

# HetSys Matters

NEWS FROM THE EPSRC DOCTORAL TRAINING CENTRE IN THE MODELLING OF HETEROGENEOUS SYSTEMS (HetSys)

## CDT Directors' Update

Welcome to the third edition of HetSys Matters! It has been a busy year for the HetSys Centre for Doctoral Training (CDT) and we have lots of exciting news to report. Since the last edition, our first cohort of students have completed their studies and moved into a range of academic and non-academic roles. Cohort 2 are busy writing their theses this summer. Cohort 3 have all successfully completed and been awarded their Postgraduate Diplomas in Modelling of Heterogeneous Systems. Many of our students have been presenting their work at a variety of national and international conferences, which you can read more about on page 3.

We're also pleased to report that HetSys has been renewed with the award of £7 million in funding from the EPSRC for a further five cohorts of entry. Over the next 8 years HetSys II will train 50 further PhD students to use computational modelling to tackle pressing global sustainability challenges including accessing clean fusion energy, controlling infectious diseases and designing energy-efficient devices such as new battery electrolytes.

The new CDT has an expanded team spanning seven departments and three university research centres, forming a national centre of excellence in computational simulation. PhD students in the Centre will work closely with industry and with international partners, gaining valuable experience in doing so. HetSys II will have 21 industrial partners (15 new since HetSys I), seven institutional and 17 international partners who have identified similar challenges; three of these partners took part in the recent Study Group described on page 4

The new Centre builds on the successes of the first phase of HetSys, and will take advantage of the ongoing artificial intelligence revolution by training students in research software engineering, uncertainty quantification and scientific machine learning. It will have new cross-cutting themes in modelling of biological systems, development of new simulation algorithms, and analysis of materials, linking mathematical modelling projects with experiments. The news comes as part of the Engineering and Physical Sciences Research Council's (EPSRC) recent announcement of £1 billion funding for 65 Centres for Doctoral Training (CDTs) across the UK.

Finally, we report some changes in the HetSys management team. James has taken over as Director of the CDT as of October 2023, with Julie moving to the Co-director role to continue to provide support for HetSys students. With the formal launch of HetSys II in October 2024, Nick Hine and Livia Bartok-Partay will take up roles as Deputy Directors of the new CDT. We will also welcome Tom Hudson as incoming Director of Postgraduate Studies, plus Heather Turner, Victoria Jelcic and Phill Stansfeld to the management team as co-investigators in the new CDT (in addition to continuing co-investigators Peter Brommer, Lukasz Figiel and Julie Staunton).

**James Kermode and Julie Staunton**

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“The best part of HetSys for me is the supportive research community. I owe a lot of my success to the many discussions and conversations with peers across departments and research groups, and I'm excited to see the family continue to grow.”

Tom Roche, Cohort 3

## New Supervisors

**We are delighted to announce that we have new supervisors joining HetSys later this year:**

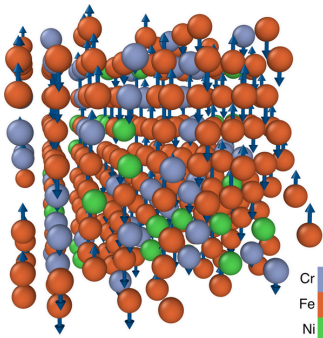
Michael Faulkner, Engineering  
Katarzyna Macieszczak, Physics  
Gareth Roberts, Statistics  
Alex Robertson, Physics  
Dimitri Veras, Physics

## New Contacts

Sarah Jarratt joins us from the Department of Physics to take up the role of CDT Administrative Officer for HetSys

## Theoretical insight meets data driven approaches

### HetSys students carry out pioneering new research on magnetic alloys



In a fantastic example of cross cohort collaboration, Lakshmi Shenoy (Cohort 2) and Chris Woodgate (Cohort 1) are lead authors on a new research article published in *Physical Review Materials*. The research work, which also involves international collaborators at EDF R&D in Paris and the University of Lille, combines first principles and machine learning modelling of stainless-steel alloys used in nuclear power plants. Linking theoretical insight with data-driven approaches gives a good balance of accuracy and transferability. Combining ideas from their respective PhD projects has led to the first joint publication between their research groups.

Chris joined HetSys Cohort 1 from Warwick's MMathPhys course for a project on the quantum physics of magnets. Lakshmi joined Cohort 2 from an MSc in applied mathematics at KCL to work on the ENTENTE Horizon 2020 co-funded project applying atomistic modelling to nuclear materials. In Chris' second year and Lakshmi's first year they took the cross-cohort PX918 Electronic Structure Theory for Experiment and Models training module to develop their electronic structure skills. Lakshmi also took PX920 Micromechanics of Materials to provide continuum scale fracture modelling skills needed for her project, while Chris chose a module on the mathematics of machine learning. Lakshmi has contributed to teaching PX914 Predictive Modelling and Uncertainty Qualification module and Chris with PX911 Quantum and Atomistic and PX912 Continuum and Mesoscale Modelling modules. They worked together on the student-initiated Multiscale Musings podcast. These activities helped to establish the scientific relationship needed for a fruitful collaboration.

Speaking about the research Lakshmi said "Discussions with Julie [Staunton] and Chris brought a physics perspective to a project that was originally more machine learning focused, and that helped us come up the new approach to model collinear spins. It's great to be part of a CDT where we can have such discussions with scientists working in related but different fields, as that can bring out new insights from angles we may not have considered before."

This research received funding from the HetSys CDT and the ENTENTE consortium and computing resources from IRENE at TGCC via PRACE, ARCHER2 via the UKCP consortium, the Sulis tier 2 facility and Warwick HPC facilities run by the Scientific Computing Research Technology Platform.

**About the Authors:** **Lakshmi Shenoy** is a 4th Year PhD student in the HetSys CDT, **Chris Woodgate** is a former HetSys cohort member and a Post-Doctoral Researcher at Warwick, **Julie Staunton** is a Professor in Theoretical Physics and a co-Director of HetSys and James Kermode is a Professor of Materials Modelling and Director of HetSys.

**Publication Details:** Lakshmi Shenoy, Christopher D. Woodgate, Julie B. Staunton, Albert P. Bartók, Charlotte S. Becquart, Christophe Domain, and James R. Kermode. *"Collinear-spin machine learned interatomic potential for Fe7 Cr2 Ni alloy"*

**Phys. Rev. Materials** 8, 033804 (2024); doi.org/10.1103/PhysRevMaterials.8.033804

## Eat, Sleep, Code, Repeat

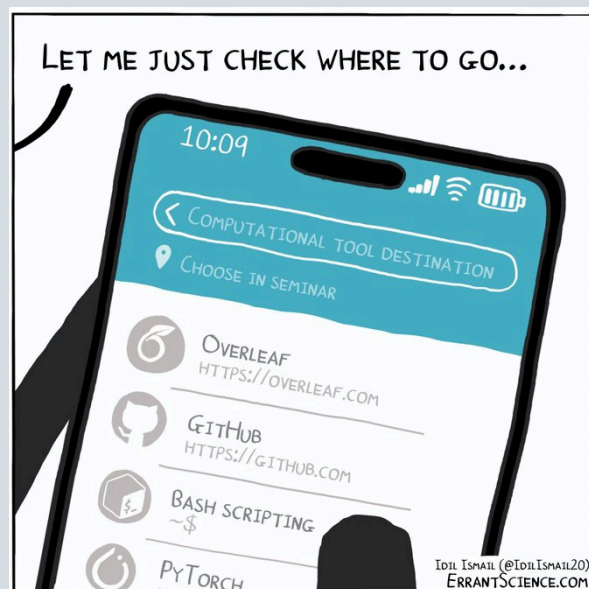
### Tips for Early-Career Researchers in Computational Science

With the increasing influx of students from diverse backgrounds joining the ever-popular field, this short guide aims to help students navigate through the various computational techniques that they are likely to encounter during their studies.

Covering a broad spectrum of techniques, including Bash scripting, scientific programming, and machine learning, among other fields, this paper is structured into nine sections, each introducing a different computational method.

This fantastic initiative of the HetSys CDT, Maths and Diamond CDT UoW students listed below is now online (arXiv.org) and published in the European Physical Journal Plus.

**Publication Details:** I. Ismail, S. Chaudhuri, D. Morgan, C.D. Woodgate, Z. Fakhoury, J.M. Targett, C. Pilgrim, C. Maino  
 "Eat, sleep, code, repeat: tips for early-career researchers in computational science"  
**The European Physical Journal Plus** Volume 138, article number 1094, (2023) (arXiv.org)



# HetSys Presents...

Our students and colleagues have attended many conferences and workshops this year presenting their work on national and international stages. Below **Chantal Baer**, a cohort 4 student talks about her time at the Faraday Institution Early Career Researchers conference and the opportunity to present her own work:



"Earlier this year I attended the Faraday Institution Early Career Researchers conference. Targeted mainly at PhD and postdoctoral researchers in the battery sector, the conference consisted of a mix of talks, training sessions, panel discussions, and a careers café. In contrast to most other academic conferences, invited keynote speakers didn't focus on their latest research but gave overviews of their career journeys, highlighting challenges they faced along the way, and sharing lessons they learned in overcoming them.

"This insight into the academic world was extremely valuable, especially when it comes to making decisions about the next step, and in my opinion such open discussion about career paths within academia should be encouraged more.

"With a focus on skills development they offered a wide range of workshops such as intellectual property, project and time management, fellowship applications, writing of academic papers, even how avoid imposter syndrome. Being quite early in my PhD journey, I chose the 'Paper Writing Masterclass' by Nature which was very informative, and the knowledge acquired will be very useful when writing my first paper.

"Talking about science was left to the early career researchers, many contributed by presenting a poster or giving a talk in one of four parallel sessions covering a huge range of different topics within battery research. I gave my first presentation of my work, this was a personal highlight for me and actually more fun than expected!

"A key part of the Faraday Institution is facilitating the connection between academia and industry, since getting the battery sector ready for net zero by 2030 is a combined effort. Getting insights into the world of industry and networking with representatives from different companies was key. One of the panel sessions had CEOs and R&D managers of three battery start-up companies to give insight into the differences between academia and industry and showcase their respective career journeys.

"Ending with a careers café and networking opportunities I appreciated the opportunities the event had provided for early career researchers. The skills, insights and networking opportunities I obtained during the two days will be very valuable for my future career."

## HetSys Community

The HetSys Coffee Club was born out of a CDT-wide Research Discussion meeting in early 2023 with a goal of encouraging collaboration within HetSys, especially across cohorts and research themes. It was felt that informal catch-ups between friends proved a successful approach, and that a shared weekly forum might be desirable. Since then, the 'HetSys Coffee Club' has been a good source of research conversation with regular members from several university departments and a great starting point for new cohorts.

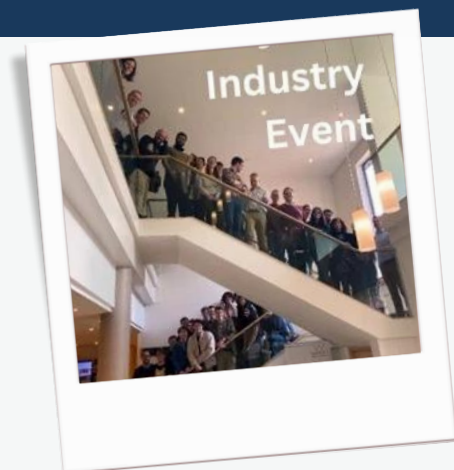
The HetSys Coding Challenge was the invention of Cohort 3 student, Tom Rocke with support from James Kermode and Julie Staunton. Each term, Tom endeavours to set reasonably short coding tasks for the CDT to solve, with the aim of creating a fun shared experience that is accessible to all. Tom hopes that it ends up as an enjoyable staple of the HetSys community, and that it might even go beyond the CDT and reach the wider university.

## Presentation Prizes and Awards

**Chris Woodgate** was selected as this year's recipient of the Winton Capital Thesis Prize for Physics. This annual award is given by the Physics department to recognise an outstanding PhD thesis examined in the preceding calendar year His thesis is entitled 'Atomic Arrangements in Multicomponent Alloys: First-Principles Theory, Atomistic Modelling, and Implications for Magnetic Properties' and was supervised by Julie Staunton. Currently working as a postdoctoral researcher in Julie's group in Physics, Chris is expanding upon the programme of work carried out in his PhD and collaborating with the research group of Laura Lewis' at Northeastern University in Boston, USA.

Several members of HetSys recently attended the 16th conference of Computer Simulation of Irradiation Effects in Solids (COSIRES) in Kingston, Canada. Congratulations to **Fraser Birks** who was presented with the award for Best Student Presentation for his talk "QM/MM Style Mixing of Machine-Learned Interatomic Potentials to Accelerate Simulations".

Held every two years COSIRES is a leading venue for presenting and discussing recent advances in the computational investigation of materials phenomena caused or influenced by all forms of irradiation. A field that connects cascade formation to irradiation creep is necessarily at the forefront of computational and experimental materials science, often driving innovation in advanced techniques across a vast range of time and length scales.



## HetSys Industry Study Group

April saw our fifth Industry Study Group. Building on previous successful events we welcomed a multidisciplinary research audience of HetSys staff and PhD students plus industry partners AWE, Johnson Matthey and Syngenta.

These three companies presented their challenges to our students and academics, who broke into groups working together and sharing their skills over the next three days to code, model, and sketch solutions to the problems.

Misbah Sarwar, Rachel Kerber and Carlos Fonte represented Johnson Matthey, a global leader in sustainable technologies bringing their chemistry and engineering backgrounds to the event and asked the group to explore machine learning approaches to modelling chemical reaction networks. Misbah Sarwar, Senior Principal Scientist explained that *“the industry day was a great opportunity to explore the use of novel Machine Learning based approaches for studying a range of catalytic systems and processes. We were very impressed by the depth and breadth of the solutions proposed and the student’s ability to think swiftly and solve complex problems efficiently while collaborating and innovating”*.

All involved brought their expertise, enthusiasm and ideas to the table and demonstrated the power of collaborative working. We hope that several of these challenges will feed into PhD projects for future HetSys cohorts.

## Theory to Application: a Cutting-Edge Secondment with Vanellus

**Earlier this year Oscar Holroyd (cohort 3) undertook a three month secondment in Industry.**

Vanellus (vanellus.tech) are building a ‘next-generation physics solver’, a new physics simulation written from the ground up integrating novel machine learning research and modern numerical programming approaches. Oscar was to use his range of programming and mathematical skills to contribute to developing their core solver, he tells us more below:

“After a rush to meet a tight deadline, my supervisors and I were fortunate enough to be successful in our application for a UKRI Impact Acceleration Account grant to fund a three month collaboration between the University of Warwick and the fluid dynamics start-up, Vanellus.

“Although the busy Cambridge commute and the fixed working hours came as a bit of a shock, I had a very fruitful 12 week stint working with Laurence Cullen, Michael Negus, and Aditi Roy.

“The plan for the placement was to try and use Vanellus’ fully-differentiable GPU-based fluids solver to machine-learn control policies, reflecting the analytical approach that my PhD takes. Although it took a little while to get my head around their codebase, I really enjoyed working on a large piece of industrial software as part of a group. The contrast between this and poorly documented, hard to understand academic codes (often including my own!) was a real treat. I’m hoping that I can take this back with me into the scientific computing I do now I’ve returned to the PhD.


“I ended up doing more work on the core solver than expected, adding features and speeding up the code to open up a wider range of problems to try and tackle with machine learning. We ended up focussing on trying to move regions of fluid tagged with a tracer to target locations with feedback controls. Despite the best efforts of the computer – which stubbornly insisted on exploiting glitches at boundary conditions to cheat the simulation – we eventually managed to corral it into success to round off the three months away.”

**EPSRC Centre for Doctoral Training in the Modelling of Heterogeneous Systems (HetSys)**

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