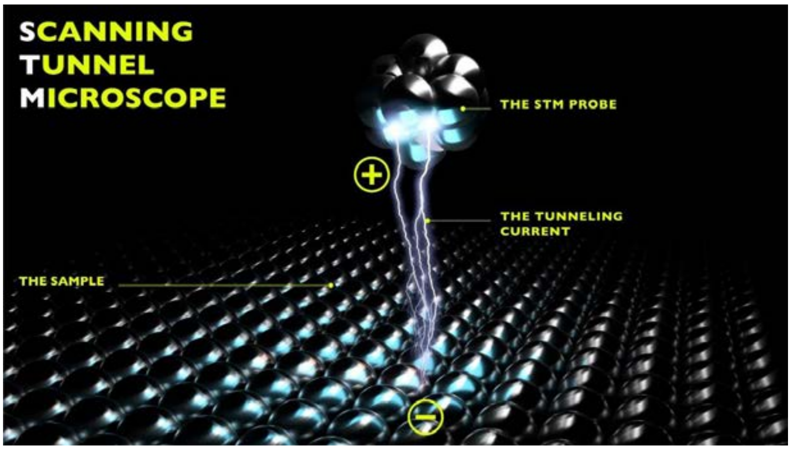
Studying 2D Materials

2D materials only a few atoms thick are one of the hottest topics in Physics. Since the discovery of the supermaterial graphene, for which two scientists were awarded a Nobel prize in 2010, hundreds of other 2D materials have been identified. These have either been made experimentally or identified through computational modelling.

Understanding the quantum properties of these new super thin materials with promising applications in electronics, healthcare, and new energy materials requires advanced scientific facilities and techniques. Exposing 2D materials to the powerful X-rays produced at a synchroton beam facility is one of the most effective ways of studying electron behaviour in the materials. The process generates vast amounts of data that we have been able to analyse using sophisticated cloud computational modelling funded by OCRE.



> My University of Bath research group uses OCRE-funded cloud supercomputing to predict new 2D materials and identify valuable properties of recently discovered 2D semiconductor materials.
>
> Professor Daniel Wolverson, University of Bath.

RESEARCHER
Professor Daniel Wolverson

ORGANISATION
University of Bath

FIELD OF STUDY
Natural Sciences

LOCATION
United Kingdom

OCRE RESOURCES USED
Cloud Services

CHALLENGE

A Fast-Moving Scientific Field

The study of 2D materials is a fast-moving scientific field. Typically, our experiments generate vast volumes of new data in short intensive experiments rather than in a steady well-paced flow. Newly produced data has to be analysed in rapid turnaround simulations that most often can't be achieved with a university's limited supercomputing resources.

Another challenge of our research is to make it accessible and engaging for undergraduate students. Apart from a few textbook calculations, there is little that students can contribute to our modelling work without using the same expensive computational tools as us. Inspired by astrophysics, where undergraduates are regularly given observational data to analyse, we wanted to explore the ability of cloud computing to deliver accelerated student training in our methodologies before giving them real scientific problems to solve.

> “It has been a pleasure to involve undergraduates in the research activity of my group, and it has been clear that they take the responsibility of making good use of HPC resources very seriously and can rise to the challenge.
>
> Professor Daniel Wolverson, University of Bath

SOLUTION

OCRE Cloud Flexibility for Time-Optimised Experiments

The cloud supercomputing resources provided by OCRE have allowed us to carry out computational work at a range of scales with widely varying numbers of cores and compute times, optimised for the requirements of our experiments. This flexibility meant we could run calculations at the optimum core numbers for given parallelisation strategies, making our calculations more efficient in terms of total core-hours used. At the same time, it has also improved turnaround time.

Our undergraduate students can now receive faster and improved critical training. For example, a well-converged scientific calculation of publishable quality requires the right balance between precision and costs but doing this can be hindered by limits on computational resources. The flexibility of the OCRE cloud-funded supercomputing solution removed this limitation. It meant the work of producing scientific results and proving their reliability could be carried out by our students, allowing them to make a substantial research contribution.

IMPACT

Going Beyond the Original Project

We have tackled the specific new 2D materials and experimental datasets on which the proposal was based – and have gone even further. In particular, we are modelling scanning tunnelling microscopy data on new 2D materials. This is a near-atomic scale investigation of the electronic states in these materials. The simulations extend the calculations carried out to model our synchrotron data. We have also simulated X-ray photoelectron spectroscopy data of our materials. With the OCRE-funded resources, we developed and validated a new methodology for this analysis, resulting in a recent publication on our computational approach.

Including undergraduate students in our OCRE project work has given them valuable experience in conducting actual scientific research within an active and diverse research group. Our students have appreciated and been inspired by the level of the resources they could access. This type of experience is vital in recruiting new researchers into the field.