HetSys Welcome Week 2023

EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

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HetSys Welcome Week 2023

James Kermode (School of Engineering), HetSys Director
Julie Staunton (Department of Physics), HetSys Co-Director
Nick Hine (Department of Physics), HetSys Director of Postgraduate Studies
Sarah Jarratt (School of Engineering), HetSys CDT Administration Officer

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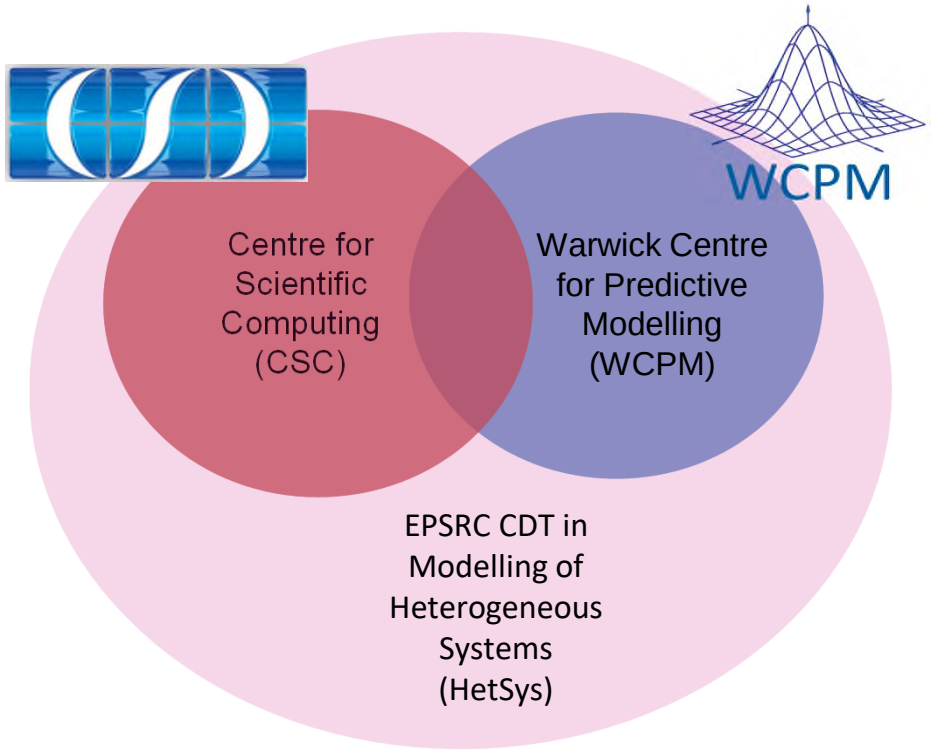
HetSys Community



Whole community together for lunchtime seminars every Monday, 1-2pm

Management Team
Julie Staunton (Phys)
James Kermode (Eng)
Nicholas Hine (Phys)
Sarah Jarratt (Admin)

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+ rest of core team of PhD supervisors

Chemistry
Livia Bartok-Partay
Scott Habershon
Bora Karasulu
Becky Notman
Reinhard Maurer
Gabriele Sosso
Phill Stansfeld

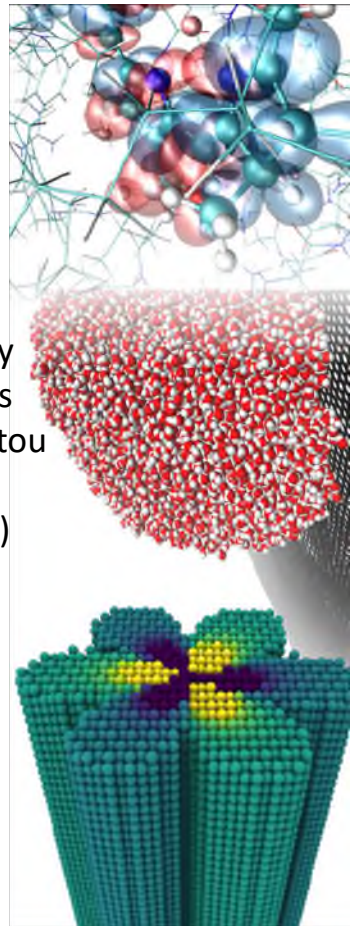
Physics
Tony Arber
Animesh Datta
David Quigley
Tom Goffrey
Ravi Desai

RSE (SC RTP)
Chris Brady
Heather Ratcliffe

Engineering
Peter Brommer
Duncan Lockerby
Phytos Neophytou
Hatef Sadeghi
Albert Bartok-Partay
Emmanouil Kakouris
Neophytos Neophytou

Łukasz Figiel (WMG)

Mathematics
Radu Cimpeanu
Thomas Hudson
Susana Gomes
Tim Sullivan
James Sprittles



HetSys Key Training Needs

1. Cross-disciplinary barriers, integrating modelling approaches

2. Assess reliability of results – uncertainty quantification

3. Emphasise robust, sustainable software development

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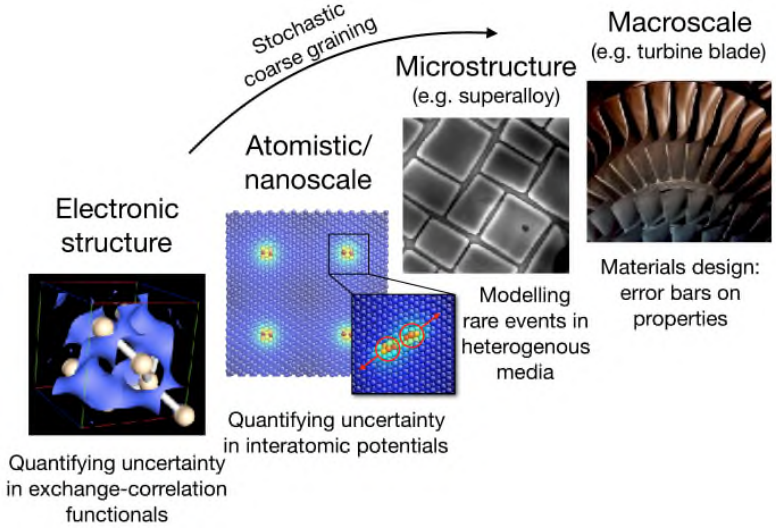

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PhD Projects 2023

EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

HetSys Welcome Week 2023

Julie Staunton (Department of Physics),
HetSys Co-Director

Student	Project	Primary Supervisor	Student Mentor
Minerva Schuler	Alternative protein sources: growing the next generation computational modelling framework	Radu Cimpeanu	Joseph Duque-Lopez
Matthew Christensen	Reliable quantum simulations of plasma and fusion physics	Animesh Datta	Ben Gosling
Nojus Plungė	Blending ultrasound data with physics-based models to predict damage in structural systems	Emmanouil Kakouris	Tom Rocke
Philip Jones	What's that made of? Modelling muonic X-ray radiation for quantitative elemental analysis	Albert Bartok-Partay	Seb Dooley
Roman Shantsila	(Inter)facing the Bitter Truth: How to Design Better Interfaces in Next-Gen Batteries using Atomistic Simulations Assisted by Machine-Learning	Bora Karasulu	Anas Siddiqui
Valdas Vitartas	Machine-learning quantum surrogate models to simulate energy transport across interfaces	Reinhard Maurer	Jake Eller
Y C Wong	Machine Learning Multiscale Simulation Of Photoconductivity In Correlated Oxides	Nicholas Hine	Fraser Birks
Yihui Tong	Developing the capability to forecast extreme Space Weather events	Ravindra Desai	Laura Cairns
Yuji Go	Complex Electronic Structures for Thermoelectric Energy Materials	Neophytos Neophytou	Matt Nutter
Zahra Bhatti	Charting a course towards new light-activated molecules	Scott Habershon	Chantal Baer

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Training Programme

EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

HetSys Welcome Week 2023

Nicholas Hine (Department of Physics),
HetSys Director of Studies

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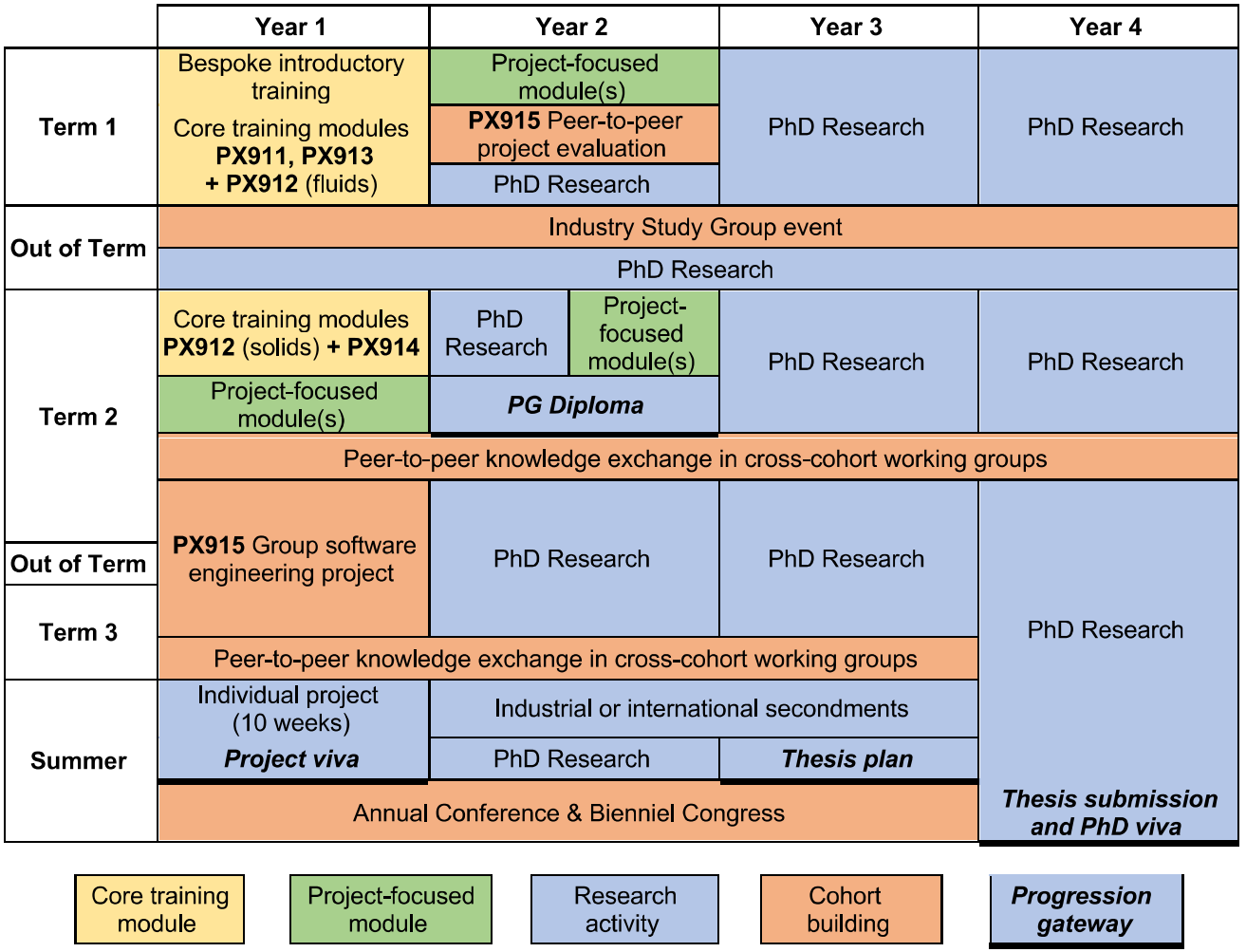
Overview of Training Programme

- Some elements of the CDT training will run throughout the four year PhD programme but most are concentrated in the **first 18 months.**
- Students associated with projects from the start, enabling **bespoke programme** for each student, with a **common core** ensuring a broad knowledge of multiscale modelling methods, plus high-level software engineering and UQ techniques.
- Training culminates in the award of a **Postgraduate Diploma** (PGCert and MSc also available as exit qualifications for those choosing not to progress to PhD).
- Years 2-4 predominantly research, with some cohort activities.



Core Modules:

PX911: Multiscale modelling methods and applications (15 CATS)

PX912: Multiscale modelling methods and applications II (15 CATS)

PX913: Introduction to Scientific Software Development (15 CATS)

PX914: Predictive Modelling and Uncertainty Quantification (15 CATS)

PX915: Software engineering group project; Peer-to-Peer Uncertainty Quantification Project (30 CATS)

Core Module Syllabus Overviews

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PX911: Multiscale modelling methods and applications I

Term 1, weeks 1-10

- Provides an introduction to atomistic modelling techniques including OFT, classical force field methods and an appreciation of how they interact with other modelling frameworks.
- Students will learn how to design atomistic simulations of condensed matter or molecular systems, and how to identify simulation methodologies appropriate to bridging multiple length scales, balancing accuracy vs. cost.
- Multiscale Modelling case studies by guest lecturers will show how problems involving heterogeneous systems are tackled at multiple length & time scales.

PX912: Multiscale modelling methods and applications II

Term 1, weeks 6-10, Term 2 weeks 1-5

- Provides a grounding in macroscopic and multiscale modelling techniques, emphasizing applications and the links between methods and across scales
- Lectures on foundations of continuum mechanics, thermodynamics, fluid dynamics, solid mechanics, and recent developments in multiscale fluid, plasma and solid mechanics
- Topics covered will range from the basics of continuum mechanics and thermodynamics concepts through to demonstrating the route from underlying models via algorithms to practical implementation in simulation packages.

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Core Module Syllabus Overviews

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PX913: Introduction to Scientific Software Development

Term 1, weeks 1-10

- Provides bespoke Software Carpentry training developed by our RSE group to ensure students understand the core principles of programming and software development, gain experience with writing, debugging and reading code in high- and low-level languages, and learn to use common tools for data analysis and visualization.
- Lectures will cover fundamental operation of a computer, use of version control, debugging tools, and approaches to group-based software development.
- Where necessary for individual projects, C or Fortran training will be provided, positioning students to follow further programming option modules, e.g. PX925: High Performance Computing.

PX914: Predictive Modelling and Uncertainty Quantification

Term 2, weeks 1-10

- Provides an introduction to predictive modelling techniques including statistics, machine learning, data analytics and data mining, essential for solving problems in the interdisciplinary area of predictive modelling.
- Lectures will cover random processes, statistical learning, Bayesian inference, Monte Carlo methods, model selection, and supervised and unsupervised machine learning techniques.
- Focus on scalable approaches to UQ and propagation in multiscale models, and concludes with an overview of Bayesian inverse problems

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Core Module Syllabus Overviews

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PX915 Part I: Software engineering group project
End of Term 2 to middle of Term 3

- Undertaken collectively by the cohort, with students designing, specifying, optimising and implementing a small-scale simulation package to model heterogeneous systems
- Examples include density functional theory, molecular dynamics, computational fluid dynamics and finite element analysis. Careful division of responsibilities and integration of work will be required.
- Module will include seminars on intellectual property and software licensing with input from Warwick Ventures, who commercialise innovations produced from research carried out in the University.

PX915 Part II: Peer-to-peer Project Evaluation (Year 2)
Around week 3, term 1 of year 2

- Builds on output of individual research projects: another cohort member will be assigned to evaluate the quality of a student's model error estimates and/or compliance with research software engineering principles
- Run models with an ensemble of inputs to enable sensitivity analysis, or on a selection of architectures, with opportunities for power-usage profiling.
- Software testers will be encouraged to discuss the process with the software authors, fostering dialogue across the cohort.

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Optional Modules:

- **At least 2 optional modules, to total 30 credits, including 15 credits from this list:**

PX917 Computational Plasma Physics (15 credits)

- **PX918*** Electronic Structure Theory for Experiment and Models (10 credits)
- **PX919*** Quantum Chemistry (10 credits)
- **PX923*** Biomolecular Simulation (10 credits)
- **PX925** High Performance Computing (10 credits)
- **ES98E** Scientific Machine Learning (10 credits)
- **IL939** Public Engagement (15 credits)

** These modules (PX918, PX919 and PX923) can be expected to run in 2024/25*

Please discuss best options to complement your PhD project with your supervisor.

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Other Optional Modules:

Any module of an appropriate level (usually 9- or 4- coded), for example:

MA6J1: Continuum Mechanics (15 credits)
MA933: Stochastic Modelling and Random Processes* (15 credits)
MA934 Numerical Algorithms and Optimisation* (15 credits)
MA930 Data Analysis and Machine Learning* (15 credits)

Core modules of the Mathematics of Real-World Systems (MathSys) CDT programme.

<u>These are pre-approved.</u>
<u>Others are subject to approval by supervisor, module leader and HetSys Director of Graduate Studies</u>

Computing

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You are being supplied with a Dell Laptop, which has been pre-installed with Ubuntu Linux and a range of scientific software packages. See:

https://warwick.ac.uk/fac/sci/hetsys/studentinformation/computing/

Please sign up ASAP for an SCRTP account:

http://www2.warwick.ac.uk/research/rtp/sc/desktop/myaccount

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Support:

- Stay in **regular contact** with your supervisor(s) and your student mentor;
- Approach module leaders **early** if you feel you are falling behind on a particular module, not understanding the material, or struggling in any way;
- Approach your supervisor or one of the HetSys management team (Julie, James or Nick) if you are having difficulties with the course **as a whole**.

We are all here to help!

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Useful Contacts

Julie Staunton (Department of Physics), Director
Room PS1.41, Physical Sciences, Department of Physics
J.B.Staunton@warwick.ac.uk

James Kermode (School of Engineering), Co-Director
Room D2.10, School of Engineering
J.R.Kermode@warwick.ac.uk

Nick Hine (Department of Physics), Director of Graduate Studies
Room PS1.40, Physical Sciences, Department of Physics
N.D.M.Hine@warwick.ac.uk

Sarah Jarratt (School of Engineering) CDT Administrative Officer, HetSy
sRoom F4.07, School of Engineering
hetsys@warwick.ac.uk

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Office Space

M NUTTER	
T ROCKE	
L SHENOY	
I BEST	

F BIRKS	Z BHATTI
A LEE	M CHRISTENSEN
G SOPPITT	Y GO
G ANIS	P JONES

N PLUNGE	**HOT DESK**
M SCHULER	R FOGHI
R SHANTSILA	Y C WONG
Y TONG	V VITARTAS

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You have all been allocated a desk in the [D2.15 open plan office space](), with docking stations for your HetSys laptops

Risk assessment for this area allows full occupancy. Full details of RA and online training courses to be completed before you work there will be sent out via email.

If you want to work elsewhere on campus, space is available in the Library or in the [Postgraduate Hub]()

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Welcome Week Schedule

EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

HetSys Welcome Week 2023

James Kermode (School of Engineering),
HetSys Director

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Monday 25th September	Tuesday 26th September	Wednesday 27th September	Thursday 28th September	Friday 29th September
10am - 12 noon **Welcome to Hetsys** Presentations from Julie Staunton, James Kermode, Nick Hine and Sarah Jarratt MAS 2.05/6	***Individual meetings with Supervisors and Mentors***	10am - 12 noon **Laptop Troubleshooting Session** MAS 2.05/6	10am - 12 noon **Mathematics Induction Session** MAS 2.05/6	**Informal activity**
12 noon - 1pm **Informal Lunch** MAS 2.05/6		2pm - 4pm **Python Programming Induction Session** MAS 2.05/6	2pm - 4pm **Quantum Mechanics Induction Session** MAS 2.05/6	
		6:00pm **Social Event** Radcliffe		**Informal Social Event**

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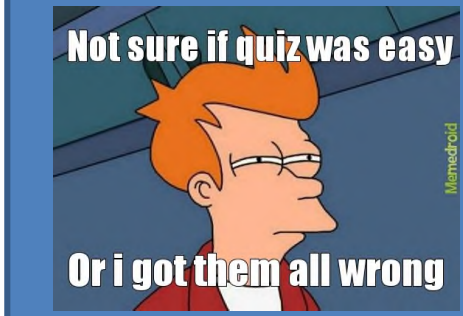

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Student Information Website

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https://warwick.ac.uk/fac/sci/hetsys/studentinformation/

includes Timetable, Induction materials and lots more

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Health and Safety

There are some University Health and Safety videos on Moodle that you should watch

Health & Safety Induction
Fire Safety Training
Display Screen Equipment

Information is linked here:
https://warwick.ac.uk/fac/sci/hetsys/studentinformation/induction/healthandsafety/

There are also tips on setting up your work environment

Up to date guidance from the University in relation to COVID-19 and support for those having to self-isolate on campus can be found here: https://warwick.ac.uk/coronavirus

These slides will be uploaded to the HetSys student information page.

Monday-Thursday
You can find me in
D215 or on Teams

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Administrative Matters

EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

HetSys Welcome Week 2023

Sarah Jarratt
CDT Administrative Officer, HetSys
School of Engineering

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Research Support and Training Grant

- Each student has a budget (£6000) for directly incurred costs required to carry out the PhD project such as travel to conferences, workshops and specialist resources.
- All expenses should be directly relevant to the PhD project's research outputs and must follow the University's expenses policy.
- Your individual expenditure code will be set up on the university's SAP finance system, which is to be used for all RTSG expenditure. https://warwick.ac.uk/fac/sci/hetsys/studentinformation/costcodes/
- It is your responsibility to ensure that you monitor their expenditure and do not exceed the budget allocation.

Research Support and Training Grant

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- Examples of allowable costs are:
    - *Software essential to your PhD*
    - *Books and other reading material not available in the library*
    - *Printing posters and lecture notes*
    - *PhD travel and subsistence for external conferences, workshops, short courses, summer schools*
    - *Support for internships where external partner is not able to support*

In additional to this, all students can either have a desktop computer or a docking station for their campus workspace from year 2 onwards

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Research Support and Training Grant

- Examples of ineligible costs are:
    - *Repair or replacement of your HetSys laptop*
    - *Costs of alcohol under any circumstances*
    - *Any costs incurred for moving to the UK, e.g. visa fees, health surcharge*
    - *Any costs incurred outside of your funding period.*

Further information can be found online:
https://warwick.ac.uk/fac/sci/hetsys/studentinformation/costcodes/

Research Support and Training Grant

Full guides to claiming expenses and booking travel can be found online:

https://warwick.ac.uk/fac/sci/hetsys/studentinformation/bookingguidance

I will run a workshop on this in term 2

Annual Leave

- Full-time PGR students are entitled to take a maximum of eight weeks/40 days holiday in the year (incl. the statutory (i.e. Bank Holidays) and customary University holidays).
- If a student is supported by a student visa, they must refer to the Immigration Team for advice prior to requesting a leave of absence as this may affect their visa.
- No single period of annual leave should exceed four weeks.
- No official monitoring through HetSys, just agree with your supervisor and keep a record of the leave you have taken – feel free to email HetSys@warwick.ac.uk if you would like me to keep a record