leading institutional HPCs within the sector and is the highest in terms of performance in the North of England.

The UCISA video shows Viper users Dr Elke Roediger and Dr Gareth Few at work

With help from academic departments from across the University and the HPC Support Team, the video highlighted Viper's fantastic achievements and industry leading research technologies that will help to continue to develop ground-breaking research for many years to come.

You can watch the video at: www.youtube.com/watch?v=uWdp-r0-2n4

HPC Special Interest Group

In September the University will be hosting the UK HPC Special Interest Group quarterly meeting along with a follow up one day workshop. Comprising of providers of HPC services at more than 40 UK universities and research institutes, the HPC-SIG aims to promote the use of HPC in academia and industry. Hosting the September meeting is a sign of the growing reputation that the University of Hull has forged in the HPC arena since Viper came online in June 2016.

During the meeting, current interns David Coulson and Matthew Summerbell will be presenting on their experience with us. Recruitment of skilled HPC staff is a recognised issue within the sector, and there has been much interest in our intern programme from those in the HPC SIG. The second day will feature a workshop on cloud computing.

New National Tier-2 HPC Sites

Six new Tier-2 HPC centres, funded by £20 million from the EPSRC, will give academics and industry access to powerful computers to support research in engineering and the physical sciences. The centres are located at the universities of Cambridge, Edinburgh, Exeter, Oxford, Loughborough University and UCL.

The new centres provide a diversity of computing architectures to meet the computational requirements of the research community (including high-throughput and GPU computing). For example, the JADE system at the University of Oxford will be the largest GPU facility in the UK while the GW4 centre will be a world-leading facility based on ARM processors. Scientists will thus be able to choose from a wide range of emerging architectures to run their applications.

Modelling Molecules In Future Oceans Using Viper

By Christina C. Roggatz

Dr. Benoit's Computational Chemistry Group

Between August 2016 and June 2017, Christina ran more than 500 jobs on Viper, in total utilising over 17,000 CPU hours

Water and computers don't mix well in reality as everyone knows. Modelling the influence of water on biological and chemical processes also poses a whole set of challenges. However, it enables me to investigate a very interesting question: What do molecules look like in future oceans and what are their characteristics?

Why are molecules in future oceans of interest?

The oceans are becoming ever more acidic as man-made, increasing carbon dioxide emissions into the atmosphere are absorbed and cause the pH in our world's oceans to decrease an effect called ocean acidification. By the year 2100, the sea surface pH is predicted to drop by up to 0.4 units to pH 7.7. This may not seem much, but it has been shown to significantly affect the fitness, physiology, reproduction and behaviour of everything in the sea from huge sharks and whales to the tiniest of plankton. My latest research [1] also reveals that smell molecules in the ocean are significantly affected by ocean acidification (Fig. 1).

Imagine you are a little crab living on a shore covered with large rocks and deep pools, and battered by tides and waves. The only way to find your lunchtime snack would be to smell it from a distance. But the same also applies to the octopus hunting you. So you, the crab, also rely on smelling the octopus first to avoid being eaten. What if this was no longer possible?

In fact, chemical communication using smell is essential for marine organisms. Its importance is comparable to the combined status of vision and hearing in humans. Smell molecules are chemicals that are produced on purpose – by females to attract males, for instance – or as a result of natural processes such as protein degradation. In both cases, they can be used by animals to smell their way around. Many smell molecules transporting information from its source to an organism are potentially sensitive to pH. This holds particularly true for peptides and proteins, which are used, for example, by crabs, barnacles and mussels as markers for food, predators, settlement spaces or during brood care and larval hatching. The main question is whether a drop in pH will affect their function and render them ineffective.

How can Viper be used to model marine molecules?

For a molecule to be "smelled" by an animal it needs to interact with a receptor located in the animal's nose – although crabs actually smell using their antennae and even the tips of their legs. Two characteris-

tics are key in this process: the molecule's conformation (3D structure) and how positive and negative charges are distributed. Both turn out to be affected by changes in pH.
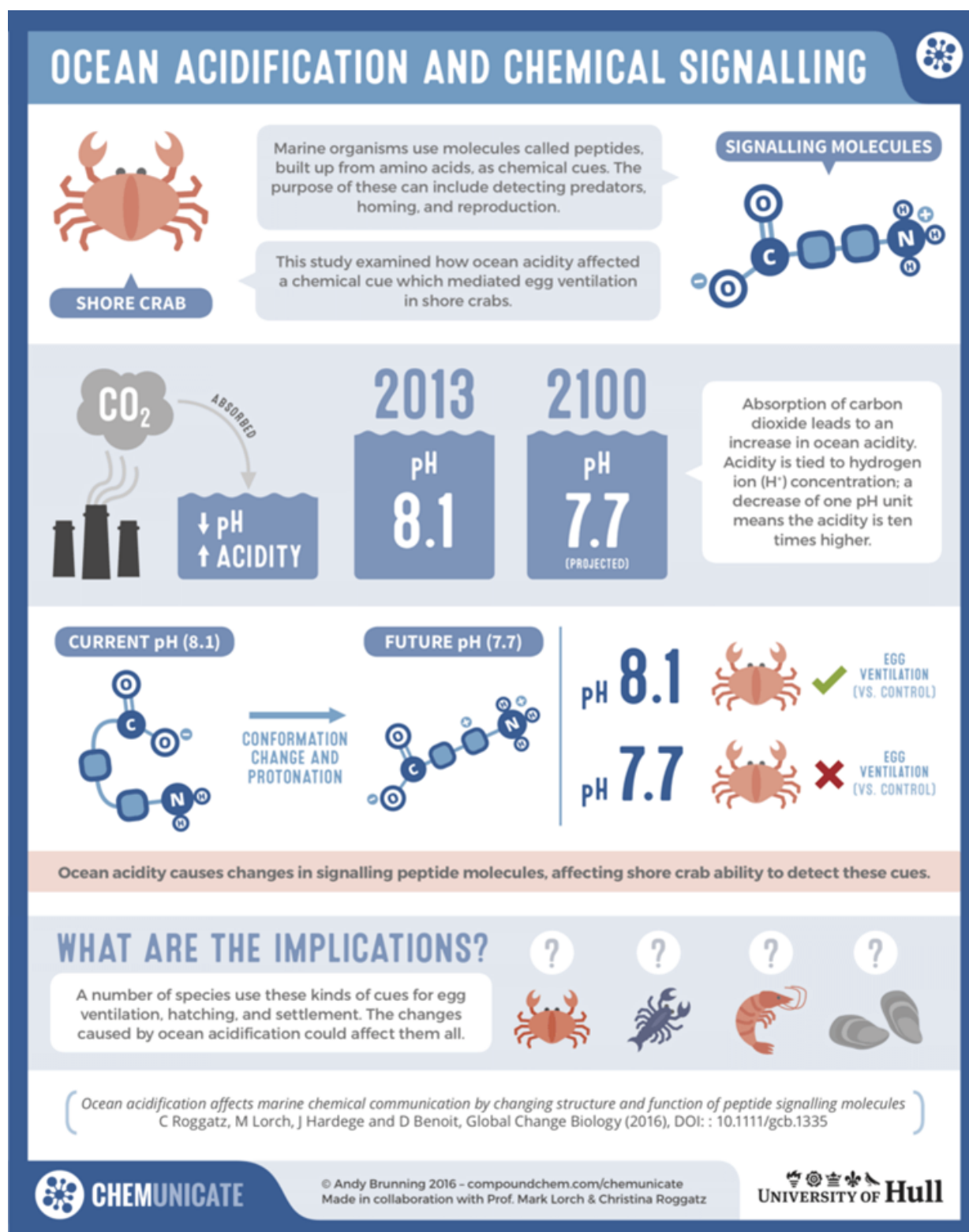

Figure 1: Infographic summarising my latest research results of effects of ocean acidification on signalling molecules of crabs and other marine animals.

Most smell molecules are too small to gain insight into their conformation using chemical analytical techniques, such as nuclear magnetic resonance (NMR) spectroscopy. Also the different pH dependent forms often cannot be studied separately. I therefore use Viper to assess what smell molecules in future ocean conditions will look like. Using quantum chemical programs, Viper allows me to calculate the most likely conformation of a molecule. This can be achieved by altering the position of the atoms in the molecule to obtain the arrangement that has the lowest possible energy and so the optimal conformation is found. Viper also enables me to visualise the charge distribution around the molecule. The differences between molecules in today's and future ocean conditions can so be shown by comparison, for example, for three

5

smell molecules used by crab larvae to communicate (Fig. 2). While in their eggs, tucked underneath the female's abdomen, the larvae release these smells to tell their mother when they need more ventilation, oxygen or assistance to hatch. Molecules responsible for the smell today are relatively compact and have very distinct areas of positive and negative charge. In contrast, the future molecules are less compact and have an overall positive charge. These changes were found to happen exactly within the ocean pH range expected from today until the year 2100.
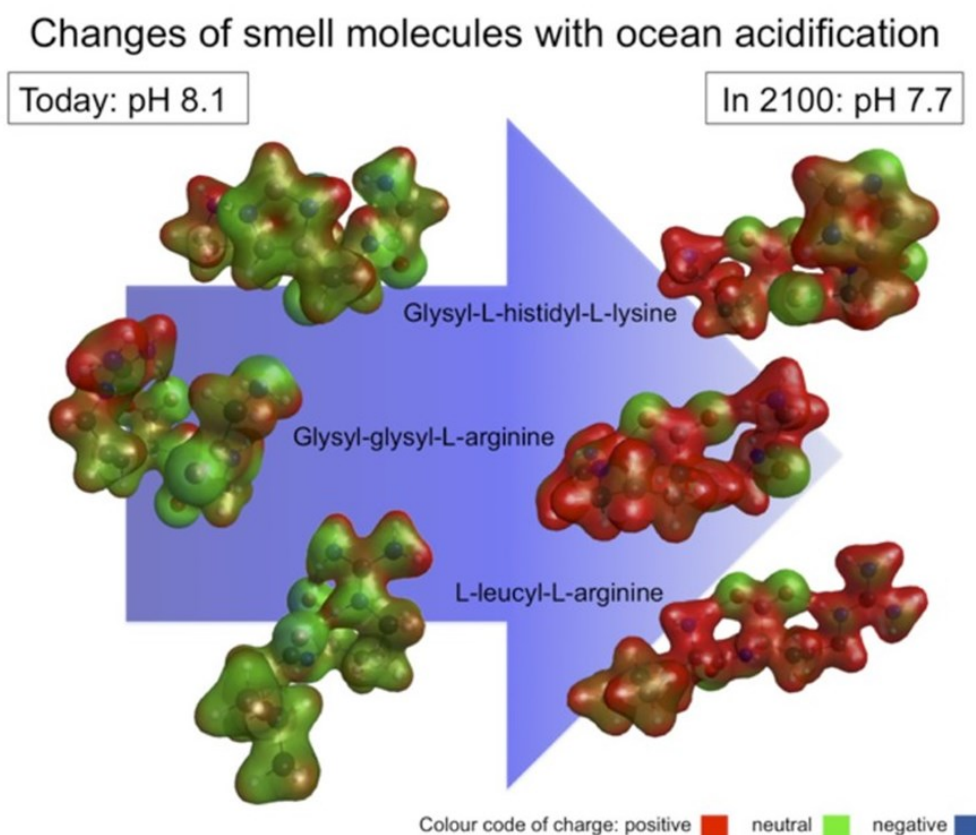

Figure. 2: Model conformers of three smell molecules in today's ocean pH (left) and in future oceanic pH conditions (right). The colour of the molecules' electron density surfaces indicated positive (red), neutral (green) and negative change (blue).

Computational models are a great way of visualising differences. However, the results are only of significance if the model conformers can be verified by experimental data. I gathered experimental data by measuring the NMR spectra for samples with a known concentration of the molecule in a buffer solution. The pH of each sample can be adjusted to a value of interest using acid or base and the buffer solution helps to stabilise the pH during the measurements and to mimic ocean conditions in a test tube to a certain extent. Verifying the computational model conformers is then possible by calculating the NMR parameters of each model conformer and comparing them to the experimental data of the molecule. During my PhD, I have been working on the development of a suitable validation method and a way to obtain the best possible model conformers. I therefore investigated in detail the effects of calculation method, molecular conformation and representation of water on the calculation of NMR parameters. Using Viper to run jobs with 14 cores in parallel reduced the computation time from more than one day to only half an hour. The detailed insights gained from those calculations are currently analysed and will soon be published in a series of papers on the effects of different factors on NMR calculations of small biomolecules.

For more information on Christina Roggatz's work, please see:
- [1]The research paper "Ocean acidification affects marine chemical communication by changing structure and function of peptide signalling molecules" available at http://onlinelibrary.wiley.com/wol1/doi/10.1111/gcb.13354/abstract
- The Conversation article "Oceans may become too acidic for animals to smell their way around" available at https://theconversation.com/oceans-may-become-too-acidic-for-animals-to-smell-their-way-around-61786
- Email roggatz@outlook.com

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

Delivering Research Outputs

A number of research outputs were produced using Viper since the last newsletter, including:

Nina Dethlefs and Ken Hawick published "**DEFIne: A Fluent Interface DSL for Deep Learning Applications**" in Proceedings of the 2nd International Workshop on Real World Domain Specific Languages in February

Siri Chongchitnan and Matthew Hunt published "**On the abundance of extreme voids II: a survey of void mass functions**" in the Journal of Cosmology and Astroparticle Physics in March

Nina Dethlefs and Alex Turner published "**Deep Text Generation - Using Hierarchical Decomposition to Mitigate the Effect of Rare Data Points**" in the International Conference on Language, Data and Knowledge, LDK 2017. Lecture Notes in Computer Science.

Y. Makina, K. Mahjoubi, D.M. Benoit, N.E. Jaïdane , M. Mogren Al-Mogren and M. Hochlaf published "**Periodic Dispersion-Corrected Approach for Isolation Spectroscopy of N2 in an Argon Environment: Clusters, Surfaces, and Matrices**" in the The Journal of Physical Chemistry A in June

In December, Dr Nina Dethlefs was invited to speak at the "**Lets Discuss: Learning Methods for Dialogue NIPS 2016 Workshop**" in Barcelona, presenting on "Domain Adaptation using Linguistic Knowledge"

Matthew Bennett, presented at the Meeting of the Materials Chemistry Young Scientists Sub Committee at Aston University 2017

Daniel Naylor gave a presentation entitled "**Prospects for THz Emission in Gunn Diodes**" at the UK Nitrides Consortium Winter Conference, held at the University of Oxford in January.

Wenjia Du presented on **Four Dimensional Real-time Studies of Metal Solidification under External Fields** at The Minerals, Metals & Materials Society 146th Annual Meeting and Exhibition at California in 2017-02

James Keegans, gave a presentation on "**Production of iron-group elements in core-collapse superno-vae**" at the Russbach School on Nuclear Astrophysics in Austria in March

David Benoit presented on **Accurate adsorbate vibrations from first principles** at Computational Molecular Science 2017 at Warwick in March

A list of outputs coming from work involving Viper can be found at http://hpc.wordpress.hull.ac.uk/research-outputs/. Any outputs missing? Please contact viper@hull.ac.uk

University HPC Symposium

On Friday September 8th the university is holding a day long HPC Symposium to celebrate the research carried out on Viper and showcase some of the most exciting research in HPC currently taking place. The day will feature leading external speakers and University of Hull academics presenting their own research.

The day will also include a lunch time poster session showing the range of research on Viper and how it is impacting research across the university. Evening refreshments will follow the days programme.

Some of the external speakers lined up to talk at the event include:

Professor Peter Coveney from UCL holds a chair in Physical Chemistry and is an Honorary Professor in Computer Science. He has broad research interests including condensed matter physics and chemistry, materials science, as well as life and medical sciences in all of which HPC plays a major role .

Dr Michel Steuwer from the Institute for Computing Systems Architecture at the University of Edinburgh, is one of the developers of domain-specific programming language LIFT, a novel approach to achieving performance portability on parallel accelerators

Dr Maciej Ginalski Application Engineering Manager at ANSYS, Inc. the leading engineering analysis software. His research interests in Co-simulation revolve around software integration and optimisation.

Dr Mark Wilkinson is a Reader in Theoretical Astrophysics at the University of Leicester and Project Director at DiRAC, the STFC supercomputing facility.

For more information and to reserve a place, please visit https://uoh-hpc-symposium.eventbrite.co.uk

£2M OF HPC ENABLED RESEARCH

Viper is already having a real effect on the research being conducted here at Hull with a number of grant proposals requiring use of the HPC having already been submitted and awarded.

The role of soft tissues in cranial biomechanics: is a project submitted by Hugo Dutel of the Medical and Biological Engineering Research Group and awarded £372k.

Theory of Transport in Semiconductor Devices: A project awarded to Angela Dyson in Physics by the Office of Naval Research and with a value of £130k.

Self assembly of two dimensional colloidal alloys for meta-materials applications: An award made to Martin Buzza and Walter Somerville; both researchers from the School of Mathematics and Physical Sciences and which had a value of £654k.

A review of recent advances in genetic methods to identify improvements in CAMERAS partners monitoring activities: awarded by the Scottish Government with a value of £75k.

Environmental genomics of Oak Processionary Moth: £5.4k awarded by Forest Research.

Determining the parasitoids of Oak Processionary Moths: a molecular approach; again Forest Research this time for £130k.

The evolutionary genomics of sexual recombination: a £212k NERC grant.

Evaluation of eDNA based metabarcoding as a monitoring tool for fish in large lakes: awarded by the Environment Agency to the value of £30k.

Do genomic regions under selection have hybrid origins in cichlids?; a further £65k from NERC.

Evaluation of eDNA based metabarcoding for as a monitoring tool for fish in large lakes – Phase 2: £60k from the Scottish Environmental Protection Agency

Using eDNA surveys to evaluate the impact of River Thames Scheme Capacity Improvements and Flood Channel Project; £79k awarded by the Environment Agency.

Environmental DNA monitoring of conservation priority fish in UK waters awarded by Scottish Natural Heritage to the value of £54k.

Development of a fish-based eDNA method for assessing the quality of lakes under the Water Framework Directive: Collection and Processing of Cheshire meres data again awarded by the Environment Agency—£3.5k.

Development of a fish-based eDNA method for assessing the quality of lakes under the Water Framework Directive: Collection and Processing of Welsh Lake data; £5k awarded by Natural Resources Wales.

Creation of eDNA metabarcoding dataset for freshwater invertebrates; awarded £3.5k from the Environment Agency.

Pond biodiversity assessment with environmental DNA: laying the foundations for testing fundamental ecological hypotheses awarded £5k from The British Ecological Society.

Lake fish classification delivery analysis of an eDNA sampling network was awarded £25k by the Scottish Environmental Protection Agency

Determining the impact of pumping stations on the migration of eels using eDNA approaches was awarded £9k by The Environment Agency

Oxford flood alleviation scheme— eDNA survey of Kennington Pond/ Oxfordshire saw the Environment Agency make a £1.6k award.

A non-invasive method for target taxa: passive vs targeted detection was awarded £4k by The Freshwater Biological Association for Environmental DNA

The Development of an eDNA based approach for fish sampling in lakes was awarded £8k by the Environment Agency

Assessing the impact of invasive freshwater fish using eDNA detection and characterisation of food webs through NGS based meta-barcoding was a PhD scholarship award from the Chinese Academy of Sciences to Jianlong Lee.

Heavy usage of Viper was made as part of the £246k allocation of HEIF funding into **developing evolutionary and environmental genomics for agri-tech, food security, and environmental monitoring.**

There were also a number of submissions which were awaiting news of whether they had been successful or not, along with a number of project proposals are also currently in preparation and are expected to be submitted in early 2017.

Finally, there is, HPC work that utilises Viper and which will be submitted to EPSRC through *Project Aura*. This proposal will be a wide scale collaboration with the HPC element examining Biomimetic blade design. The whole proposal is expected to be valued at around £7.5m.

Computing Insight Conference

Computing Insight UK is the country's leading scientific computing conference, that combines the latest technology trends and roadmaps, with showcasing HPC led research. The university sent members of the Viper support team to attend, alongside **Dr David Benoit,** one of the key academics behind bringing HPC to Hull and member of the HPC Steering Group. Dr Benoit reports on his experience of the event.

In December 2016, I attended the Computing Insight UK 2016 conference in Manchester, along with members of the Viper support team (Darren Bird, David Coulson and Matthew Summerbell). The meeting lasted two days and was a mixture of trade fair and a more traditional set of talks presenting research done on HPC. The range of talks was quite diverse and covered both technical aspects, such as the upgrade of the DIRAC service in Durham, to applied big-data for clinical applications and drug discovery.

Dr David Benoit presents: Accelerator-enabled quantum chemistry: a viable path to high-throughput HPC?

The event was organised by the Science and Technology Facilities Council (STFC) and included delegations from the major players in HPC (Intel, ClusterVision, SGI, Cray, OCF, HP, Atos). We also met up with the team from Red Oak who were giving a number of presentations on how to manage large-scale HPC projects. The trade fair enabled us to find out more about the latest technologies in HPC, such as SSD mass storage, hybrid HPC (with Intel's Knight's Landing Xeon Phi and Nvidia's latest P100 cards) and the latest networking fabric (both from Mellanox and Intel). The trend was very much towards active networking, energy efficient computing and accelerator cards, which should all feature prominently in future HPCs.

In this context, I gave a talk on how HPC evolved in Hull and the journey that took us from a University that had no HPC to speak of to the creation of one of the major facilities in the UK with the installation of Viper. I also showcased our research on hardware acceleration applied to quantum chemistry applications and described how we used both Xeon phi and Nvidia graphic cards to cut down computational time dramatically. I showed in particular that using hardware accelerators is a cost-effective path to high-throughput HPC for some applications.

Amongst the many exhibitors, it was notable that most of them had either heard of Viper or Hull as a new member of the HPC community. It was also clear that our presence at the event further reinforced the message that HPC at Hull was here to stay and that we intend to play an active part in the UK HPC community. Overall a very positive meeting that helped both advertise Viper and grow our contact base in HPC at national level.

"It was excellent meeting people from the world of HPC, and visiting the many booths from world leading HPC companies. Our very own Dr David Benoit presented on accelerator enabled quantum chemistry and Viper, which was well received. The audience asked many questions regarding Viper's use of containers.

I enjoyed Professor Martyn Guest's presentation on Application Performance on Multi-Core Processors, which went into detail benchmarking the differences between Intel processor architectures, Omni-Path and Infiniband interconnect and Intel vs IBM. Mark Thomas of Red Oak Consulting presented 'Confessions of an HPC Project Manager' highlighting the pitfalls of HPC projects and how to ensure projects are a success, which was very enlightening and entertaining. I also enjoyed Craig Petrie from Nallatech's presentation on FPGAs on the growing usage and performance benefits over GPUs"

Matthew Summerbell, HPC intern

International Supercomputing Conference

In June, Darren Bird, HPC Software Support Engineer in the Viper team, visited Europe's leading HPC conference, the International Supercomputing Conference in Frankfurt

For the first time the Viper Team were able to visit ISC, the International Supercomputing Conference in Frankfurt, Germany. ISC High Performance focuses on HPC technological development and its application in scientific fields, as well as its adoption in commercial environments. It is not only an exhibition of HPC manufacturers but it also included talks, tutorials and workshops on all aspects of HPC. This year there were 13 fascinating HPC topics grouped under three categories: systems, applications, and emerging technologies. All topics were addressed in different power-packed sessions. The ISC tutorials, workshops and the exhibition complemented these sessions.

An example of immersion cooling,
an alternative to air cooling in the data centre

The Top 500 HPC List

On June 19th, the latest Top500 list was released at the International Supercomputing Conference in Frankfurt. The Top 500 list ranks the fastest HPC systems from across the world, based on their performance running a High Performance Linpack (HPL) test. The list, which is updated twice a year, was first produced in 1993 and raises the profile of supercomputers, with new lists featuring on the BBC news website.

On the June 19th list the world's top ranked system is the Sunway TaihuLight at China's National Supercomputing Center. Third in the list is the Swiss Piz Daint supercomputer, which is the top rated GPU system on the list and also one of the greenest, ranked 6th for energy efficiency.

The top UK HPC in 11th spot is the Cray system at the UK Meteorological Office, with the EPSRC system ARCHER at the University of Edinburgh 73rd. The University's HPC partner ClusterVision have two HPC installations in the top 500 list, an oil immersion cooled system in Vienna at 329th on the list, and the UK Tier-2 site HPC Midlands Plus based in Loughborough in 415th.

Exhibitors this year included Intel and AMD, with many manufacturers now looking at ARM in the server space too. Those familiar with ARM probably know they have been used extensively in mobile devices and other small scale computing areas. Many of the exhibitors and researchers using HPC now believe ARM processors will provide a different path to offerings by Intel and AMD with core-count having more of a priority than single core speed. Here, Mont Blanc (part of the Barcelona Supercomputing Centre) have done a lot of the work recompiling and resolving dependencies in transferring code packages from x86 to ARM64. Also, Isambard, the University of Bristol's new ARM system will form part of the work towards ARCHER-2 and its use of ARM processors. This will also use a large amount of different technologies e.g. Omni-Path/InfinfiBand based on Cray Linux.

AMD used the exhibition to launch the new processor range called EPYC which highlights a core count of 32 with a 128 PCIe lanes for high connectivity. There was also a group from China's Tianhe-2 or TH-2 which is a 33.86-petaflop supercomputer located in National Supercomputer Centre in Guangzhou and was the fastest super computer until June 2016.
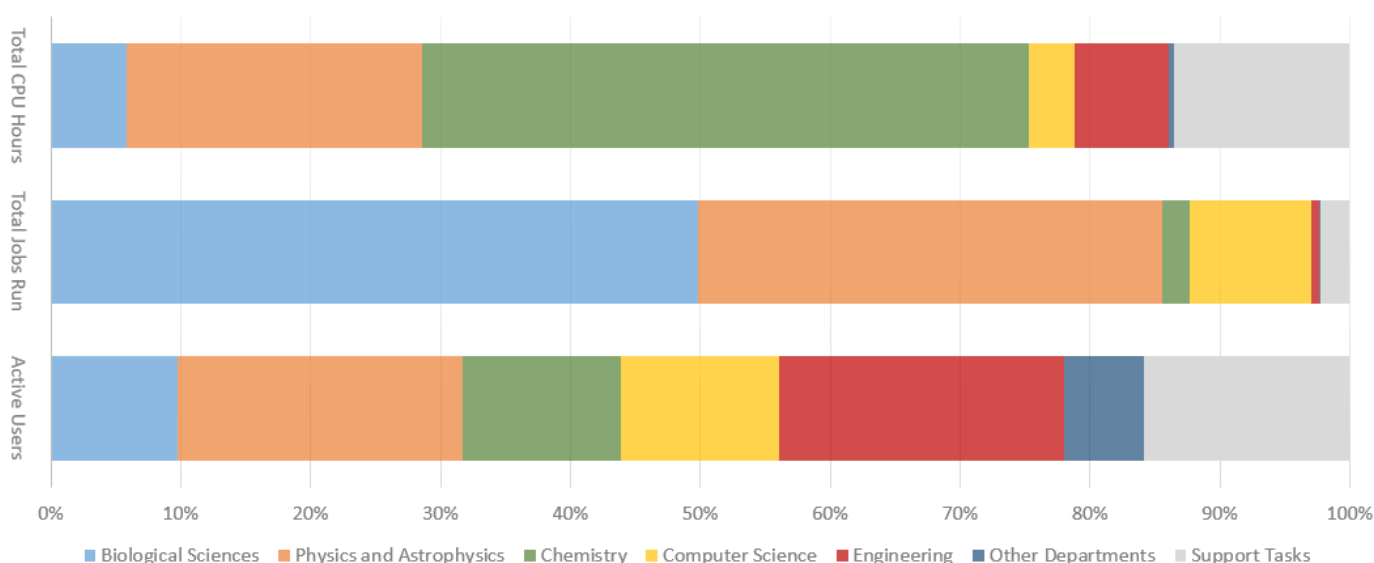
Deep learning was strongly promoted at the exhibition and within the various talks. ISC this year devoted a whole day to 'deep learning'. Talks included the use of this new technology to autonomous cars and the use of deep learning to help research dig deeper into data sets, meta-data and multiple-sourced data sets. The extensive Watson API was referred to within the talks along with Intel's Knight's Landing (and Knight's Mill) processors, women in HPC, I/O in HPC and the steering of ISC into next year.

12 months of Viper

The 12 months since Viper went live has flown by and we've met with many users, seen many jobs and many CPU hours of research help produce world class and world changing research as shown by our example research outputs. Viper has been kept pretty busy:

13.8 million CPU hours of research has been carried out on Viper (nearly 1600 years)!

More than 388,000 jobs have been run

Legend: Biological Sciences | Physics and Astrophysics | Chemistry | Computer Science | Engineering | Other Departments | Support Tasks

Categories: Total CPU Hours, Total Jobs Run, Active Users

Earlier in the year we surveyed our HPC users:

100%
Were satisfied or very satisfied with Viper

96%
Rated support received as being satisfactory or very satisfactory

Some user comments from the survey:

- Fast & efficient. Opens up an entire new range of questions to be investigated thanks to the speed

- I wish Viper was here at the start of my PhD

- The service has met and exceeded my needs and allowed me to produce much more detailed simulations than I would have otherwise been able to. I'm very happy that I was able to make use of it

- Viper performance has enabled calculations that were previously not realistic on local clusters

- The use of Viper has been a very positive experience; the knowledge of Viper staff has significantly helped in achieving research results

Viper Support Services

Viper is supported by a dedicated team of 6 support staff, taking care of the day to day management of the software and hardware infrastructure that makes up the Viper environment. The team, who are all certified to ITIL Foundation level, the industry standard IT Service Management certification, have a wide range of expertise and experience from Linux and HPC system administration to code development and software engineering.

As well as the day to day running of the HPC facility, we also provide the following services to the research community to help them make the most of the resources available include:

- Training on topics such as Linux, High Performance Computing and software development
- Support and advice on areas such as migrating tasks from the desktop to HPC and HPC workflows
- Software engineering resource to work with researchers and research groups to develop and optimise code to run on the HPC
- Advice and assistance on the inclusion of HPC in research proposals

We regularly hold open surgery sessions which give users the opportunity to talk directly to team members about possible workflows and HPC issues or even go through some informal training. Come along to the ICT Consultation Room by the IT Service Desk, Monday's 2-3pm. The Viper team are happy to meet with any researchers interested in looking at how Viper may be used in their research, and can also organise group sessions or school seminars focussed on the usage of HPC to specific research topics.

Getting Information

The main HPC website is at http://hpc.wordpress.hull.ac.uk/home/ and includes information about:

- The research carried out on Viper, including case studies, research areas and research outputs
- The support team and the HPC Steering Group
- The support FAQ
- How to apply for an account

Our documentation and technical support wiki can be found at http://hpc.mediawiki.hull.ac.uk which includes:

- General pages with information on Viper, HPC concepts and basic usage
- Training pages including guides on getting connected to Viper, working remotely and Introductions Linux
- Application pages with detailed information on the hundreds of applications, tools and libraries available on Viper, including typical usage instructions

To contact the team, please use one of the following email addresses:

- For support enquiries, please raise a ticket via the University of Hull Service Desk by emailing help@hull.ac.uk
- For queries regarding the use of Viper, please email the team directly on viper@hull.ac.uk
- Please feel free to contact the HPC Systems Manager, Chris Collins, directly on chris.collins@hull.ac.uk

@hull_hpc_viper   Viper HPC