Boosting the Welsh economy through the power of supercomputing

UNDEB EWROPEAIDD
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Llywodraeth Cymru
Welsh Government

Cronfa Datblygu Rhanbarthol Ewrop
European Regional Development Fund

SUPERCOMPUTING WALES
UWCHGYFRIFIADURA CYMRU

Atos

Supercomputing is changing the world we live in

Supercomputing is everywhere, changing the world we live in for the better. Helping to develop medicines, personalise healthcare, design cars, generate finer-grained weather forecasts and mitigate climate change: the extreme power of supercomputers makes all of these technological advances possible.

As the world faces continued pressure across many areas of society and the environment, supercomputers will continue to play an ever more important role in determining the future.

It is vital that universities in Wales, being at the forefront of ground-breaking, world-class research, can take advantage of the transformative power that High Performance Computing (HPC) and data analytics can bring.

Unlocking world-class research capabilities for Wales

As an HPC centre of excellence, Supercomputing Wales facilitates world-class research at Welsh universities and is internationally recognised across academia, industry and government.

Wales, and indeed the world, benefits from better informed patient care, understanding of dementia, improved speech recognition, increased social and behavioural insight, and breakthroughs in our understanding of the universe, all underpinned by research conducted using Supercomputing Wales facilities.

Supercomputing Wales: The national supercomputing research facility for Wales

Supercomputing Wales provides an innovative, state-of-the-art supercomputing and big data facility for Wales.

Part-funded by the European Regional Development Fund (ERDF) through the Welsh Government and match-funded by university partners, the £15m programme is a collaboration between Cardiff, Swansea, Bangor and Aberystwyth universities. It represents a step-change for academic and collaborative research with industry in Wales.

Two supercomputing hubs based in Cardiff and Swansea, accessible from across Wales via a high-speed network, allow users to perform complex calculations and simulations that wouldn't otherwise be possible.

Expert Research Software Engineers support users to develop software to utilise the facilities, simulate complex problems and enable world-class, innovative research that will lead to important breakthroughs.

Facilitate innovative scientific collaborations with industry and other partners

Capture more research funding and allow Wales to compete globally for research and innovation projects

Enable and support complex projects with modelling, simulation and data analysis

Support from a network of expert Research Software Engineers

Develop expertise with training and software carpentry workshops for users

Users supported by a specialist national team of technical staff

Internationally recognised research

Cardiff University

Researchers:
Dr David J Willock
Dr Sachin Nanavati

Research Software Engineer:
Dr Sachin Nanavati

The effect of Chromium in surface coatings made up of Aluminium Phosphates

Electrical steel is a specialist material used in electrical motors and transformers to produce desired magnetic properties.
They are crucial components of the electrification of modern society. The steel plates are typically coated with aluminium metaphosphates with key additives like chromium, to increase its overall efficiency. However, chromium is expensive and can be difficult to process safely.

This project's aim is to understand the role of the chromium in the aluminium metaphosphate coatings by using high performance computing resources to calculate the material properties of metaphospates at different levels of chromium doping. By harnessing the power of the supercomputer, the models will be capable of including the chemical interactions at an atomic scale. Understanding the role of the chromium in the material will enable the local company Cogent to design a suitable, environmentally friendly alternative to chromium.

This project is in collaboration with the experimental group of Prof P. Davies, Lee Edwards (School of Chemistry, Cardiff University), Dr P. Anderson (School of Engineering, Cardiff University) Dr F. Robinson, and M. Cicuta (Cogent Power Ltd, part of Tata Steel). With the aid of electronic structure calculations, they will try to develop a fundamental understanding of the effects observed experimentally.

3D black-hole-binary simulation

Researchers:
Prof Stephen Fairhurst
Prof Mark Hannam

Research Software Engineer:
Kieran Phillips

2016 announced the first ever detection of gravitational waves as part of the LIGO

At Cardiff University, the Gravitational Physics Group who in 2016 announced the first ever detection of gravitational waves as part of the LIGO (Laser Interferometer Gravitational-Wave Observatory) consortium benefit from the upgraded Supercomputing Wales (SCW) facilities.

Kieran Phillips, the SCW Research Software Engineer (RSE) embedded within the research team, has optimised the 3D black-hole-binary simulation code used to calculate the gravitational-wave signals that Einstein's general theory of relativity predicts are emitted when two black holes spiral together and merge.

These calculations are used to identify signals from real astrophysical sources in the LIGO and Virgo gravitational-wave detectors, and to measure their properties. The results of this code were previously used to construct the theoretical models that were used to measure the properties of the first direct detection of gravitational waves in 2015 (which subsequently lead to the 2017 Nobel Prize in Physics), and all later detections.

Kieran has achieved impressive performance gains in the code, delivering a circa 50% increase in speed and a factor-of-two reduction in memory footprint. This significantly increases the number of simulations that can be performed for the same computational cost, and of course the speed at which the results can be produced.


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Internationally recognised research

Swansea University

Researchers:
Prof Gert Aarts
Prof Biagio Lucini

Research Software Engineers:
SCW RSE group at Swansea University

Studying the Universe at the smallest scales

Research groups in the College of Science at Swansea are studying the nature and effects of the fundamental laws of physics at the smallest scales. Current projects include looking at the behaviour of matter at very high density and temperature, comparable to that found in the first seconds after the Big Bang, studying the properties of fields living in two-dimensional universes such as a sheet of graphene, and investigating candidate's theories that may give us a better understanding of the true nature of the famous Higgs boson discovered at the Large Hadron Collider.

SCW Research Software Engineers have worked and are working on all three of these projects: for the first case, working on improving performance of the state-of-the-art openQCD code on the latest Intel Xeon Phi and Xeon Scalable processors; in the second case, taking the prototype single-threaded code and making it a robust parallel application; and in the third case, using mathematical trickery to reduce the memory footprint of the application by half.

"Supercomputing Wales enables researchers to do bigger, more complex and higher impact research through the use of supercomputers. Researchers in all domains are under pressure to push to more computationally demanding problems. This is particularly challenging in domains which haven't historically been compute intensive. For many, supercomputing is also an unfamiliar technology, which makes it difficult to fully appreciate the possibilities it could offer. We provide both expertise and a compute platform to researchers in Wales, working in diverse domains including the study of the human genome, computational fluid dynamics and the science of the beginning of the universe. This not only enables the consortium universities to produce world-leading research, but has an impact far beyond Wales, through robust collaborations with institutions around the world."

Dr Mark Dawson, Supercomputing Wales Research Software Engineer at Swansea University

Lattice Gauge Theory

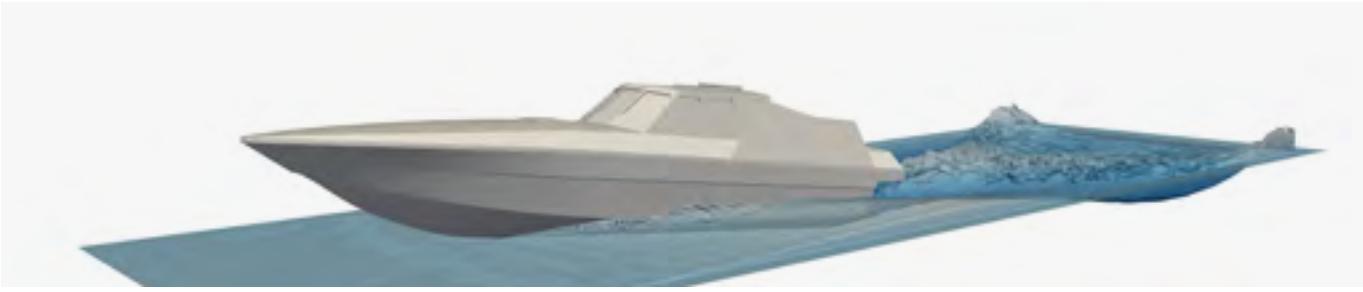
Researcher:
Dr Ben Evans

Research Software Engineers:
SCW RSE group at Swansea University

Hydrodynamic design of high-speed boats

Computational methods for simulation of high-speed boats remains an under-developed field, in particular when compared to the prevalence of aerodynamic design. The complex behaviour of spray and turbulence need to be accounted for, as well as an interaction surface between the boats which is dynamically-changing and a complicated shape.

Research at Swansea University has allowed the extension of methods used widely in aerodynamics to the optimisation of the design of high-speed boats. Parallel computing allows simulation of these complex interactions for real boat designs and RSEs at Swansea have optimised these algorithms to reduce reliance on high-latency processes.



Internationally recognised research

Aberystwyth University

Researcher:
Dr Pete Bunting

Research Software Engineer:
Dr Colin Sauze

Estimating the total mangrove biomass using remote sensing satellite data

The Global Mangrove Watch project is seeking to produce an estimate of the total mangrove biomass using remote sensing satellite data.
It will continue to track this over time to help safeguard mangrove forests against further loss and degradation.

The Global Mangrove Watch (GMW) is an international initiative led by the Japan Aerospace Exploration Agency (JAXA) in collaboration with the University of New South Wales (Australia), Aberystwyth University (U.K.), solo Earth Observation (Japan), Wetlands International and the World Conservation Monitoring Centre (UNEP-WCMC).

Bangor University

Researcher:
Dewi Bryn Jones

Research Software Engineer:
Aaron Owen

Welsh language speech recognition toolkit

At Bangor University, the language technologies unit (Canolfan Bedwyr) are developing an open-source speech recognition toolkit for the Welsh language.

Being able to interface and control electronic devices through the human voice is becoming an increasingly prevalent technology.
If Welsh cannot be used in these environments, then the language will be excluded from the digital world.

In order to train the acoustic model which forms the basis of the speech recognition system, a large number of Welsh audio samples are required. Due to the popularity of crowdsourcing tool Paldaruo, which records people reading Welsh prompts aloud, the computational requirements of the project have exceeded the capabilities of the research team's development machine.

Aaron Owen, a SCW Research Software Engineer at Bangor University has been working with Canolfan Bedwyr to provide training and software development support. Together, by utilising the new SCW systems, they have achieved impressive performance gains.
As a result, many acoustic models can now be trained in parallel which would not have been previously possible.

A powerful alliance of market leaders

DELL EMC | Atos

Supercomputing Wales has two supercomputer hubs based at Cardiff and Swansea universities, with research teams across the consortium universities accessing the facilities.

Together, the hubs represent a full suite of HPC and High Performance Data Analytics (HPDA) hardware and software with added benefits, including:

- 13,000 cores, tens of terabytes of memory and hundreds of terabytes of high performance storage
- Atos BullSequana S Datalake appliances
- Dell EMC PowerEdge R640, R740 and C6420 Servers with Intel® Xeon® processors
- Dell EMC Networking S3048 & PowerVault MD3420 storage
- Atos extreme Factory software, which allows the facility to be accessed as a service, across Wales
- Extensive technical support, education and training.

The programme brings together the expertise, experience and dedication of global partners, Atos and Dell EMC, to create Wales' first Supercomputing Centre of Excellence. The programme delivers:

- A high performing, high density, energy efficient supercomputer delivering low Total Cost of Ownership (TCO)
- Internationally recognised research capabilities and facilities
- A shared facility with access across all of the consortium university locations
- A lasting legacy of supercomputing skills in Wales
- Engagement with wider partners including Intel, Mellanox, Nvidia and Micron.

Developing supercomputing expertise in Wales

It is increasingly important for Wales to continue developing skills in HPC and data analytics as technologies such as Artificial Intelligence (AI) develop, and advances continue in the high performance computers which are able to process it.

In order to develop the existing expertise in Wales, the right training and development needs to take place. Atos helps further the professional development of the highly-skilled workers at Supercomputing Wales by supporting PhD students, providing technical training, and facilitating new relationships.

Supercomputing Wales is a key enabling infrastructure for several large-scale multi-million pound research and innovation projects across Wales, where access to high performance computing facilities and expertise is essential to their delivery.

"Supercomputing Wales represents a step-change in university research in Wales. Supercomputing Wales contributes a huge amount to the Welsh economy; not only through the research funding the programme has helped to secure, but also through the creation of highly-skilled jobs. The cohort of 15 Research Software Engineers represents one of the largest groups in the UK.

At Supercomputing Wales we have established a hub for high-performance computing, data-science and AI. Through our facilities, new research breakthroughs are possible; handling increased complexity, additional variables, new dimensions and new problem domains, leading to research outcomes that change lives."

Professor Roger Whitaker, Academic Director for Supercomputing Wales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APC

About Atos

Atos is a global leader in digital transformation with over 110,000 employees in 73 countries and annual revenue of over € 11 billion.

European number one in Cloud, Cybersecurity and High-Performance Computing, the Group provides end-to-end Orchestrated Hybrid Cloud, Big Data, Business Applications and Digital Workplace solutions. The group is the Worldwide Information Technology Partner for the Olympic & Paralympic Games and operates under the brands Atos, Atos Syntel, and Unify. Atos is a SE (Societas Europaea), listed on the CAC40 Paris stock index.

The purpose of Atos is to help design the future of the information technology space. Its expertise and services support the development of knowledge, education as well as multicultural and pluralistic approaches to research that contribute to scientific and technological excellence. Across the world, the group enables its customers, employees and collaborators, and members of societies at large to live, work and develop sustainably and confidently in the information technology space.

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Let's start a discussion together

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