BEAR

BIRMINGHAM ENVIRONMENT FOR ACADEMIC RESEARCH

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Foreword

Professor Andrew Morris
Chair of Research Computing Management Committee

I'm delighted to introduce this fourth Bear Case study. Bear – the Birmingham Environment for Academic Research provides compute, storage, training and research software engineering support. Bear's computing resource is provided as BlueBEAR, a heterogenous system comprising the latest CPU and GPU hardware connected to fast, secure storage. Access to Bear is provided free of charge to University of Birmingham researchers, funded from university central funds. This ensures that all researchers have a baseline access to the machine to try-out research computing and develop new projects.

Once again the breadth of the simulations carried out on BlueBEAR is staggering, modelling everything from price-setting behaviour, thermoelectrics and proteins to stars. Artificial Intelligence (AI) and Machine Learning continues to play an important role in research, in this case study including high entropy alloys and linking environmental policy to impact. This and the previous Case studies demonstrate the scientific and societal value of having such a resource and -- in a tough climate -- help justify its continued support.

Abstract

This collection of case studies highlights the breadth and variety of research supported by the University of Birmingham's Environment for Academic Research (BEAR). BEAR comprises modern IT resources designed to facilitate research. The case studies illustrate how BEAR services, including the Research Data Store (RDS), BEAR software, and the University supercomputer BlueBEAR, are essential to advancing significant research across various disciplines.

BlueBEAR, a crucial part of BEAR, offers free compute power and specialized applications to help staff and students delve deeper into their research. Upgraded in 2025, the cluster features numerous large memory nodes and a GPU service alongside standard compute nodes. Additionally, the RDS is a favoured option among researchers for securely storing their active research data.

As of publication, over 5,000 researchers from all five colleges were actively using BlueBEAR and/or the RDS. This volume presents case studies showcasing diverse research from each college. From estimating snow coverage to modelling second language acquisition, these examples demonstrate how BEAR services are enabling exciting and important research throughout the university.

Contents

Contributors

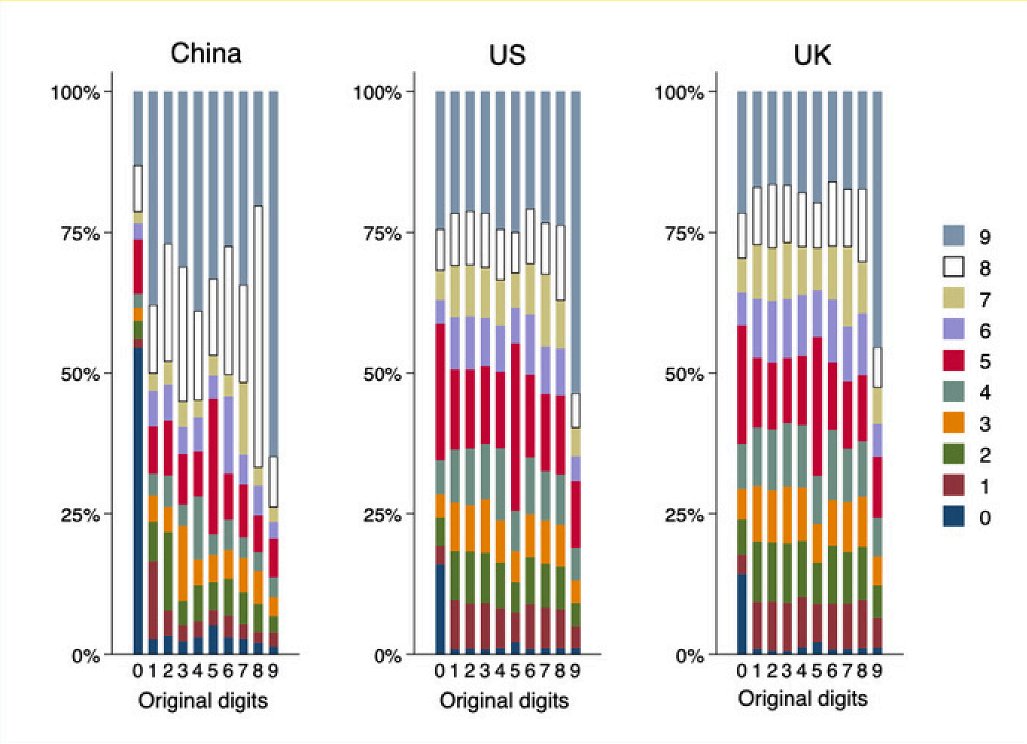
Understand price-setting behaviour

Zhuangchen Wu - PhD Student

My research examines price-setting behavior using daily data from online sellers, which is crucial for macroeconomic modeling and monetary policy design. Unlike monthly or quarterly inflation statistics, daily price listings reveal various pricing patterns. BlueBEAR's High-Performance Computing (HPC) service is essential for handling this large-scale data.

One project focuses on price-ending digits. Prices often end in "99" or "9" to appear cheaper and boost consumption, leading to price rigidity. In China, the digit "4" is considered unlucky and "8" lucky, unlike in the US and UK. I explore the prevalence of these digits in price endings and their impact on price-setting.

Our findings show that "8" and "9" are favored in China, influenced by numerology, while US and UK sellers are not significantly affected. BlueBEAR's HPC service is vital for processing large datasets and running complex regressions efficiently, enhancing research quality and productivity.



The transition matrices of price endings

Understand the relationship between outdoor temperature and decision-making

Haonan Tian - PhD Student

Haonan's research focuses on understanding how temperature shocks influence energy assessors' scoring decisions during property evaluations. In the UK, EPCs provide vital information about a property's energy efficiency to potential buyers and tenants, playing an indispensable role in real estate transactions. To delve into this area, I analyze a massive dataset comprising approximately 17 million EPC records from 2008 to 2023. Given the extensive scale of this dataset, the high-performance computing (HPC) services of BlueBEAR are not just necessary but crucial to my research.

One of my research projects examines the impact of temperature shocks on EPC scores. We find that higher average temperatures are associated with a statistically significant increase in EPC scores. Specifically, a one-standard-deviation increase in temperature anomalies leads to a 7.7% increase in EPC scores. This temperature effect is particularly important for properties below the EPC rating band threshold, as temperature-driven score increases can push them into a higher band and potentially boost their market value. To explain these findings, we identify effort and cognitive performance as two primary mechanisms. When assessors invest less effort (on weekends or during a narrower scope of work) or face higher cognitive load (heavy precipitation or sleep deprivation), the temperature impact intensifies.

BlueBEAR's HPC capabilities are crucial for my research, particularly in managing and analyzing the extensive EPC data.

Panel A. Day of week / Property types Panel B. Precipitation

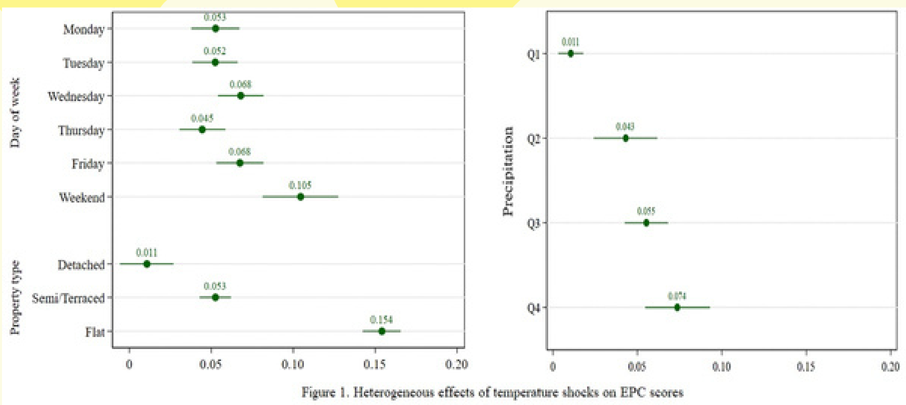
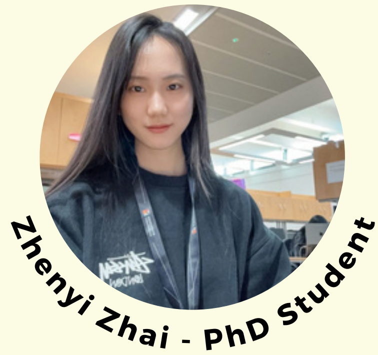


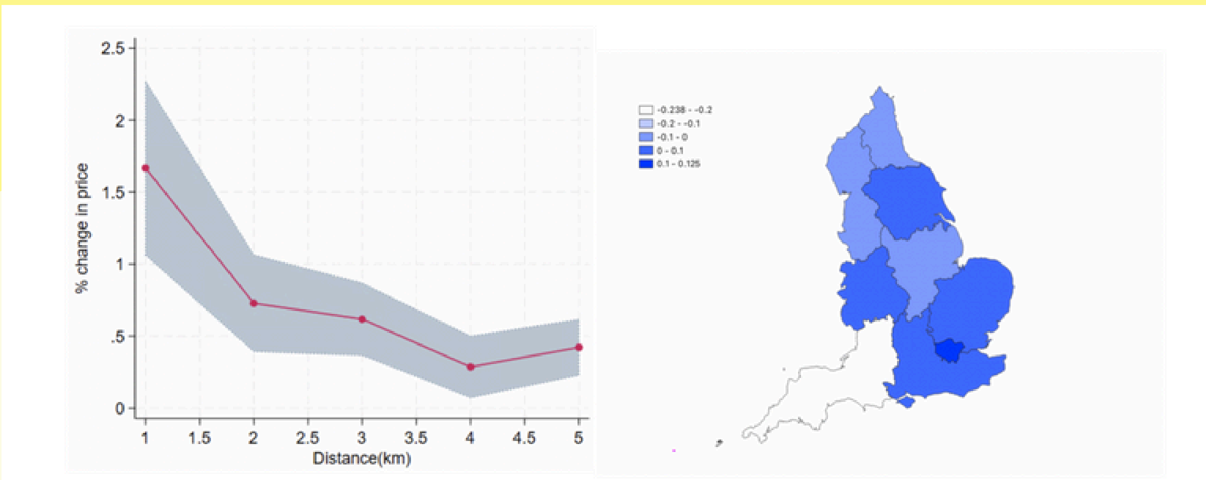
Figure 1. Heterogeneous effects of temperature shocks on EPC scores

The impact of free schools on neighbourhood house prices



A study by Zhenyi Zhai, a PhD student in Economics, who investigates how the establishment of free schools in England affects nearby house prices. Using a method called "difference in differences" and analysing data from 2011 to 2019, Zhai examines changes in property prices within a 5 km radius of new free schools. The study finds that house prices generally increase within 1 km of a new school, but the impact varies by region. For instance, house prices rise significantly in London and the East of England, while they decrease in the North East and North West.

The research relies on BlueBEAR, a high-performance computing service, to handle the large dataset of over two million property transactions and school attributes. BlueBEAR's powerful computational resources enable efficient data processing and analysis, which is crucial for understanding the dynamic effects of free schools on local real estate. This study highlights the importance of educational resources in influencing housing markets and demonstrates how advanced computing can support complex economic research.



Panel A: Distance and effects of free school establishment

Panel B: Effects of free school establishment in different areas

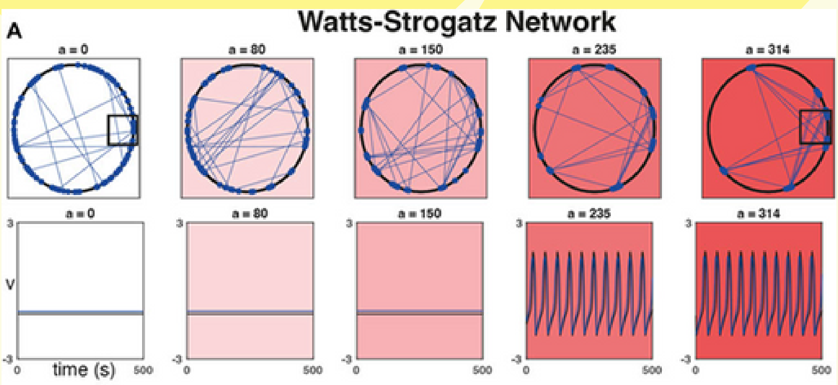
House prices increase near new free schools, with significant regional variation

Too many networks, not enough time

Daniel Galvis, who studies how network structures and differences within nodes influence complex behaviors in systems like the brain and pancreas. By using BlueBEAR, a high-performance computing service, Daniel conducts Monte Carlo experiments to simulate and analyse these networks. This method involves running numerous simulations with random inputs to understand how specific network features, such as connectivity patterns, affect overall system behaviour.

His research is particularly focused on understanding how these network features predict diseases like epilepsy and diabetes. For example, he examines how the arrangement of cells in the pancreas affects glucose metabolism, developing measures to quantify the likelihood of cells with similar properties forming connections. This helps in identifying patterns that could indicate the onset of diseases.

The relevance of this research lies in its potential to uncover the underlying mechanisms of complex biological systems, leading to better predictions and treatments for various diseases. By leveraging advanced computational tools, Daniel's work demonstrates the importance of interdisciplinary approaches in tackling intricate scientific problems, ultimately contributing to advancements in healthcare and biomedical research



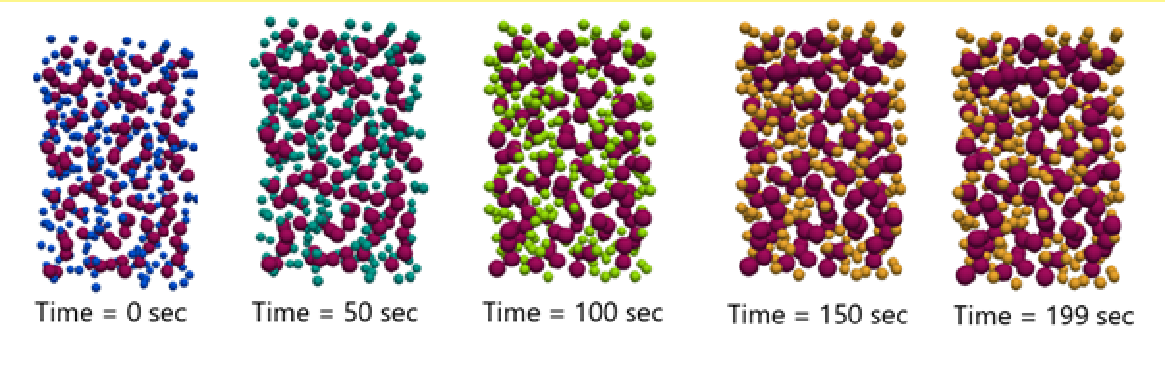
networks where similar units are increasingly likely to form cliques

Transforming powder dissolution challenges into opportunities

Khizra Abdul Wadood - EngD Student

Khizra, is leveraging BlueBEAR to simulate the complex dynamics of how powders mix with solvents. This research is crucial for industries ranging from pharmaceuticals to personal hygiene, where understanding powder behaviour can lead to more efficient and effective product formulations. Traditional methods often rely on inconsistent empirical data, making computational simulations more reliable and cost-effective alternative

By employing advanced simulation tools like LIGGGHTS, OpenFOAM, Lethe, and DualSPHysics, researchers can model particle-fluid interactions with remarkable precision. These simulations shed light on key behaviours, such as powder swelling, offering insights that were previously unattainable. Running these complex models on BlueBEAR enables researchers to refine their processes virtually, cutting down on the need for costly and time-consuming physical experiments.



DEM Simulation of Swelling Particles

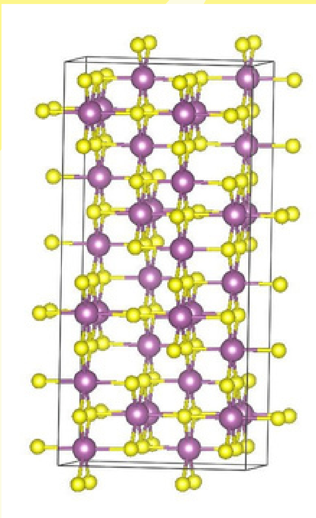
Characterising novel materials for renewable energy applications

Philippa Cox - PhD Student

Philippa uses the Birmingham Environment for Academic Research (BEAR) high-performance computing resources to investigate novel materials that could be used in renewable energy technologies. Her research primarily focuses on understanding the structure, electronic properties, and defect chemistry of these materials through computational methods.

Her work is particularly significant in the fields of thermoelectrics and photovoltaics. She explores how the symmetry and disorder within a material's structure can influence its electronic properties and efficiency in energy conversion. By using advanced computational techniques such as Density Functional Theory (DFT), cluster expansions, and Monte Carlo integration methods, she can model and analyze these materials at an atomic level. This detailed analysis helps in predicting the behaviour of materials under different conditions, which is crucial for developing more efficient renewable energy technologies.

This emphasizes the importance of high-performance computing in modern scientific research. Philippa's ability to perform complex simulations and analyses using BEAR's resources allows her to gain insights that would be impossible with standard desktop computers. This capability not only accelerates her research but also contributes to the broader goal of developing sustainable energy solutions.



Unit cell for Sc_2S_3

Simulating fuzzy protein complexes

Thomas utilizes the BlueBEAR high-performance computing resources to develop and apply integrative structural biology techniques to study biomolecular complexes. His work is part of a collaborative effort involving the School of Biosciences, the School of Chemistry, and the Institute of Cancer and Genomic Science, under the guidance of Professor Teresa Carlomagno.

His research focuses on the formation of high-affinity complexes between disordered protein regions, known as "fuzzy" protein complexes. Unlike traditional protein interactions that rely on complementary shapes, these fuzzy complexes do not exhibit site-specific interactions or structure formation. One notable example is the acetylation mechanism of the histone 3 (H3) tail, which plays a crucial role in modulating chromatin structure and DNA accessibility. This process involves the histone chaperones Asf1 and Vps75, which form a large complex with the acetyltransferase enzyme Rtt109 and the histone dimer H3:H4.

By using BlueBEAR, Thomas can perform complex molecular dynamics simulations of protein-protein interactions at an atomic level using a combination of biased and unbiased techniques. These simulations, which model systems containing hundreds of thousands of particles and span timescales from nanoseconds to microseconds, are essential for understanding the detailed mechanisms of fuzzy protein interactions. This research not only advances our knowledge of protein chemistry but also has potential implications for developing new therapeutic strategies

Structure of the complex formed by the histones H3 and H4, the enzyme Rtt109, and the histone chaperones Asf1 and Vps75.

Using computational and laboratory research to unravel genome plasticity in plants

Katie Jeynes-Cupper - PhD student

Katie Jeynes-Cupper, a PhD student in Biosciences, is conducting research on genome plasticity in plants using the BlueBEAR High-Performance Computing (HPC) cluster at the University of Birmingham. Her work, which earned her the best presentation award at the BEAR Conference 2024, aims to address food security issues and advance crop breeding and biofuel production. The Catoni Research Group, where Katie is based, focuses on understanding the genetic and epigenetic mechanisms driving plant traits and evolution. This research involves a combination of greenhouse and laboratory experiments, as well as computational analysis using next-generation sequencing data.

The group has developed several open-source tools, such as DMRcaller, PackFinder, and mobileRNA, to analyze genomic data. Katie's specific research investigates the link between RNA mobilization and phenotypic changes in crops, with the goal of leveraging these mechanisms to support crop breeding efforts. The computational power of the BlueBEAR HPC cluster has been crucial in handling vast quantities of genomic information and optimizing analysis pipelines. Katie's work highlights the importance of HPC resources in advancing plant research and addressing global challenges related to food security and sustainable agriculture.

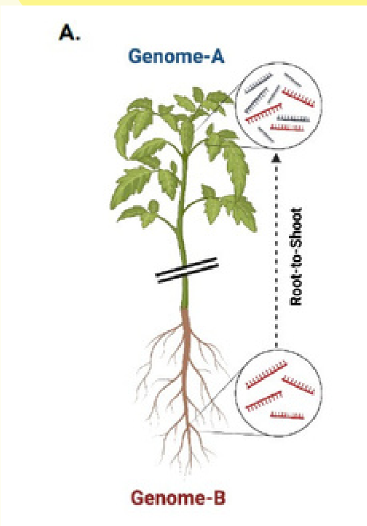


Diagram of a grafting experiment involving mobile RNA molecules (movement assumed in the root-to-shoot direction). The sampled material (assumed as scion) will include molecules produced by the genome A (in blue) as well as mobile molecules that have travelled from the Genome B (in red). Computational work is required to determine mobile molecules, by analysing their nucleic acid sequences produced with genomics approaches

Predicting the wind characteristics around high-rise buildings

Jose Romero - PhD Student

Jose Romero is utilizing the BlueBEAR High-Performance Computing (HPC) cluster to predict wind characteristics around high-rise buildings. His research focuses on understanding the effects of wind on the built environment and mitigating associated risks. This includes applications ranging from analysing wind impact on structures, to pollutant dispersion or ground vehicle interaction. The importance of this research is highlighted by the example of Bridgewater Place, where wind amplification at street level led to a devastating accident, prompting the City of London to adopt guidelines to limit the impact of new high-rise developments on pedestrians and cyclists.

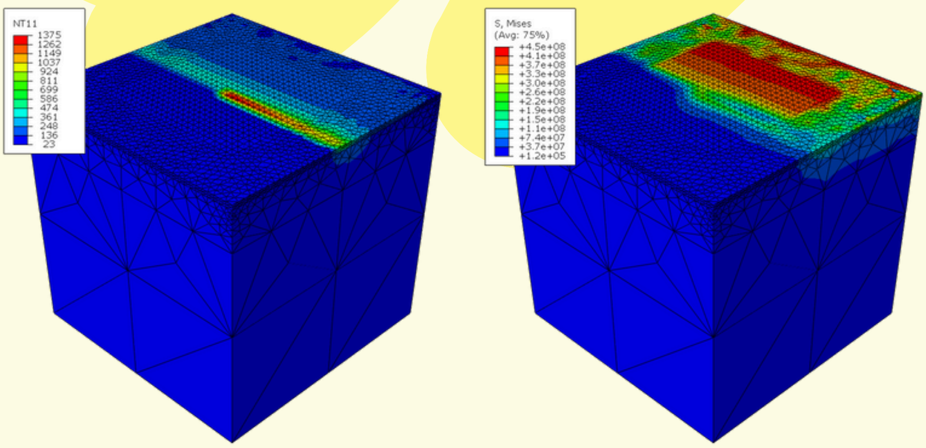
The BlueBEAR HPC cluster is crucial for Jose's work, significantly reducing the time required to run Computational Fluid Dynamics (CFD) simulations from months or years to just hours or days. The cluster's ability to handle large datasets and provide extensive computational power and memory is essential for solving the complex Navier-Stokes equations that describe fluid flows. The support and resources provided by the BlueBEAR team, including documentation and workshops, are invaluable to Jose's research, enabling him to produce and store large datasets and accelerate his simulations.

Bridgewater place: A case study on the importance of wind engineering Bridgewater Place puts 'wings' in place to block wind – BBC News – Picture taken from BBC News article

Predicting residual stresses in additive manufacturing

Vincenzo Brachetta, a researcher in the School of Metallurgy and Materials at the University of Birmingham, is using the BlueBEAR High-Performance Computing (HPC) cluster for his computational studies. During his PhD, he used BlueBEAR to predict residual stresses in additive manufacturing and his research focused on the finite element modelling of the additive manufacturing process, particularly for titanium alloys, to understand and minimise the material and energy waste associated with the production and repair of mechanical components like turbine blades. Residual stresses, which are internal stresses that remain after the manufacturing process, can reduce the fatigue life of components and are a significant challenge in additive manufacturing.

The BlueBEAR HPC cluster enabled Vincenzo to run multiple high-fidelity numerical simulations concurrently, significantly reducing the time required for these complex computations. The comprehensive IT infrastructure at the University of Birmingham, including the reliable Research Data Store and the advanced software management systems, supported his research. By using tools like SIMULIA/Abaqus integrated with FORTRAN and Python, Vincenzo was able to accurately predict residual stresses and the formation of brittle phases like martensite, which further impact the lifespan of components. His work highlights the critical role of HPC resources in advancing materials science and improving manufacturing processes.

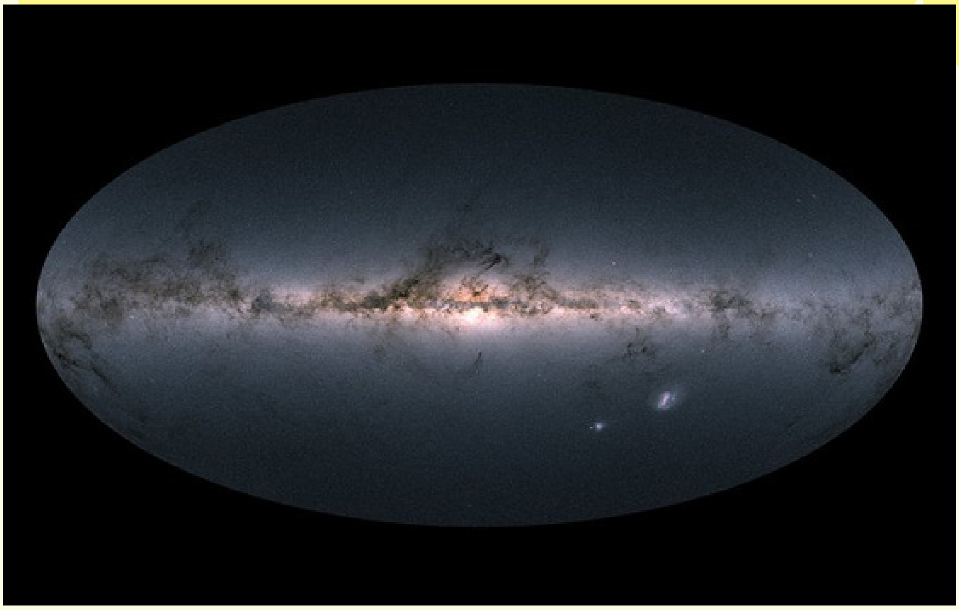


Simulation of development of residual stresses during laser scanning calculated using SIMULIA/Abaqus (left: temperature field, right: von Mises stress).

Studying stars across the Milky Way

Amalie, a research fellow at the School of Physics and Astronomy, is using the BlueBEAR High-Performance Computing (HPC) cluster to study stars across the Milky Way. Her research aims to understand the history and evolution of our galaxy by analyzing the intrinsic properties of stars, such as their masses, chemical compositions, and ages. By simulating and modeling thousands of stars, Amalie can reconstruct the timeline of key events in the Milky Way's history, providing insights into how the galaxy has evolved from the Big Bang to the present day.

The stars Amalie studies are similar to our Sun but are more advanced in their evolution. These stars have exhausted the hydrogen in their cores and now generate energy through fusion processes in surrounding shells, causing them to expand and appear more orange or red. The computational power of the BlueBEAR HPC cluster is essential for handling the vast amounts of data and complex simulations required for this research. Amalie's work highlights the importance of HPC resources in advancing our understanding of galactic evolution and the broader context of stellar properties

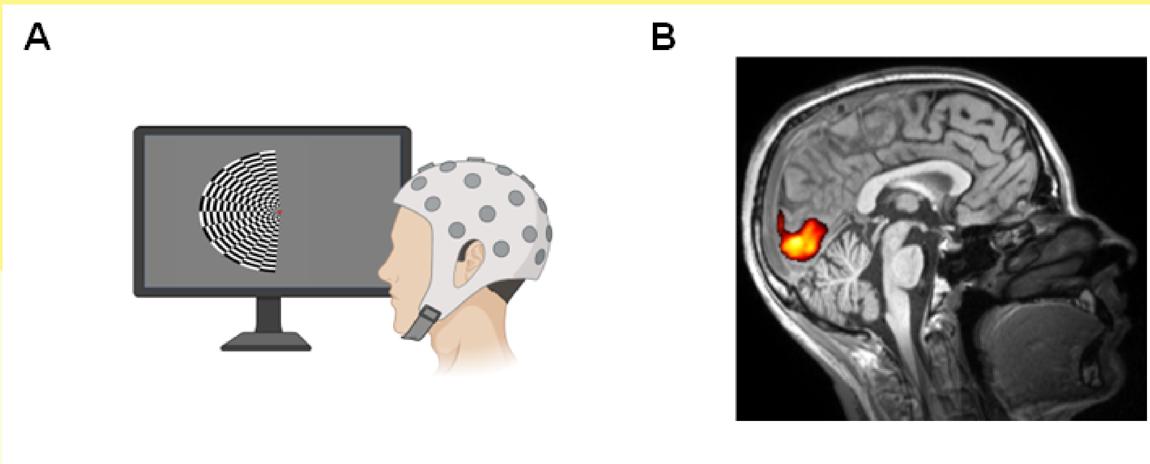


The most detailed view of the stars in the Milky Way. Credit: ESA/Gaia/DPAC

Investigating the brain

Brandon, is using the BlueBEAR High-Performance Computing (HPC) cluster to investigate how our brains interpret visual stimuli. His research integrates electroencephalography (EEG) and functional magnetic resonance imaging (fMRI) to gain a comprehensive understanding of visual processing. EEG measures brain activity through electrodes on the scalp, providing fast but surface-level data, while fMRI records slower changes in brain activity by tracking blood flow, offering detailed localization of brain activity.

Combining these methods presents computational challenges due to the large volume of data and intensive pre-processing required. The BlueBEAR HPC cluster helps overcome these challenges by providing the necessary computational power and storage solutions. This allows Brandon to process data from both modalities in parallel, significantly reducing the time needed for analysis. His work highlights the importance of HPC resources in advancing our understanding of brain function and visual processing



Examples of the visual stimuli used to elicit visual activity in the brain and EEG electrodes

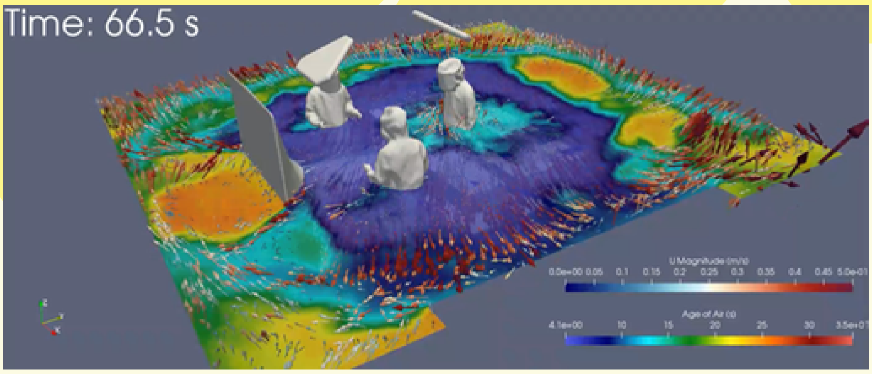
A computational fluid dynamic model of an ultra clean air operating theatre

Andrew Thomas - Orthopaedic Surgeon

Andrew Thomas, a Consultant Orthopaedic Surgeon at the Royal Orthopaedic Hospital, Birmingham, is collaborating with researchers including Professor Mark Simmons from the Department of Chemical Engineering, University of Birmingham, Professor Federico Alberini and Jairo Murillo-Rincón, University of Bologna, Dr Carlos A. Duque-Daza, National University of Columbia and Andrés S. Espinosa-Moreno, Basque centre for mathematics to develop a Computational Fluid Dynamic (CFD) model of an ultra-clean air operating theatre. This model aims to address the problem of deep infections in joint replacement surgeries by optimizing airflow patterns to minimize airborne contamination.

The research team used laser imaging and ultrasound-based anemometry to gather comprehensive data on airflow velocities. The Orthopaedic Hospital also contributed by commissioning detailed measurements of input airflow and thermal data was acquired using an high resolution thermal camera.

This collaborative effort highlights the importance of HPC resources in advancing medical research and improving surgical outcomes. The work was acknowledged with an HPC Wire readers’ choice award in 2021. The initial model has been published and presented at numerous educational and training events. The data is informing work such as the Healthcare Infection Society guidance on commissioning and testing of operating theatres and the Institute of Environmental Science and Technology Working group CC055 on testing and measurement in surgical areas.



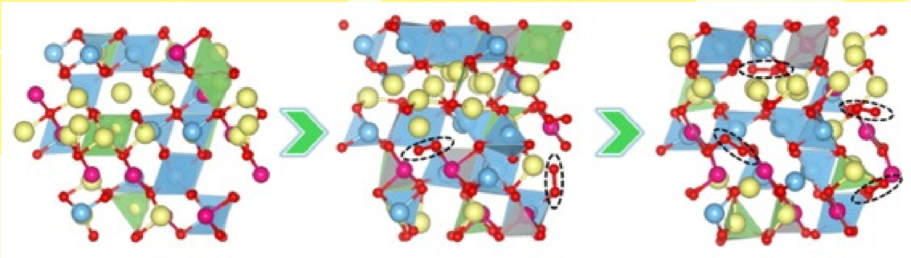
The velocity and direction of airflow in an ultra clean air operating theatre. The background colour is the age of the air, a measure of stagnant areas in the system

Studying battery materials

Sandeep Das - Postdoc

Sandeep Das, a postdoctoral researcher and computational chemist in the Scanlon Materials Theory Group at the University of Birmingham, is utilizing the BlueBEAR High-Performance Computing (HPC) cluster to design novel lithium-ion (Li-ion) battery materials. His research focuses on developing advanced cathode materials with higher energy density and specific capacity compared to current technologies. This is crucial as existing Li-ion battery technologies have mostly reached their performance limits, and there is a growing need for improved batteries to support renewable energy sources and electric vehicles.

Sandeep's work involves studying disordered rock salt (DRX) structures as potential cathode materials. These structures feature a mixture of lithium and transition metals (TMs) at the cation site, which enhances lithium transport and overall battery performance. However, the oxidation of oxygen anions in these materials can lead to issues like voltage hysteresis and irreversible phase transitions. The BlueBEAR HPC cluster allows Sandeep to perform large-scale density functional theory (DFT) calculations, enabling a deeper understanding of the electrochemical behaviour of these materials and helping to stabilize the oxygen anion reduction process. This research is essential for developing practical, high-capacity cathode materials for the next generation of Li-ion batteries



Evolution of a discharged cathode material showing O2 formation

Training accurate Machine Learnt Interatomic Potentials (MLIPs) for High Entropy Alloys (HEAs)

Joseph Arnold - Postdoc

Joseph, a postdoctoral research fellow in the Gurrutxaga-Lerma research group at the University of Birmingham, is developing machine learning-based interatomic potentials (MLIPs) for High Entropy Alloys (HEAs). HEAs are a unique class of metal alloys composed of five or more elements, capable of forming both highly disordered solid solutions and structures with varying degrees of ordering. To accurately model the properties of HEAs, large supercells and a significant number of k-points are required, which translates to high computational demands.

The BlueBEAR High-Performance Computing (HPC) cluster is essential for Joseph's research, allowing him to optimize large structures and perform extensive simulations that would be otherwise impossible. The HPC resources provide the necessary computational power and memory, with 6 TB of RAM available per user, to handle the complex calculations involved. The support from Advanced Research Computing has been invaluable in establishing Joseph's computational workflow, enabling him to make significant progress in understanding and predicting the behavior of HEAs

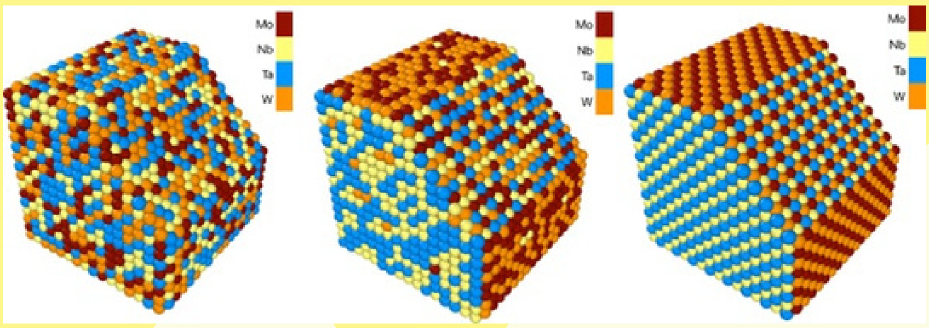


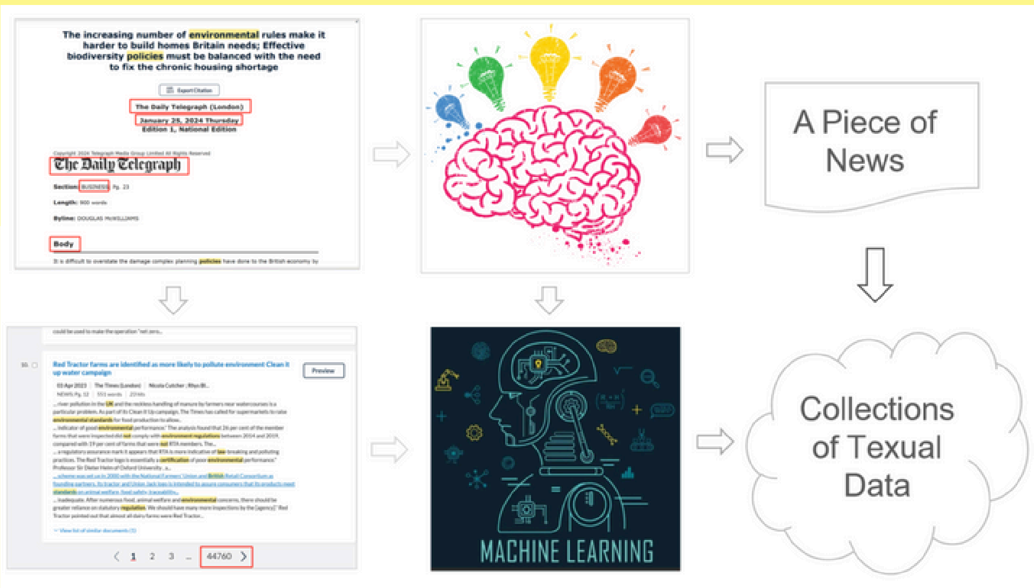
Figure – Examples of ordering which can occur in HEAs. (left) disordered solid solution – some short-range ordering present. (middle) B2 long range ordered structure – NbTa and MoW sublattices. (right) Long range ordered structure. Images generated by Dr. Christopher Woodgate.

Unlocking the power of BlueBEAR for social science research

Shuyu Li - PhD student

Shuyu Li, a PhD student in Environmental Economics at the University of Birmingham, is leveraging the BlueBEAR High-Performance Computing (HPC) cluster to tackle complex environmental economics problems. Her research focuses on applying Machine Learning (ML) techniques to analyze the evolution of environmental policies and evaluate their impacts. By using advanced ML models like BERT and T5, Shuyu can process large datasets of text, such as online news articles, to identify and classify content related to environmental policies. The computational power and storage capabilities of BlueBEAR have been crucial in making her work feasible and efficient, transforming her workflow and allowing her to focus on refining research questions and interpreting results

The integration of ML and HPC has opened new avenues for social science research, enabling the analysis of vast and diverse datasets, including news articles, videos, conference transcripts, and social media imagery. BlueBEAR provides a comprehensive ecosystem that supports researchers at every stage of their projects, offering reliable data storage and powerful GPU resources. This has been particularly beneficial for Shuyu, as it has allowed her to manage terabytes of data securely and accelerate her research significantly.

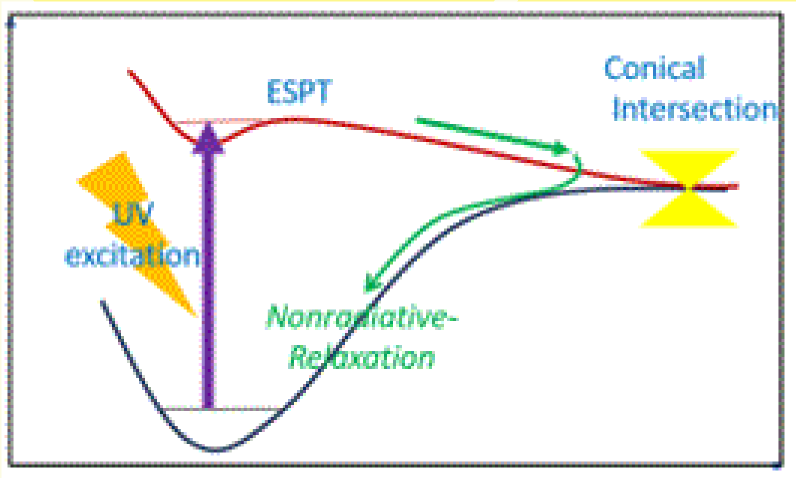


Molecular Photophysics: a connection between Theoretical Chemistry and Ultrafast Spectroscopy

Dr Reza Omidyan - Associate Professor

Reza Omidyan, an associate professor of Physical Chemistry, is utilizing the BlueBEAR High-Performance Computing (HPC) cluster to study molecular photophysics. His research focuses on predicting the photophysical properties of biological and chemical compounds, such as photostability, photoisomerization, and photoswitching. These properties are crucial for applications in health and material sciences, including sunscreens and photostabilizers. Reza employs high-level ab initio and nonadiabatic dynamics (NAD) simulation methods to determine optimized geometries, electronic structures, and potential energy surfaces of large molecules

The BlueBEAR HPC cluster is essential for running hundreds of trajectories in NAD simulations, which track the evolution of excited state populations over time. These simulations address critical questions about photoisomerization and relaxation mechanisms. For example, Reza's research on the molecule Astragalin revealed that its deactivation mechanism involves an excited state proton transfer followed by ultrafast internal conversion. The computational power of BlueBEAR makes these complex calculations feasible, enabling significant advancements in understanding the interaction of light with matter.



Deactivation mechanism proposed for this system.