UKRI Science and Technology Facilities Council

Scientific Computing

Where Advanced Computing Accelerates Discovery

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STFC Scientific Computing

Use the QR code
to visit our website:

STFC Scientific Computing

An international centre of excellence for advanced computing expertise and digital research infrastructure.

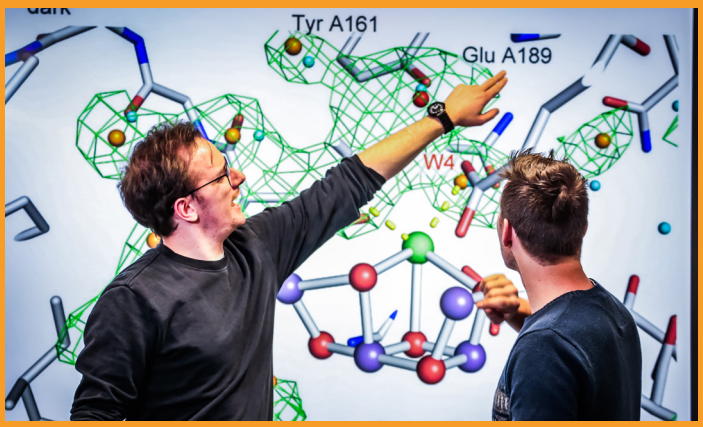
For more than 50 years, we have provided a foundation for research partnerships, building pioneering research communities and collaborating on a global scale with researchers and forward-thinking businesses.

We have a multidisciplinary, collaborative approach to addressing complex research and development challenges. Whether it's accelerating new drug discoveries, finding sustainable materials and new methods of tackling climate change, supporting the detection of gravitational waves or unlocking the secrets of the universe, we generate new technologies and discoveries that have real-world applications to benefit people worldwide.

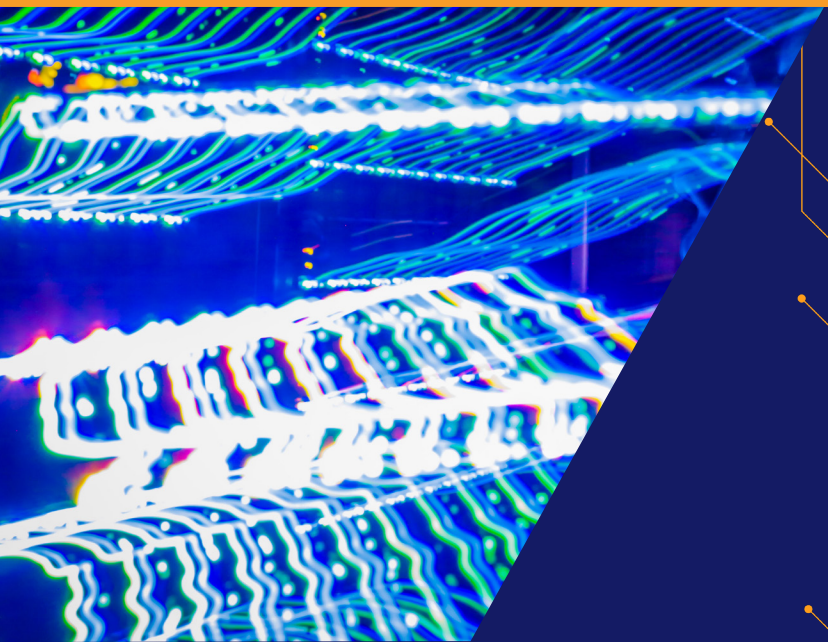
STFC Scientific Computing -
where advanced computing accelerates discovery

How Scientific Computing Makes a Difference:

In the following pages you will find brief information about some of the expertise we bring to research projects, such as speeding up drug discoveries and helping to predict climate change; and activities such as leading the UK's premier computing conference and inspiring young people to take up science as a career.



There are QR codes for each project which, when you scan them using your mobile device, will take you to a web page with more information.



Fast Tracking Drug Discovery Via the STFC Cloud

On average, it takes a new medicine 10 years to complete the journey from initial discovery to the clinic. The cost to research and develop each successful drug is estimated to be $2.6 Billion (USD). Scientists at the Diamond Light Source in Oxfordshire are carrying out research to speed-up this process, and they are being helped by the STFC Cloud.

The STFC Cloud is a dedicated cloud infrastructure, developed and managed by Scientific Computing, which provides access to computing resources for users across STFC facilities and other partners.

The scientists at Diamond used the Cloud to collaborate on the COVID Moonshot programme, in which scientists, research organisations and industry partners are dedicated to the discovery of affordable drugs to combat COVID-19 and future viral pandemics. The STFC Cloud has enabled the sharing of data in almost real time. This has shortened the process of finding preclinical candidates for antiviral drugs from years of research to less than 12 months.

Use the QR code to read the full case study:

Nature Inspires New Engineering Designs

Researchers from STFC Scientific Computing are collaborating with the University of Manchester to use the surface patterns found in nature to find ways to reduce fuel consumption and increase aerodynamic efficiency for aircraft, ships, and cars.

When air passes over an aircraft wing the flow is disturbed by surface friction, which separates the flow and leaves a gap above the surface, creating drag on the wing. This is a common phenomenon in air, road, and water vehicles, and can have a huge impact on fuel consumption, endurance and overall efficiency.

The research team used computer simulations to study the airflow process and explore new ways to improve vehicles' aerodynamic efficiency. Inspired by the natural streamlined movement of birds and fish as they glide through air and water, the team investigated the micro-scale pattern of ridges and grooves on bird feathers and shark skin.

"Sharks and birds are both well adapted to moving efficiently through fluid, be it water or air. If you examine shark skin or bird feathers under a microscope, they both share a common feature: small directional grooves, invisible to the naked eye, that are used to control the flow of fluid over the surface."

Dr Jian Fang, Senior Computational Scientist

Learn more about our innovative design approach here:

Predicting Climate Change

Climate change is now top of the world's agenda. Climate scientists have developed detailed computational models to project the likely effects on our climate of continuing to emit carbon. If we are to understand the risks of climate change we need to study how these new weather patterns will affect our lives. Will our streets flood after heavy rainfall? What effect will rising temperatures have on the food we grow?

This is where Scientific Computing's Data and Analytics Facility for National Infrastructure (DAFNI) is helping. DAFNI is involved in the OpenCLIM project, which concentrates on a diverse set of risks and their possible effects on anything from the streets and houses we live in, to yields of crops like wheat or potatoes.

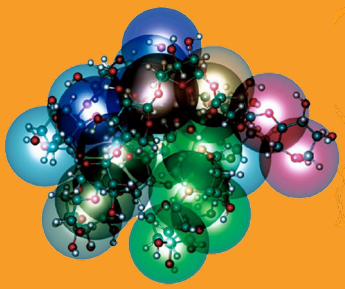
The DAFNI computing platform enables the models of different scenarios to be brought together. For example, growth in urban areas can be combined with models of flooding caused by rising water levels to predict what could happen. This in turn will enable plans to be put in place to reduce the impact on our homes and businesses.

Use the QR code to read more about this initiative and DAFNI in our Annual Review, page 30:

OpenCLIM is funded by the UKRI-Natural Environment Research Council

Addressing Industry Challenges With Materials Modelling

A major challenge we face today is understanding the effects of materials used in everyday products and services, from plastics in food to storage containers for nuclear waste. Computational Scientists at STFC Scientific Computing are addressing these challenges by developing software tools that can help a diverse range of researchers and industries.



See more information using the QR code:

The software, which was developed by our Computational Chemistry group based at the Daresbury Laboratory in Warrington, Cheshire, is already being used in a variety of different industries and applications, including:

- Developing a tool designed to simulate the effects of radiation damage in materials, which has become incredibly useful in experimental and theoretical research into the ageing of materials exposed to radiation.
- Designing and developing new pharmaceutical products or improving existing products.
- Testing the damage and micro-structural changes of spacecraft surfaces when they collide with microscopic meteor particles in space, an experiment that would be impossible to perform on Earth.
- Investigating why plastic particles penetrate into food, how they can be used in cosmetic products, and exploring the effects they may have on cell membranes either in the food or in the human body.

Collaborating to Advance Solar Energy Technologies

Computational scientists from STFC Scientific Computing are working with two UK universities, using real experiments and advanced computer modelling to improve the component of solar cells that absorb energy. They are testing dyes rather than using rare-earth metals, which are expensive and difficult to obtain, as a component to capture the sun's radiation for use in solar panels and other products. Improving this technology should make solar cells cheaper to produce and, subsequently, more affordable to consumers.

"Taking advantage of these abundant organic dyes, which are more sustainable and less devastating to the environment than their counterparts, will push us closer and closer to realising the full potential of renewable energy."

Dr Ya-Wen Hsiao,
Senior Computational Scientist, STFC

Find out more using the QR code:

Using Computers to Design Safe and Sustainable Nuclear Reactors

As the UK's net-zero goals loom, computational scientists within STFC Scientific Computing are carrying out research to model and simulate designs for the next generation of safe and sustainable nuclear reactors. Molten Salt Fast Reactors, which use a molten salt mixture to carry the radioactive material, have the potential to improve the sustainability of the nuclear cycle since they can use current nuclear waste as fuel and at the same time generate more, emission-free, energy.

Making these designs a reality still requires a lot of research. Numerical models, new relevant data stacks and datasets are still needed for us to fully understand the reactions and mechanics that will be going on in these machines.

Use the QR code below to learn more:

Computing Insight UK (CIUK) – Our Flagship Conference

We organise and run STFC's increasingly popular annual High Performance Computing conference, held in Manchester each December. Due to its successful growth in recent years we are confident that Computing Insight UK is now the UK's premier HPC conference and exhibition.

In 2022 CIUK attracted over 500 attendees, a diverse range of exhibitors, guest speakers and industry professionals. The conference revolved around the theme of 'Sustainable HPC' and many sessions reflected this, with talks ranging from the challenges of designing and developing more modern, environmentally sustainable data centres to the feasibility of Net Zero HPC systems.

"It's great to see so many people here...I think the theme of sustainable computing has really attracted people – it's clearly a hot topic!"

Tom Griffin, Director, STFC Scientific Computing

Find out more about CIUK:

Inspiring a New Generation of Computer Scientists

Remote^3: Engaging Schools and Beyond

One of STFC's popular public engagement projects is a partnership between Scientific Computing, the Boulby Underground Laboratory and the STFC Public Engagement Team. The Remote^3 project was adapted from a small initiative designed to help students from remote schools in the Scottish highlands into a far wider reaching project adapted to continue remotely through the coronavirus pandemic.

Children all over the country attended weekly webinars during the summer months that introduced a coding challenge using Lego Mindstorm robotic rovers, and provided information about the uses of robots all around the world.

Boulby Underground Laboratory is home to a Mars Yard, where Mars Rover prototypes are tested for international space research. The extremely salty, hot and dusty environment there simulates conditions found on other planets and this is exactly where the students' rovers are tested.

"We want the project to inspire creative design, encourage teamwork, and develop presentation skills in a diverse environment, as well as provide awareness of the remarkable front-line science taking place. In doing so we hope to encourage the next generation of young people into a career in STEM subjects."

Dr. XinRan Liu, STFC Leadership Fellow, University of Edinburgh

Further Career Opportunities with STFC Scientific Computing

Are you looking to pursue a career in Scientific Research? STFC offers a wide range of exciting career opportunities, including **apprenticeships** within one of our teams, **industrial placement years** for university students looking to broaden their horizons, or **graduate positions** within the department, working on a number of projects to find a field you are truly passionate about.

The combined years of experience for current and past Scientific Computing graduates makes a total of **223 years**

"I knew that I wanted an industrial placement that would prepare me for a job in scientific research, and the ethos of STFC and the opportunities it offered were exactly what I was looking for."

Harriet Jones, Industrial Placement Student

There are no limits to what you can achieve at STFC.

Tom Griffin, Director of Scientific Computing, originally joined STFC as an industrial placement student!

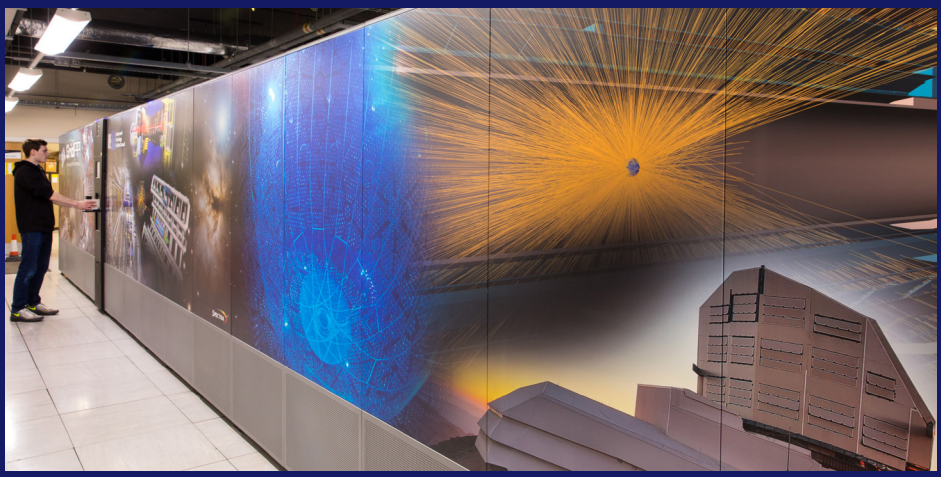
Find more about our career options here:

Record-Breaking Tape Robots!

In the Spring of 2023 we upgraded our tape storage systems in STFC's scientific data centre at the Rutherford Appleton Laboratory (RAL) in Oxfordshire. We now hold the record for having two of the largest TFinity automated tape libraries, also known as 'tape robots', in the UK and Europe.

These libraries can store up to 440 petabytes of research data. To give an idea of just how much data that is, **one petabyte** of data is equivalent to **500 billion pages of text,** so you can see how effective these tape robots are!

Users can call up the data on their laptops, and within a few seconds the tape robot will have located and scanned the relevant tape and made the data available. Affectionately named Asterix and Obelix, these automated tape libraries are a cost effective way to store the huge amounts of data generated through scientific research.



Find out more about STFC's innovative data storage solutions here:

For more information about STFC Scientific Computing visit our website: **scd.stfc.ac.uk** and our exciting **Virtual Exhibition,** where you'll find displays, posters, podcasts and videos, links to schools activities and even a **virtual tour** of the **RAL Data Centre.**

Follow the QR code for the Virtual Exhibition:

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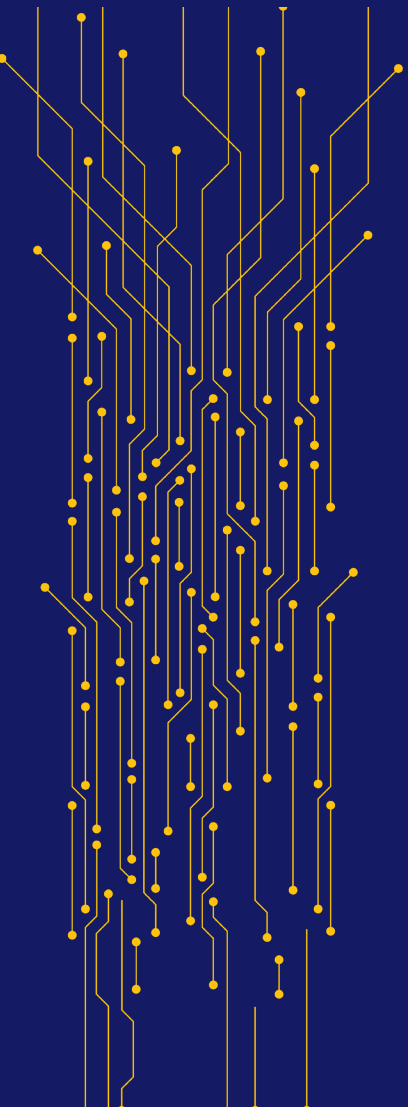
Scientific Computing



STFC Scientific Computing is based at the Rutherford Appleton and Daresbury Laboratories.

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