Viking Annual Report 2022/2023

HPC Management Committee

Introduction

In January 2018, University Executive Board authorised £2.5M for the purchase and support of a new central high-performance computing facility for the University of York, supplied by Dell and supported by Alces Flight. This aimed to accelerate research in the university across all of the faculties and to provide a focus for developing interdisciplinary activities across the University. On February 14th 2019, Viking went live, providing 7000 cores, 42 TB of memory, 2.5 PB of storage, free at the point of delivery, to staff, postgraduates, and undergraduates. This is a major university facility comparable to that provided by institutions much larger than York. This report describes the activity with Viking over the final year of its expected 5 year lifetime.

Summary

Despite being in its final year, Viking usage has continued to grow to 350 projects and 1500 registered users. The number of research outputs associated with Viking is 212, and Viking has supported upwards of £20M in funded research. Whilst still predominantly used by the Faculty of Sciences, it has been encouraging to see increased uptake in the Faculties of Social Sciences and Arts and Humanities.

With Viking now coming to end-of-life, focus has been the procurement of its successor, VIking2. Viking2 will be built and designed with a similar ethos, free at the point of use and with hardware that reflects the diversity of the research within the University. One major difference with Viking2 will be the move to a more sustainable data centre, EcoDatacentre in Falun, Sweden. This data centre has a negative carbon footprint, achieved with using sustainable building materials and also harnessing the heat produced by computer hardware to be used to dry wood pellets that are used to provide heating to businesses and homes. Viking2 is expected to come online in September 2023.

Thanks to support from several funding sources, we have expanded our capacity for GPU computing, allowing researchers to explore a technology that is rapidly growing in popularity. This capacity will be attached to Viking2 to offer researchers a seamless transition between traditional computing resources and the cutting edge.

The Viking support team has expanded, bringing broader knowledge and expertise. Lower resolution times on support cases are being delivered as a result, and we have further outreach to the University research community through Research Coding Club.

Statistics

- 1500 registered users across 382 projects, spanning 18 schools and departments
- At least £20 million in grant funding where Viking has contributed compared to an investment of £4.02 million (dedicated hardware, services and staff).

- 212 recorded research outputs
- 48 million CPU hours of work done over 4.4 million jobs
- Computing resources have been allocated to user jobs for 76% of the time in 2022
- 63% of Viking users are undergraduate/postgraduate taught students

Year Overview

Viking has continued to provide a valuable research facility for staff and students across the university. In addition to research, Viking is also used for three undergraduate modules, two based in the School of Physics, Engineering, and Technology (PET) and one based in Computer Science. We have seen an increased uptick in use and outputs from the Department of Biology, showing the growing need for computational resources in this area. In addition to this, the Viking team also branched into cloud, in conjunction with Alces and Azure and academics in the Department of Psychology. The project was a success which resulted in the team being shortlisted for an award at Supercomputing 2022, a large, international HPC conference. Viking was competing against Tier 1 and 2 facilities, which is a testament to innovative work continuing in the Viking team.

Whilst computing facilities of this nature tend to be science-focused, Viking has managed to capture a user base across 18 academic schools and departments.

Faculty of Sciences	Faculty of Social Sciences	Faculty of Arts and Humanities
Biology	School for Business and Society	Archaeology
Chemistry	Economics and Related Studies	School of Arts and Creative Technologies
Computer Science	Education	Language and Linguistic Science
Environment and Geography	Centre for Health Economics	Philosophy
Health Sciences		
Hull York Medical School		
Mathematics		
School of Natural Sciences		
School of Physics, Engineering and Technology		
Psychology		

Figure 1: Departments with registered Viking projects

The Department of Biology (80) has submitted the largest number of project applications on Viking, with a similar number in the School of Physics, Engineering and Technology (72),

Chemistry (66) and Computer Science (58). We have seen some growth in the number of users from the Faculties of Arts and Humanities and Social Sciences (92 user applications) and we are working to further improve these figures.

Research Outputs

Using the University Research Database (Pure) and user surveys, we have recorded a total of 212 research outputs (papers, articles, datasets, software etc.) that have been produced using Viking. Another 37 research outputs are also in preparation. The split of outputs by department roughly reflects the departmental split of researchers on Viking.
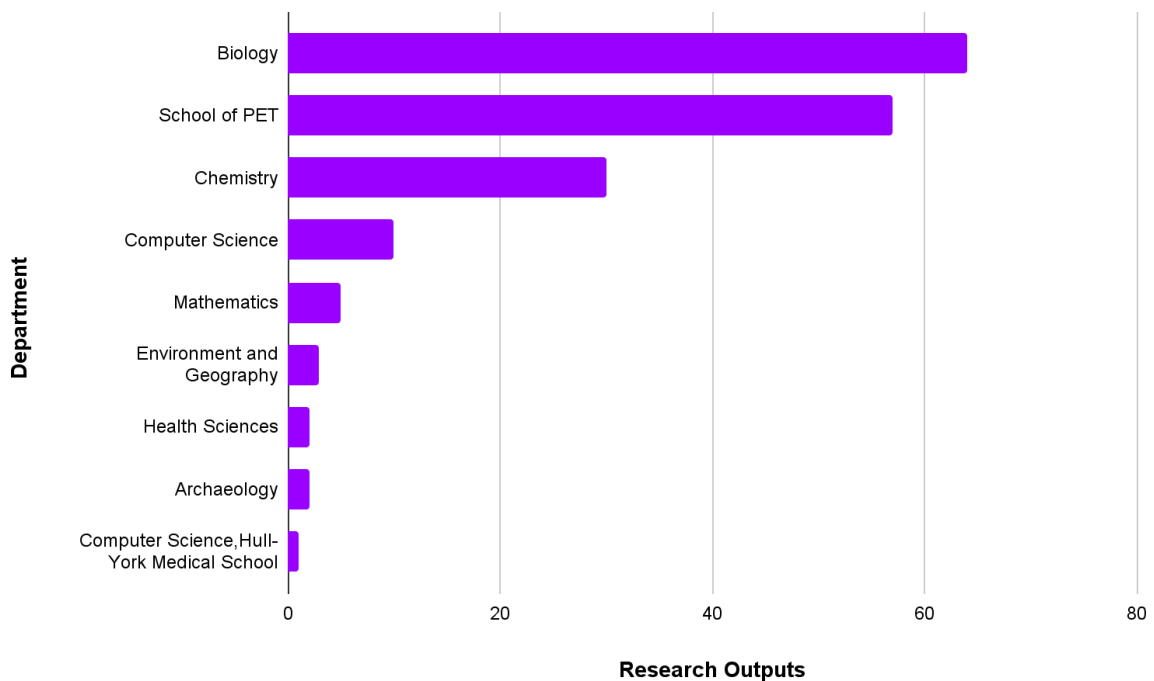

Figure 2: Research outputs which made use of Viking, counts by department. Data generated from Pure and user submissions.

This year Biology have significantly increased their outputs from 14 to 64. Although still STEM heavy we are seeing increased usage from other faculties however there is always a lag between usage and research outputs.

Case Studies

We have selected highlights of research completed on Viking. We present case studies from Physics, Atmospheric Chemistry, and Language & Linguistic Science.

Nuclear moments of indium isotopes reveal abrupt change at magic number 82

In a famous experiment performed in 1820, Danish physicist and chemist Hans Christian Ørsted demonstrated that an electric current deflected a compass needle from magnetic north. As we understand it today, the electric current generates a magnetic field. In a similar way, a charged rotating body generates a magnetic field and acquires a so-called magnetic moment. Nuclear magnetic moments relate to the orbital and spin components. Experiments showed that the spin components were weaker than those of isolated protons and neutrons. So far, a common practice was to attenuate the spin components and employ a blanket common reduction factor called the effective g-factor.

This simplistic approach to magnetic moments abruptly ended with a breakthrough experiment performed on heavy indium isotopes. An international team of scientists showed that the almost constant value of nuclear magnetic moments measured in the past in the indium isotopes with neutron numbers from N=64 to 78 is continued till N=80, but then jumps to a much larger value at N=82.
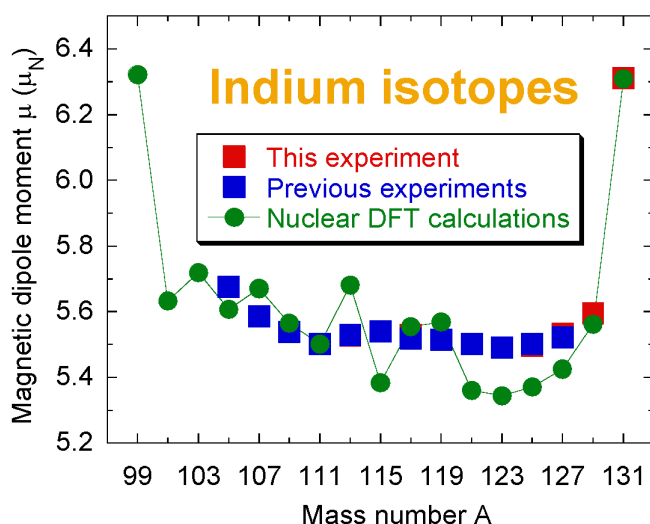
Such a jump is a surprise and does not support the earlier assumptions of an effective g-factor but, rather, calls for invoking specific nuclear-structure effects. Advanced calculations, performed on Viking by Bonnard and Dobaczewski showed that the magnetic moments of the indium isotopes (proton number Z=49) are generated not only by the single odd-proton hole in the magic proton closed-shell corresponding to Z=50 but also by self-consistently polarised states of the entire Z=50 core.

In a mature domain of physics such as nuclear physics, it is not often that one has a chance to rewrite the textbooks written by the giants of the field. New ideas and breakthrough understanding come from combining the most advanced experimental and theoretical capabilities. A new chapter appears to be opening in the story of nuclear magnetic moments, for which the HPC calculations are, and will be of paramount importance.

The Nuclear-DFT calculations are particularly voracious in the consumption of processor time. They are typically performed in an embarrassingly parallel mode, whereupon a single self-consistent solution is determined within about 12h-24h of CPU time but has to be obtained for many different nuclei, configurations, deformations, etc. In addition, reliable estimates of various observables (nuclear moments in particular) require symmetry restoration, which multiplies the CPU times by factors anywhere between a few and a million. It is clear that progress in this domain of theoretical physics will be tightly governed by the availability of advanced computation capabilities.

Improving the Modelling of Atmospheric Volatile Organic Compounds

M. Rowlinson, M. Evans

Volatile organic compounds (VOCs) play an important role in regulating atmospheric chemistry and can lead to the formation of ozone, a greenhouse gas and air pollutant. Two of the most important VOCs are ethane and propane, but we don't understand where these chemicals are coming from in the atmosphere. We use the GEOS-Chem chemical transport model (www.geos-chem.org) on Viking to simulate the chemistry of the atmosphere and understand the sources of these molecules. GEOS-Chem is a well used open-source community atmospheric chemistry model used by groups around the world (Harvard, MIT, CalTech, NASA, Edinburgh, UCL, Peking University etc) to understand the composition of the atmosphere.
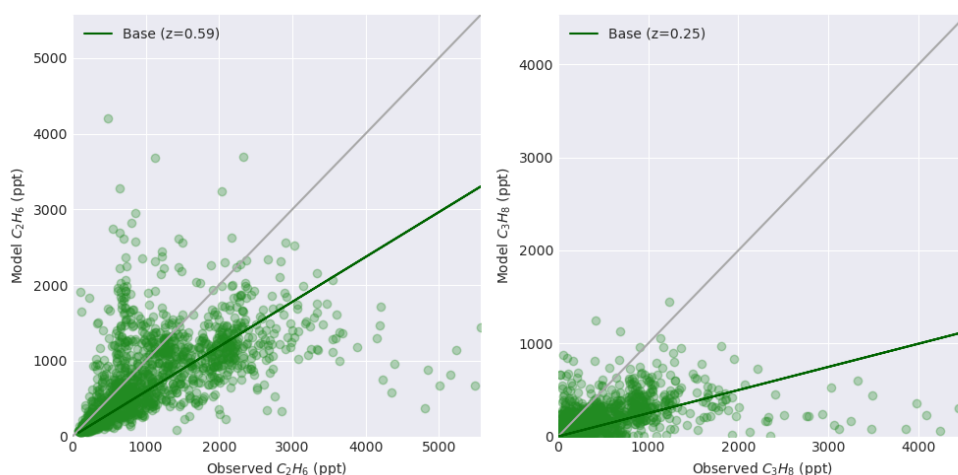

Figure 1.

Simulated concentrations from our model are compared to measured values from around the world in Figure 1. This shows the model underestimates both ethane and propane. Comparing the default emissions inventory to regional emissions estimates for Europe, USA and China, it was found that ethane and propane emissions were substantially lower in the global database than in the regional. We then adapted the emissions of VOCs in the model, to match each of the regional estimates.

We run the model again on Viking with the new emissions, and compare the change in model performance in Figure 2. When using the adapted emissions the concentrations of ethane now compare much better with measurements, and there is also a smaller improvement for propane. Viking was vital for this study as it allowed us to run large simulations very efficiently, whilst also providing computing resources for the processing and analysis of the model output.
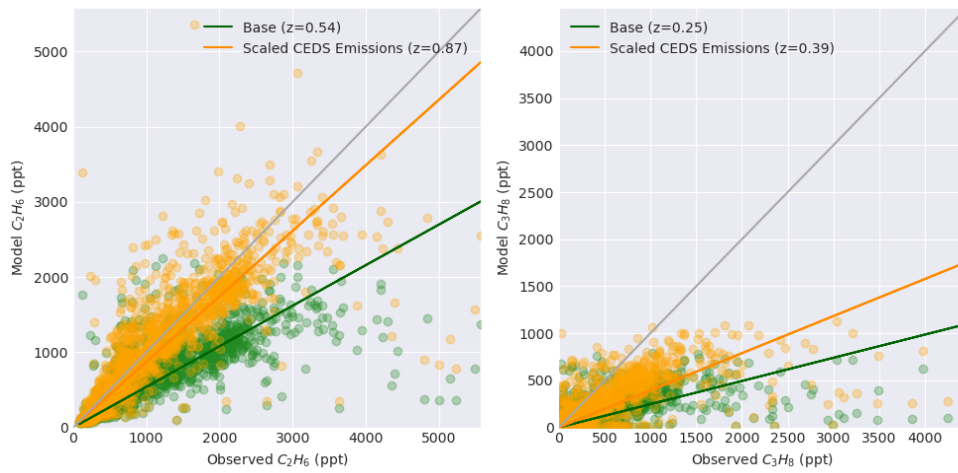
Figure 2.

Self-Calibration for γ-ray tracking array

S. Chen, S. Paschalis, M. Petri, M. Bentley, M. Labiche, F. Holloway and S. Heil

High precision γ-ray spectroscopy is one of the most powerful tools to study nuclear structures. In the last decades, the frontier of γ-ray spectroscopy was moved to the development of γ-ray tracking arrays based on highly segmented High Purity Germanium (HPGe) detectors, that allow for a better determination of the incoming γ-ray direction and the full deposited energy. The most advanced implementation of such a technique is in two arrays: the AGATA (Advanced Gamma Tracking Array) in Europe and the GRETA (Gamma Ray Energy Tracking Array) in the US. The tracking ability of these arrays very much relies on the precise determination of the interaction positions within the detector volume, which is realised by comparing the experimental signals against a pre-generated library of signals (signal basis) that maps the detector response at different interaction positions. A novel method, called Self-Calibration, is proposed to generate a reliable signal basis from a large experimental data set. Starting from the assumption of segment-sized position resolution for all signals, and using an iterative minimization procedure based on the Compton scattering formula, this method improves the position assignment for signals and converges to their real positions after a few iterations.
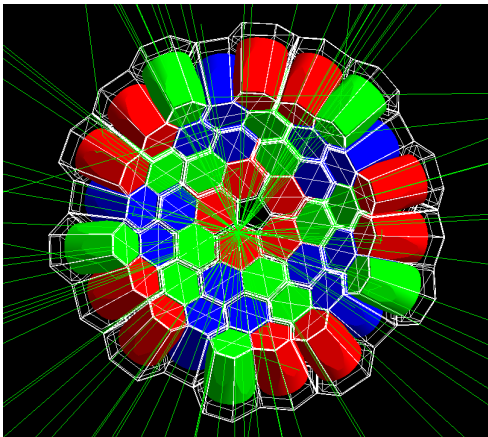
The simulation of AGATA with 45 detectors (3 types with different geometries in red, green and blue). Every detector is segmented by 6 sectors x 6 slices (36 segments). A radioactive source is placed at the centre of the array, emitting γ-rays (green lines) in 4π. Only Compton scattering events are saved for analysis. For every detector, signals are read from all segments as well as the core, which give 37 channels in total. Signal shape from each channel is recorded with 60 sampling points, leading to 37x60=2220 data points per detector per event.

To achieve the converging condition and generate signal basis with enough density, the order of 10^8 Compton events need to be accumulated and analysed, which uses hundreds of GB of memory and thousands of hours of CPU time. The large number of CPUs and large size of memory in Viking allow us to process this work in a highly parallelized way - the program is developed with multi-threads and the analysis of each detector can be separated in parallel processes - eventually, hundreds of CPUs can be utilised simultaneously to make the program two orders of magnitude faster. With Viking, this method can be completed in a reasonable time scale, therefore, becoming really practical.

Forced-Alignment of Large Speech Corpora to Facilitate Forensic Speech Research

Harrison, P., Xu, C., Hughes, V., Foulkes, P., Welch, P., Wormald, J.

'Person-Specific Automatic Speaker Recognition (PASR): understanding the behaviour of individuals for applications of ASR' is a 3-year, £1 million ESRC funded project in the Department of Language and Linguistic Science in the Faculty of Arts and Humanities. The project is investigating the characteristics of people's voices that influence the performance of automatic speaker recognition systems used in forensic casework. To discover which characteristics are important to an ASR, the results of more traditional and interpretable phonetic analyses are being used to provide insights into the opaque statistical speaker models generated by ASR systems and identify groups and patterns within the results of automatic speaker comparison tests.

Many types of phonetic analysis require the timing location of different categories of speech sounds (e.g. vowels, consonants) within a recording to produce meaningful measurements. This segmentation process is often manual and very labour intensive. To ensure the findings are robust, large speech corpora containing thousands of speakers with diverse characteristics including age, regional/ethnic accent are being used but this makes the manual segmentation approach impossible. Instead, a process known as 'forced alignment' is used to automatically align a written transcript of a recording with the audio signal at the level of individual speech sounds, (i.e. individual vowels and consonants).
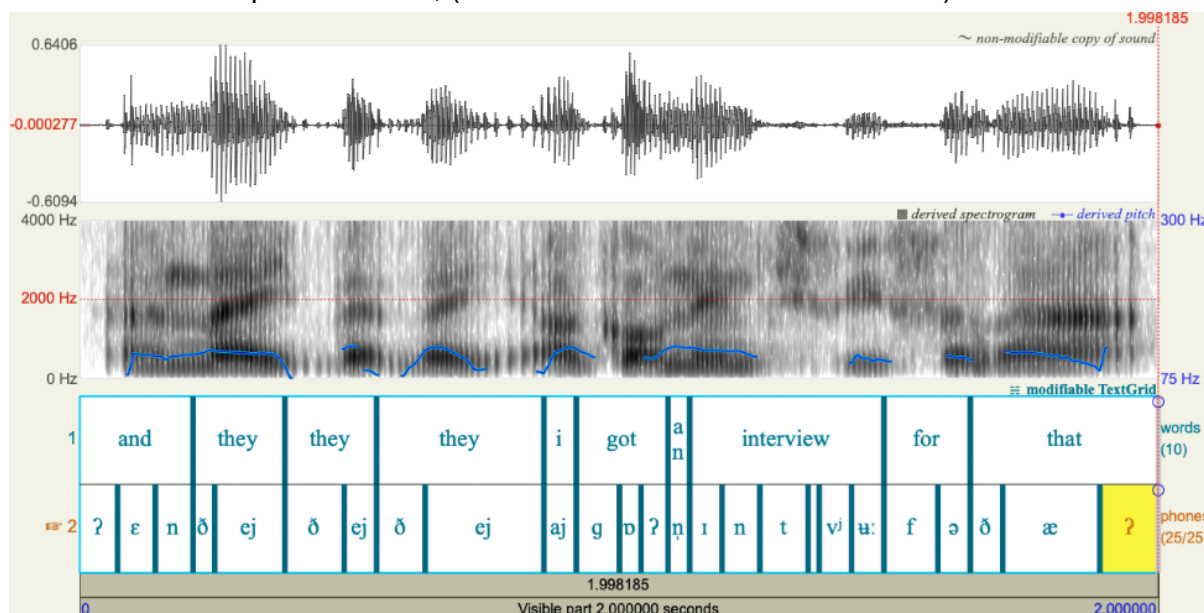
Word and segment (phone) level segmentation (bottom half) of a short section of a speech recording generated from a written transcript using the Montreal Forced Aligner. The amplitude waveform and spectrogram are also shown in the top and second panels.

The large number of CPU cores available on Viking allows effective use of the parallel processing capabilities of the Montreal Forced Aligner (MFA) software. This significantly reduces the time taken to process thousands of recordings compared with researchers'

laptop and desktop computers. The time savings have allowed exploration of the impact on the alignment accuracy of varying a range of MFA's parameters including different language models and dictionaries. This is particularly important as the recordings are of telephone calls with reduced quality and the language models are not optimised to the speakers' accents.

The development of a straightforward and simple to use pipeline for using Montreal Forced Aligner on Viking paves the way for other researchers in the Department of Language and Linguistic Science to use this tool in the future for larger-scale analyses. As researchers in the department are beginning to use increasingly larger speech corpora the need for such tools and the large processing capability of Viking will no doubt grow.

Support and Training

Research Software Engineering Team

The [Research and High Performance Computing Support Team](#) continues to grow in the past year with two new [research software engineers](#) which broadens the existing available support and now adds robotics, environment, geography and The Plasma Institute knowledge into the mix. A new role of Research Software Engineer Team Lead has been created to manage and support the RSE team. These new positions increase the RSE team to 6 people.

Research Infrastructure Team

The Research Infrastructure Team continues to provide support for users across the university. We have 1 FTE devoted to Viking, with 1 FTE in physics and 1 FTE in CS.

York has continued its contribution to EasyBuild. [EasyBuild](#) is a software build and installation framework that simplifies software management on HPC systems. The Team has not only contributed significantly to the Easybuild community with code, but one of the Research Infrastructure Team members (Jasper Grimm) is now an EasyBuild maintainer. York has made 900 contributions in the last 12 months. Easybuild is a framework used in a number of HPC facilities both nationally and internationally, with York now being a major contributor.

These new team member additions have resulted in lower case creation to solution time for the Research IT team and a marked increase in positive user feedback. Service Level Agreements (SLAs) are being met for cases to receive responses in less than three days (accounting for weekends) and often cases are solved in one response with a friendly and informative approach. Additionally, some in-person sessions have been delivered when requested by users, this allowed us to deliver focused support tailored to the user's specific needs.

[Research Coding Club](#) continues its outreach for anyone who works with research software. Offering both informal drop-in style clinics, which not only invite participants to problem solve each other's work but also just a friendly chat, and also structured seminars where short talks of one hour or so on interesting topics are delivered by anyone within the University. Some more recent topics include version control through Git and parallel problem solving which often finish off with some lively discussion within the group.

MATLAB is a popular application in use on a range of University systems, but it can have a steep learning curve for some users when running it remotely on Viking as they are unfamiliar with the additional layers. Listening to user feedback, a new solution to streamlining this use case has recently been introduced, gaining recognition of its unique approach from the wider MATLAB community.

Finally, various user surveys have been conducted throughout the year focussing on their use of Viking to help the team better structure the upcoming Viking 2 project. Focusing on the users feedback here allows the upcoming Viking 2 to deliver on their use cases and overall needs, drawing from their day to day experiences with the current Viking HPC.

Regional and National Links

The N8 Centre of Excellence in Computationally Intensive Research (N8CIR) was awarded £3.1M in 2019 from EPSRC, supplemented by £5.3M from N8 member institutions, to establish a new research computing facility in the North of England. **Bede** offers access to a large GPGPU cluster using novel technology. You can find more information about this facility on the N8 CIR website. The University of York is one of the biggest users of the Bede facility. We have also contributed to a number of case studies with places for more in the future. The Director of N8 CIR is also a member of the University of York.

The ARCHER2 Service is a world class advanced computing resource for UK researchers. ARCHER2 is provided by UKRI, EPCC, HPE Cray and the University of Edinburgh. The new national facility, having received £79M of government funding in early 2019, went live in July 2021. There were delays due to the impact of Covid but ARCHER2 passed the benchmarking and user testing period and is now available for general use. ARCHER2 has the potential to benefit more computationally experienced University researchers, with Viking acting as a stepping stone on which to develop necessary skills. More information about the new ARCHER2 system can be found on the ARCHER2 website.

Plans for the Future

Viking entered its final year of operation in 2023. Viking has proven to be an important resource for research and teaching. Going forward we intend to build on this success with Viking2. Viking2 will follow in a similar vein to Viking except with improvements to the hardware technologies used, more cores, GPUs and some backup storage. The Research IT team also intends to improve the sustainability of the Viking service - the University aims to achieve net zero by 2030, therefore Viking2 has been designed with this in mind.

Viking2 will be housed in a carbon negative facility, in the nordic regions where greener and more cost effective power is available. [The EcoDataCenter in Falun, Sweden](), achieves this by using sustainable building materials and the heat produced by computer hardware to dry wood pellets that are used to provide heating to businesses and homes.

The Viking2 procurement has now been completed with an aim to go live September 2023.

In addition to Viking2 we have other initiatives in progress for Research IT which include:

- Trusted Research Environment for sensitive data (Azure cloud)
- Azure Virtual Desktop for research. To assist non Linux users who do not need a large HPC facility for their research.
- Two Research Software Engineer sustainability posts to improve code efficiency and sustainability.

Appendix

Publications & Outputs

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