

HETSYS MATTERS

NEWS FROM THE EPSRC CDT IN MODELLING OF HETEROGENEOUS SYSTEMS

CDT Directors' Update

Welcome to the sixth edition of HetSys Matters.

It's been another busy and exciting year for the HetSys Centre for Doctoral Training, and we're delighted to share a snapshot of what our community has achieved.

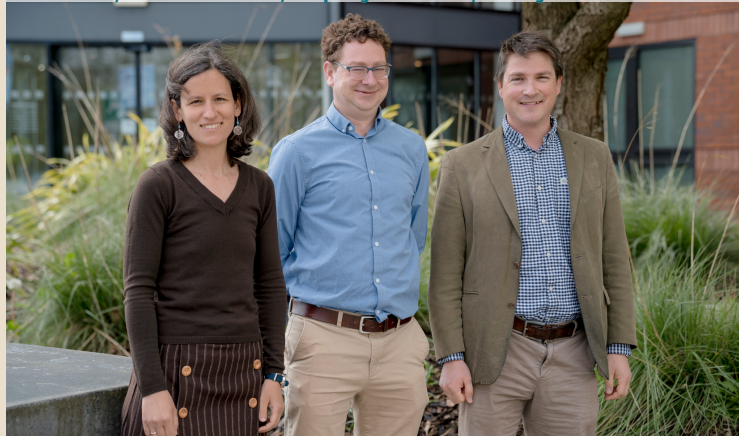
Our students continue to make a strong impact: presenting at international conferences, publishing high-quality research, and earning awards for their contributions to computational modelling. We're also looking ahead to welcoming Cohort 8, our largest yet, of 15 students, a clear sign of the CDT's growing strength and reputation.

One of the standout moments this year was our Industry Study Group, bringing together researchers from across Warwick to tackle real-world challenges set by Amentum, JLR and James Walker. Working closely with industry, students developed innovative solutions across energy materials, battery technology and advanced manufacturing, highlighting the power of interdisciplinary collaboration.

Outreach and engagement have been a major focus. From the Resonate Festival to the Big Bang Fair and local activities, our students have inspired future scientists and engineers while sharpening their own communication and leadership skills.

Closer to home, our HetSys Happenings event explored the importance of impact and science communication, while the ever-popular summer barbeque brought students and staff together for sunshine, rounders and a strong sense of community.

L:R Livia Bartók-Pártay, Deputy Director; James Kermode, Director; Nicholas Hine, Deputy Director, HetSys



We've also embraced new opportunities in cutting-edge technology. Access to Isambard-AI, one of the world's most powerful AI supercomputers, is opening up exciting possibilities in machine-learned interatomic potentials and computational materials science. During July we will hold our HetSys Annual Conference, where our community will come together to showcase the latest research. We'll also be celebrating a major milestone as Cohort 3 graduate later this summer, marking the next generation of HetSys researchers moving into careers across academia and industry.

Finally, thank you to our students, supervisors, partners, alumni and colleagues, HetSys thrives because of you.

James Kermode, Director - HetSys Centre for Doctoral Training

A Summer Evening of Food, Fun and Friendly Competition

HetSys students and academics took time out in late June to connect beyond their research, enjoying a barbeque and a relaxed game of rounders in the summer sunshine.



Industry Study Group: modelling innovative solutions



Three teams of HetSys researchers spent three days developing innovative solutions for Amentum, JLR and James Walker at our Industry Study Group.

The annual Industry Study Group is an important date in the HetSys diary. These type of study groups have been a tradition for over fifty years, originating with pioneering work in the UK during the 1960s and continue to provide valuable problem-solving and insights for a wide range of organisations.

We invite our industry partners to present challenges they'd like assistance with. In response, our HetSys academics, postdoctoral researchers and PhD students collaborate over three days to devise, model, code and compute solutions to these complex problems using a variety computational and mathematical techniques and theories. This event really demonstrates the highly collaborative and interdisciplinary nature of HetSys.

On the final day, the teams present their ideas, with the goal of providing companies with data they can use to advance towards a solution, or to potentially spark a new PhD project through HetSys.

"We were extremely impressed by the scientific ability and motivation that the students brought to the study group. Their results will have direct impact on the development of our engineering-scale materials models. The event provided an excellent opportunity to engage with early-career researchers and explore state-of-the-art modelling approaches."

Peter Hatton, Amentum

In April, the HetSys Centre for Doctoral Training hosted its annual Industry Study Group (ISG) at the University of Warwick's Radcliffe Conference Centre.

The event brought together 40 researchers, including HetSys PhD students, postdoctoral researchers and academic staff, to tackle real-world challenges posed by three industrial partners: Amentum, JLR and James Walker.

Working in self-organising interdisciplinary teams, participants were given just three days to develop solutions to complex industry problems. Beginning with a challenge statement, access to relevant data and a shared development environment, each team worked intensively to produce prototype tools, benchmarked results and proposals for future research directions.

"It was great to work collaboratively at pace on a challenge with significant industrial relevance. We were very pleased with the contributions we were able to make over the three days."

Matt Christensen, HetSys Cohort 5 (Year 3)



"The ISG team did a fantastic job working with limited real-world laboratory data. I was particularly impressed by their willingness to listen, understand the challenge and ask insightful questions throughout the event. A big thank you to HetSys for organising such a valuable collaboration."

Andrew Douglas of James Walker

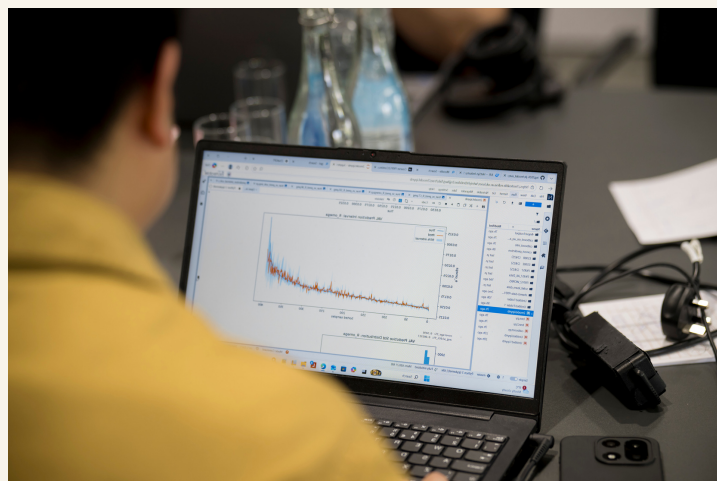


Addressing Challenges Across Three Sectors

The challenges spanned nuclear engineering, battery technology and advanced elastomer materials, showcasing the breadth of expertise within the HetSys community.

For Amentum, the team investigated machine-learning interatomic potentials for radiation-tolerant FeCrAl nuclear alloys. Researchers developed a reproducible testing framework to compare different modelling approaches and identified chromium precipitation as a likely contributor to material ageing, consistent with experimental observations. The team also demonstrated how active-learning techniques could be used to improve model performance using targeted density functional theory calculations.

The JLR challenge focused on predicting battery state-of-health using electrochemical impedance spectroscopy. The team developed a machine-learning workflow capable of extracting physically interpretable features from impedance data and using them to predict battery degradation. Alongside this, researchers explored a Neural ODE approach capable of modelling the full impedance spectrum, laying the foundations for future predictive studies of battery ageing and performance



"Great to take part in such an inspiring event and see the impact of collaborative, interdisciplinary research! This was a fantastic showcase of how academia-industry collaborations can accelerate innovation. In just three days, the team delivered practical, well-structured outputs that effectively balance data-driven models, physical insights, and system-level integration for next-generation battery pack design in electric vehicles."

David (Weiqun) Li, JLR



Developing Future Research Opportunities

Beyond delivering technical solutions, all three teams identified promising directions for future collaborative research, many of which align closely with the HetSys training programme and could form the basis of future doctoral projects.

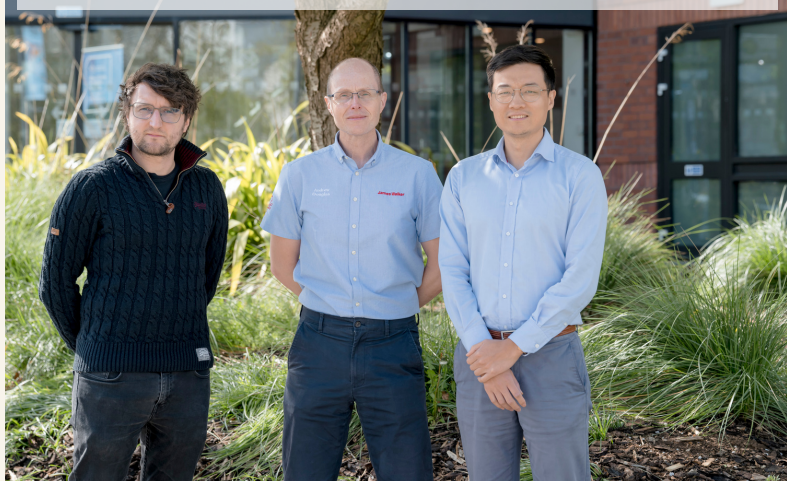
The HetSys CDT extends its thanks to colleagues from Amentum, JLR and James Walker for providing the challenges, data and expertise that made the event possible, as well as to all participating students and staff. The CDT also gratefully acknowledges the support of the Engineering and Physical Sciences Research Council (EPSRC).

If you would like to find out more about how you could take part in our next study group, please get in touch by emailing hetsys@warwick.ac.uk.

"Collaborating with industry to apply my research skills to a new area has been incredibly rewarding. The fast-paced, team-driven nature of the project made it a truly engaging and impactful experience."

Luca Seafood, Cohort 6 (Year 2)

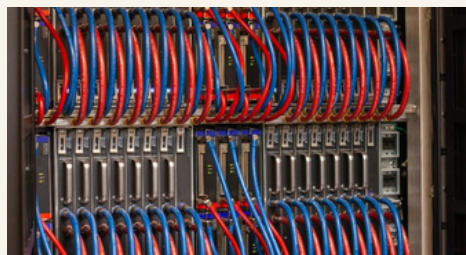
L:R Peter Hatton of Amentum, Andrew Douglas of James Walker and David (Weiqun) Li of JLR



HetSys Students Tap into Isambard AI Power

Students in the HetSys CDT recently gained access to the UK's new, leadership-class supercomputer Isambard-AI, one of the world's most powerful computers (11th in the Top 500 list in 2025). Nicholas Hine, James Kermode and Bora Karasulu, along with Chris Skylaris at Southampton, were awarded funding via UKRI's "AI for Science" scheme as part of the "AI Research Resource" for a project to apply Machine Learned Interatomic Potentials to Simulation of Interfaces in Energy Materials.

HetSys students including Luca Seaford, Fraser Birks, Chantal Baer, Roman Shantsila and Matt Nutter have already made good use of this exciting new resource, which contains the new Nvidia Grace Hopper GH200 Superchips, combining powerful GPU and CPU compute integrated in the same system. These are absolutely ideal for the combination of large-scale DFT for generating training data, training MLIPs and then running Molecular Dynamics for studying these interfaces. Efficient MLIP training requires a "closed-loop" on one machine, where workflows iterate over training data DFT, MLIP training, running MD with the MLIP for more training data, until the MLIP is sufficiently accurate for longer-timescale MD.



Just one Isambard-AI cabinet contains enough Nvidia GH200 Grace Hopper Superchips to outperform the ARCHER2 supercomputer.

Machine-learned interatomic potentials (MLIPs) are transforming computational materials science, enabling quantum-accurate simulations at unprecedented scales. Interfaces control the functionality of all energy materials, from batteries, fuel cells and electrocatalysts, to materials for fusion containment. The simulations planned will address critical challenges for the UK's clean energy transition: electrochemical interfaces governing battery and catalysis performance, and structural integrity of materials for fusion energy and safety-critical applications. What links the four workpackages of the project is production MD simulations at substantial lengthscale: 10-100s of nanometers, meaning 10^3 - 10^5 atoms, and long timescales: 10^3 - 10^6 picoseconds, with a timestep 1-10 femtoseconds, which is revolutionary for ab initio-quality MD!

HetSys Research Afternoon - showcasing student research and progress

The Annual HetSys Research Afternoon provides students with an opportunity to present updates on their current research, reflect on technical and practical challenges encountered during their PhD projects, and exchange ideas with fellow researchers working across a wide range of computational and interdisciplinary fields.

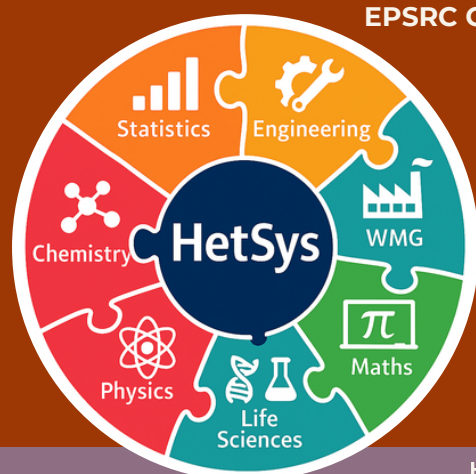
A key focus of the event is to encourage collaboration and open discussion between cohorts, creating a supportive environment where students can explore creative approaches to research challenges and learn from one another's experiences. The event also offers valuable opportunities for networking, interdisciplinary discussion, and community building within the CDT.



This year, the Research Afternoon welcomed participation from students across multiple cohorts, including four incoming members of Cohort 8, who are due to officially join the CDT in October 2026. Their attendance provided an early opportunity to engage with the HetSys research community and gain insight into the breadth of research activity taking place across the programme.

One of the highlights was the presentation delivered by Roman Shantsila (Cohort 5, year 3) who was awarded Best Talk within his session. Roman presented research focused on atomistic modelling of solid-state electrolytes and sulphur cathode interfaces, discussing his experience working with both foundational and custom Machine-Learned Interatomic Potentials, including active learning approaches and methods for comparing models using geometry optimisations, molecular dynamics, and phonon calculations.

The event showcased the high quality and diversity of research taking place across HetSys CDT and reinforced the importance of creating spaces where students can openly discuss ideas, share challenges, and build interdisciplinary connections.



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