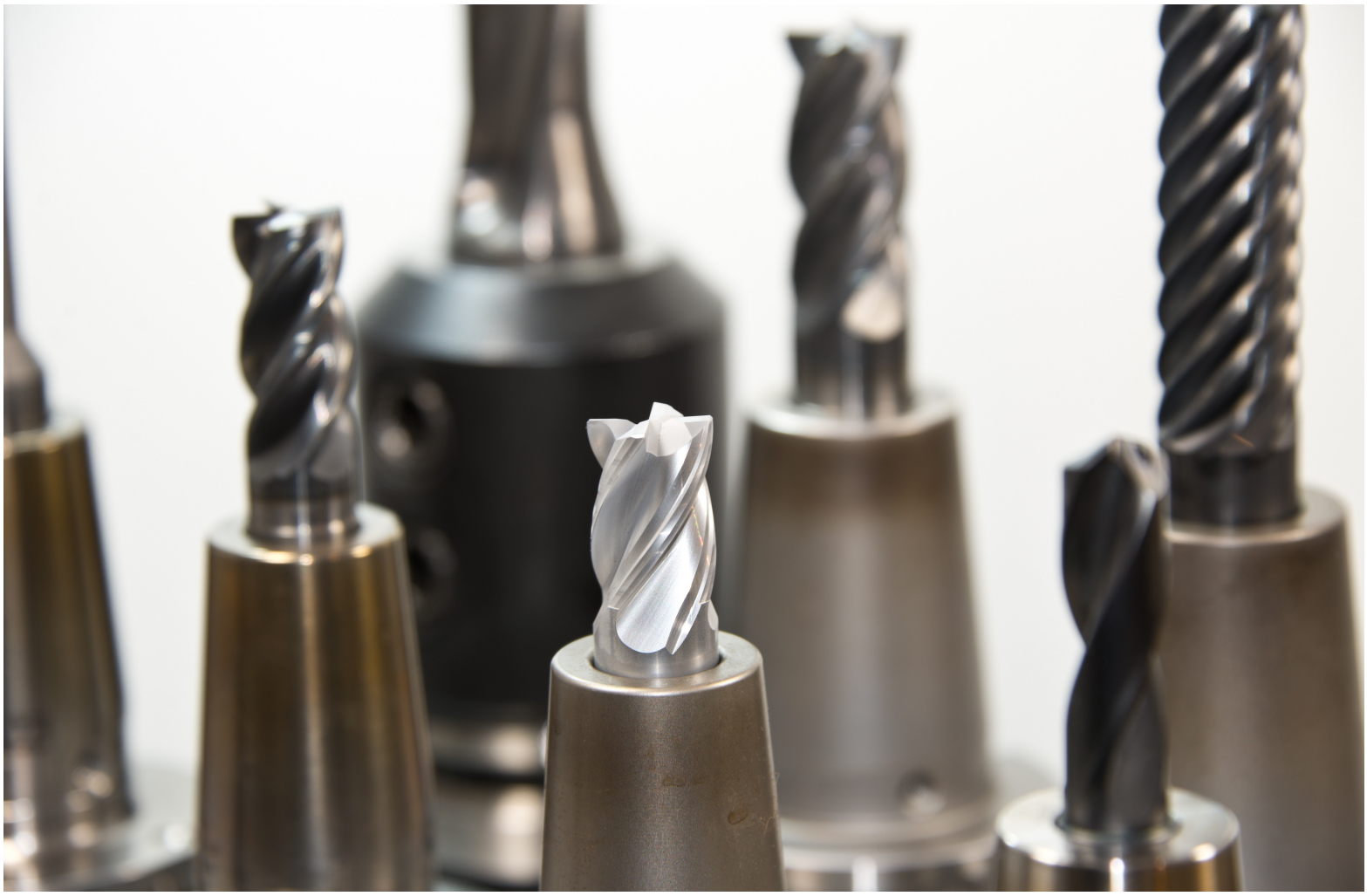


Fourth Uncertainty Quantification & Management with Industry

20th - 22nd March 2019

Innovate UK
Knowledge Transfer Network

UNIVERSITY OF LIVERPOOL

WARWICK

Contents

Problems posed by:

1 Study Group Information

The Study Group is an opportunity for industry to gain access to UK excellence in the fields of mathematics, statistics, engineering, and computer science. The structure of the Group allows for this to be done in a structured, intense session over three days.

1.1 Background

This Study Group with Industry is being run by the Warwick Centre for Predictive Modeling, and the Knowledge Transfer Network (KTN), with additional support from the University of Liverpool's Institute for Risk and Uncertainty.

Between 2014 - 2018, KTN ran the Uncertainty Quantification and Management (UQ&M) Special Interest Group (SIG). The SIG looked to draw together a UQ&M community and provide a structured meeting space where all the players could share their aspirations, knowledge and expertise.

Whilst formally wrapping up in 2018, the Study Groups have survived, and thrived in cooperation with the University of Liverpool's Institute for Risk & Uncertainty, and the University of Warwick. These Study Groups represent a vital part of the SIG's progress in identifying state of the art approaches to deal with industry problems and identify where there are UK strengths and weaknesses. It is expected that the outputs of the Study Group will be of great use to the industries posing specific problems, but also in the approaches generated, wider industry can get a sense of 'good practice' in an industrial context.

Over the course of the three years, the SIG has investment around £50,000 in activities held around the country, aiming to become a highly visible network for researchers and industrialist alike. From this investment we estimate below the values as returns on investment. We expect these values to increase as new introductions bear fruit, new ideas are implemented, and the less tangible benefits permeate into organisations.

- 11 case studies
- 12 Business to Research collaborations
- 300 SIG members
- 5 new studentships
- £40k for external money to SIG activities
- £258k of new projects initiated by the SIG

The primary mechanism we used in the SIG to drive B2R engagement was via the use cases generously supplied by our industry partners. These use cases were worked through in three

three-day Study Groups; two at the Institute for Risk and Uncertainty in Liverpool and one at the Warwick Centre for Predictive Modelling. Over these groups eleven problems were tackled encompassing aerospace, drugs discovery, automotive, and many more. These groups have bought together over 43 distinct organisations and over 175 unique participants; when added together these groups amount to over 1.5-person years of collaboration between businesses and researchers. Many of the solutions discovered at these Study Groups have created new research plans within industry and have led to collaborations with universities.

1.2 Who will be attending?

The Study Group will consist of researchers from various fields, including, but not limited to mathematics, statistics, computer scientists, and engineers. As well as university researchers, we strongly encourage registrations from Ph.D students, postdoctoral researchers and early-stage researchers.

As well as these researchers, the Study Group will be attended by industrial representatives limited to those offering problems to the group. **We are not accepting registrations from any industry not directly involved in the problems**. In addition to these attendees the Study Group will host a number of Public Sector representatives from the Research Councils, and Department of Business, Energy and Industrial Strategy. We expect to host around 60 people to this Study Group from across these sectors. Attendees can be found in Section 3.

1.3 How does it work?

The format of the Study Group will be following the highly successful European Study Groups with Industry. Industry present their problems on the morning of the first day to the Group. The researchers ask questions and choose which group they may be able to help with.

The groups (around 10 researchers per group) will move to their own working space. An academic Project Lead will be nominated. They will discuss with the group what aspects of the problem should be addressed, and how these may be approached. It is likely that the group will subdivide, but this will depend on the problem.

It is expected that the industry representatives will be on hand to answer questions, provide access to codes, data and generally ensure that the problem context is clear throughout the Study Group.

Conversations often continue during the evening, and as such the Study Group provides dinner for all delegates. This often provides an environment for cross-fertilisation of ideas between groups and disciplines.

Group work continues until the Friday lunchtime for final presentations. It is likely that the Project Lead will provide these presentations. Following the Study Group, the industry presenters will receive a report detailing what was done during the three days. Again, the Project Lead will coordinate this and draw on assistance from members of their team. The Project Lead will aim to get this report to the industrialist by the end of July 2019.

1.4 A Note Regarding Study Group Outputs

For researchers: all work demonstrated at this Study Group should be considered as open disclosure. All codes used to generate results should be made freely available to the working group and industrial partner. If you are not comfortable sharing code, please do not bring it to the Study Group.

For companies: it is understood that all insight and code generated over the course of the Study Group is research output. The research participants offer no guarantees on the code or results generated and therefore outputs are not expected to be ready for commercial application, it is not to be used in a commercial, or clinical setting. All data shared at this group will be considered open disclosure.

1.5 Agenda

	Tuesday 19	Wednesday 20	Thursday 21	Wednesday 22
09:00 onwards		Registration (D2.02 WCPM)	Group Work	Group Work
10:00		Welcome, Introductions and Problem Presentations (D2.02 WCPM)		
11:00			Tea and Coffee	Tea and Coffee
11:30		Group Work (Individual Rooms)	Group Work	Group Work
13:00		Lunch	Lunch	Lunch
14:00		Group Work	Group Work	Final Presentations (D2.02 WCPM)
15:30		Tea and Coffee	Tea and Coffee	Tea and Coffee
16:00		Group Work	Group Work	FINISH
17:00				
18:30 onwards	Pre-Study Group Drinks (Varsity Bar (on Campus)	Dinner (Pizzas at Engineering Department)	Dinner (Arden Conference Centre)	

1.6 Do I need to pay?

The sponsoring parties are grateful to Warwick School of Engineering, University of Warwick Impact Acceleration Account (IAA) for supporting the Study Group, and Innovate UK for sponsoring the Study Group through the KTN. We are pleased to cover delegates accommodation on the 19th - 22nd March, including breakfast and lunches. We do however ask for a nominal payment of between £ 15 - 35 depending on whether you are from the University of Warwick, or elsewhere. Additionally, we do ask that researchers and industrialists cover their own costs for travel to and from the venue.

1.7 Pre-Study Group Actions

To make sure the group progresses well, it is important that researchers read and study the problem statements provided by industry prior to the Study Group. It would be helpful for the researchers to have ideas on how they might approach **all** of the problems and be willing to work in any of the groups in case adjustments need to be made to balance capability and numbers in each group.

1.8 Check-in, Accommodation and Dinners

The organisers have arranged for a number of rooms to be held for Study Group members at Arden Conference Centre for the Tuesday, Wednesday and Thursday nights - requests for these should be indicated at Registration. These (en-suite) rooms include breakfast. Check-in time on the Tuesday is 16:00 and delegates should go to Arden Conference Centre on arrival. Buffet lunches will be provided at the WCPM, a buffet dinner will be available on the Wednesday night at the WCPM, and a conference dinner will be held on the Thursday evening (below).

For those traveling down on Tuesday, there will be an informal reception in the evening starting at 18:30 at the Varsity Pub. It will also be a good opportunity to discuss research ideas and how problems may be addressed in an informal manner.

1.9 Conference Dinner

The dinner on Thursday will be held at Arden Conference Centre at 19:00. Please arrive promptly at the bar in Arden from 18:30. Additionally, if you have not indicated to the organisers in your registration any allergies, we request that you do so as soon as possible.

2 Study Group Challenges

2.1 A Computational Framework to Address Materials Ageing Behaviour

Presenting Institution: Atomic Weapons Establishment

Problem Presenter: Mark Storr, Alexander Lewis, Phil Monks, Poppy Di Pietro

Overview: Modern computational methods such as those applied in Chematica [1] are able to take a target compound and successfully apply retrosynthetic techniques to determine practical synthetic routes. The aim is to identify routes which significantly improve on previous approaches, increase synthetic efficiency, or where previous synthetic attempts have failed. This project proposes to investigate a related application, i.e. determining the likely potential breakdown products for a given generic polymeric material using a combination of artificial intelligence, machine learning and modern computational chemistry.

Incorporating the long timescale (years) ageing behaviour of any proposed new material is a considerable aspect of the materials qualification process. Often such assessments rely on *prior art*, subject matter expert (SME) guidance or small-scale laboratory studies and hence can add significant cost to any manufacturing process. Furthermore, with the adoption of Registration, Evaluation, Authorisation restriction of Chemicals (REACH) legislation across the European Union (EU), there is a need to investigate a range of replacement materials. The ability to identify computationally the likely ageing behaviour of a given material species (in terms of breakdown products liberated and the timescales over which such processes occur) would be a significant step forward in the adoption of model-based assurance methodologies.

Challenge Statement: This project is based upon a self-contained decomposition mechanism for nitrocellulose ageing and is summarised below for which indicative rate equation information is available.

$$2\,\mathrm{HNO_2} \longleftrightarrow \mathrm{N_2O_3} + \mathrm{H_2O}$$
$$\mathrm{N_2O} \longleftrightarrow \mathrm{NO} + \mathrm{NO_2}$$
$$2\,\mathrm{NO_2} \longleftrightarrow \mathrm{N_2O_4}$$
$$\mathrm{N_2O_4} + 2\,\mathrm{H_2O} \longleftrightarrow \mathrm{HNO_2} + \mathrm{NO_3} + \mathrm{H_3O^+}$$
$$2\,\mathrm{HNO} \longleftrightarrow \mathrm{HON{=}NOH(trans)} \longleftrightarrow \mathrm{N_2O} + \mathrm{H_2O})$$
$$\mathrm{HNO} + \mathrm{NO_2} \longrightarrow \mathrm{NO} + \mathrm{HNO_2}$$
$$2\,\mathrm{NO} + \mathrm{O_2} \longrightarrow 2\,\mathrm{NO_2}$$
$$\mathrm{NO} + \mathrm{HNO_3} \longrightarrow \mathrm{NO_2} + \mathrm{HNO_2}$$

Simplified nitrocellulose ageing mechanism

In the first stage of the project it is proposed that a computational framework is derived to efficiently and accurately reproduce and confirm this reaction mechanism. This integrated framework should then be used to quantify the effects of uncertainty in the rate information regarding the ageing process over long time-scales and hence guide further study. Imperative in any solution is the ability to efficiently and accurately explore the sensitivity of the system to key material parameters.

In the second stage, the nitrocellulose parent is itself considered. Given the structure of a nitrocellulose monomeric repeat unit, can a computational framework be derived which is able to identify the likely key ageing mechanisms, and also predict the probability of individual reaction products appearing or accumulating within the system? Ideally this framework will be able to reproduce the results of stage one without prior knowledge of the true mechanistic pathway. This would provide confidence in future applications to other compounds.

[1] Klucznik *et al.*, Efficient Syntheses of Diverse, Medicinally Relevant Targets Planned by Computer and Executed in the Laboratory, *Chem*, **4**, 522-532, 2018.

2.2 Uncertainty Management Framework for Evolving Electrical Power Generation & Distribution Test Environments

Presenting Institution: BAE Systems Maritime - Naval Ships

Problem Presenter: Neil Harrison, Gordon McKinstry

Abstract (Technical Topics and Desired Outcomes): The desired outcome of this study group challenge is to develop a comprehensive framework for robustly handling the uncertainties that arise from a mix of stochastic and epistemic sources within an evolving system performance analysis environment. This analysis:

- starts with pure synthetic modelling, transforming data subject to various types of uncertainty and degrees of validation;
- growing to encompass cyber-physical hybrid elements, such that integrated hardware test results can be taken full advantage of via continuing analysis;
- finally incorporating gradually acquired sensor readings from the first complete real-world system, as it progresses through increasingly taxing in-service demands and contexts.

The overall aim is to generate clear understanding of the validity and bounds of the various analysis outcomes throughout, to underpin progressive assurance of system performance and extract maximum value from our models, alongside the programme of land-based and at-ship physical integration. The framework should be specific enough to inform data collection, pre-processing and analysis techniques, and abstract enough to be reapplied to other relevant areas of systems integration.

The provision of system assurance through land-based test & integration facilities is not a novel practice to de-risk system development and nor is the application of machine learning to handle uncertainty effects. However, the growing complexity, cardinality and software dependency that systems exhibit to meet stretching performance requirements makes the value of a framework for rigorously handling uncertainty across a gradually evolving landscape of models and real-world systems, an area of increasing importance in successful complex system design, development, delivery and in-service exploitation.

BAE Systems is delivering a £5.6 million contract to establish an Electrical Integration and Test Facility in Whetstone, Leicestershire, to enable critical de-risking integration tests for the Type 26 propulsion systems.

2.3 Understanding Metal Spray Deposition Variation

Presenting Institution: GKN Aerospace

Problem Presenter: Guillaume Saint-Cirgue, Tim Greenaway, Paul Clarke

Abstract (Technical Topics and Desired Outcomes): To develop the understanding and control algorithms through machine learning to dynamically control process input variables to maintain desired (fixed) output attributes of the metal spray process to reduce component key characteristic variation.

Challenge Statement: GKN Aerospace - Luton use flame spray with wire feed to create resistive circuits for electro thermal ice protection applications. The current processes are heavily reliant on either skilled operators or automation using a measure - spray - measure feedback loop to achieve the desired resistance element by element. The flame spray process is not repeatable, partly because the substrate "catch rate" can vary but also the deposition rate of the metal spray gun is variable.

Efforts have been made to reduce deposition rate variation by better control of process inputs including process gasses by mass flow controller and direct measurement of wire feed rate. This has improved variation but there are a number of variables outside of our direct control, which can contribute to deposition rate, including temperature and humidity and nozzle condition.

It is possible to directly measure and characterise the particles coming from the gun, and by adjusting the input variables this output can be controlled enabling compensation for external variables and ensuring a consistent deposition rate.

2.4 Probabilistic Frameworks for Nuclear Integrity Assessments

Presenting Institution: Rolls-Royce

Problem Presenter Michael Martin, Robert Marshall

Background: The Nuclear Industry has typically avoided probabilistic methods in structural integrity assessment as they are perceived to be less safe than deterministic design-code methods. Improved knowledge in the structural integrity field continues to highlight that the unquantified margins associated with current design-codes do not provide a consistent measure of risk. Consequently, optimal designs and the focus of effort or finance are constrained. Whilst safety remains the number one priority, life-cycle cost is also a key consideration. The benefit of probabilistic methods, in conjunction with target reliability acceptance criteria, is considered to be a more consistent approach for quantifying component margin. Subsequently, valuable opportunities for trading excess margin for simpler manufacture, Non-Destructive Examination (NDE) or analysis exist.

Challenge Statement: This case complements ongoing industry collaboration and international aspirations to change the perception of probabilistic methods. It is also well aligned with the aims described in the UK Government's June 2018 Nuclear Sector Deal. This case supports continuing regulatory engagement, codes and standards development and advancing capability and awareness in the use of nuclear structural integrity probabilistic methods.

This case considers a typical nuclear piping arrangement subject to thermal and pressure cycling. The system has an initial design life based on an anticipated operational transient history and a deterministic view of cyclic loading (pressure and temperature). This deterministic view is also used to set inspection intervals and the ensuing inspections are used to justify continued operation - this could be a highly conservative approach.

Questions to be Considered:

- How could structural reliability methods be used to extend the operational life of this system?
- Structural Health Monitoring (SHM) systems, where cracks are monitored in-situ (for example using ultrasonic techniques) are potentially useful here, also more sensors (eg temperature / pressure / other?) could potentially be employed. Is there an optimum data strategy? What are the implications to design and manufacture?
- How could a pragmatic engineering approach be developed that provides an up-to-date prediction of reliability of this system, what infrastructure / tools / research are required?

Resources Available for this Challenge:

- Geometry
- Design transient information (pressure, temperature, cycles)
- Operational history (pressure, temperature, cycles)
- Inspection history
- Fatigue initiation and crack growth data
- Target reliability

3 Participants

First Name	Surname	Institution
Antonios	Alexiadis	University of Liverpool
Gautam	Anand	University of Warwick
Mohd Haniff	Bin Osman	University of Birmingham
Liam	Birkinshaw-Doyle	University of Liverpool
James	Brixey	University of Warwick
Peter	Brommer	University of Warwick
Matt	Butchers	Knowledge Transfer Network
Dominic	Calleja	University of Liverpool
Jonathan	Carter	University of Coventry
Martyn	Cherrington	Innovate UK
Yongmann	Chung	University of Warwick
Marco	De Angelis	University of Liverpool
Poppy	Di Pietro	AWE
Alex	Diaz	University of Liverpool / Turing Institute
Matthew	Ellison	University of Liverpool
Hector Diego	Estrada Lugo	University of Liverpool
Jose	Freedman	Knowledge Transfer Network
Ander	Gray	University of Liverpool
Nick	Gray	University of Liverpool
Tim	Greenaway	GKN Aerospace
Petr	Grigorev	University of Warwick
Scott	Habershon	University of Warwick
Neil	Harrison	BAE Systems Maritime – Naval Ships
Peter	Hristov	University of Liverpool
Thomas	Hudson	University of Warwick
Ryan	Jackson	University of Liverpool
James	Kermode	University of Warwick
Gustavo	Krupa	Cranfirld University
Alexander	Lewis	AWE

First Name	Surname	Institution
Joe	Loxham	Cranfield University
Robert	Marshall	Rolls-Royce PLC.
Michael	Martin	Rolls-Royce PLC.
Lynne	McGregor	Innovate UK
Gordon	McKinstry	BAE Systems Maritime – Naval Ships
Mohad	Nezhad	University of Warwick
Berk	Onat	University of Warwick
Edoardo	Patelli	University of Liverpool
Guillaume	Saint-Cirgue	GKN Aerospace
Gabriele Cesare	Sosso	University of Warwick
Mark	Storr	AWE
Harry	Tunstall	University of Warwick
Juan	Ungredda	University of Warwick
Alexander	Wimbush	University of Liverpool

4 University of Warwick Information

Warwick consistently ranks in the top ten of all major domestic rankings of British universities. It was ranked 8th in the UK amongst multi-faculty institutions for the quality (GPA) of its research and 15th for its Research Power in the 2014 Research Excellence Framework. Entrance is competitive, with around 7 applicants per place for undergraduate study. Warwick has been ranked as the world's 20th best university based on employer reputation.

The Warwick Centre for Predictive Modelling (WCPM) is an interdisciplinary research centre focussed on providing a framework for the application of predictive modelling and uncertainty quantification (UQ) tools in science and engineering research. These mathematical tools provide a powerful new way of thinking about how to model complex systems and how to translate research outcomes into improved technology and design. WCPM was established at the University of Warwick in 2014 with a two-fold mission:

- To provide research leadership for UQ in the UK and worldwide, building on the best existing methodologies as well as developing new ones
- To combine UQ tools - traditionally developed in the mathematical sciences - with the application domain expertise of the physical and life sciences to produce scientific and engineering applications in areas aligned with national and global priorities, e.g. in sustainability, high value manufacturing, and advanced materials.

4.1 Travel to the University of Warwick

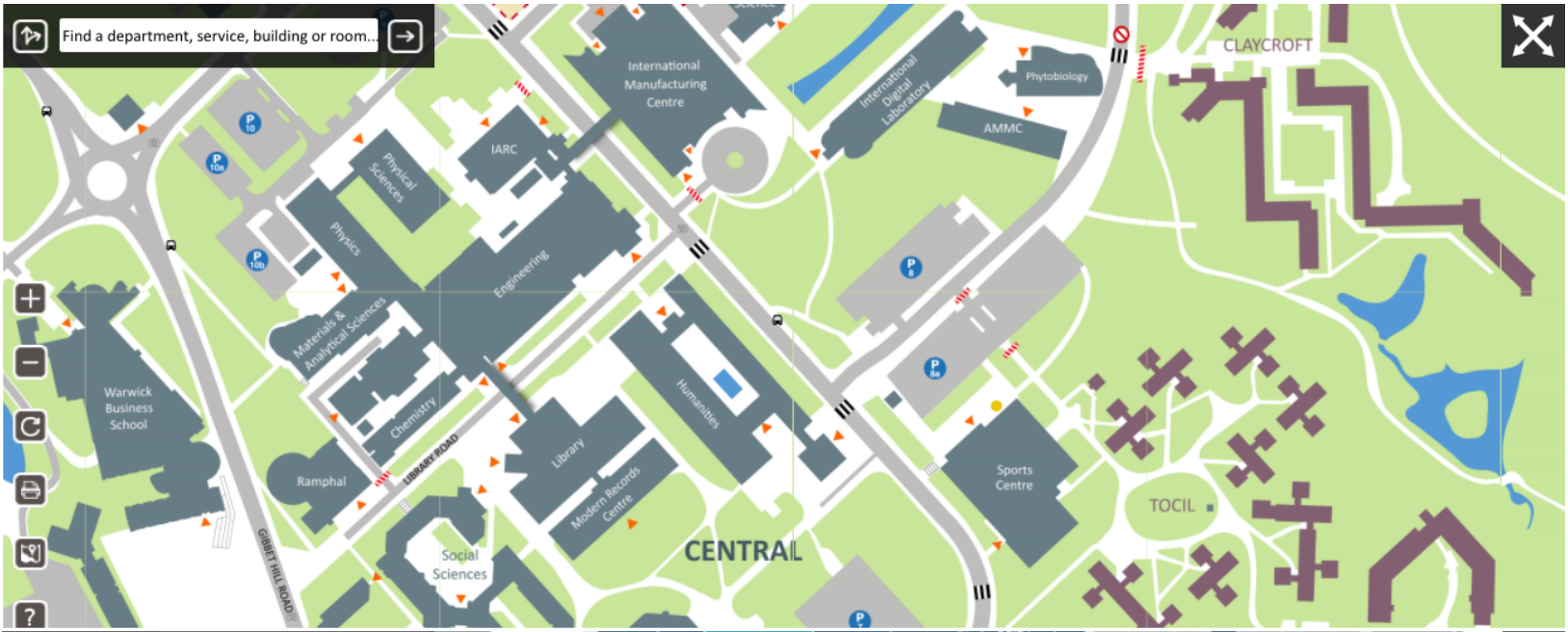
The Study Group will take place in the Warwick Centre for Predictive Modelling at the University of Warwick. Registration will take place outside room D2.02 on the 2nd floor of the School of Engineering from 9:30am on Wednesday 20 March; see campus map for details. For those staying overnight, parking is available at the Arden Conference Centre where you will be staying. Please display a copy of the attached permit in your vehicle. Some general travel information is also available.

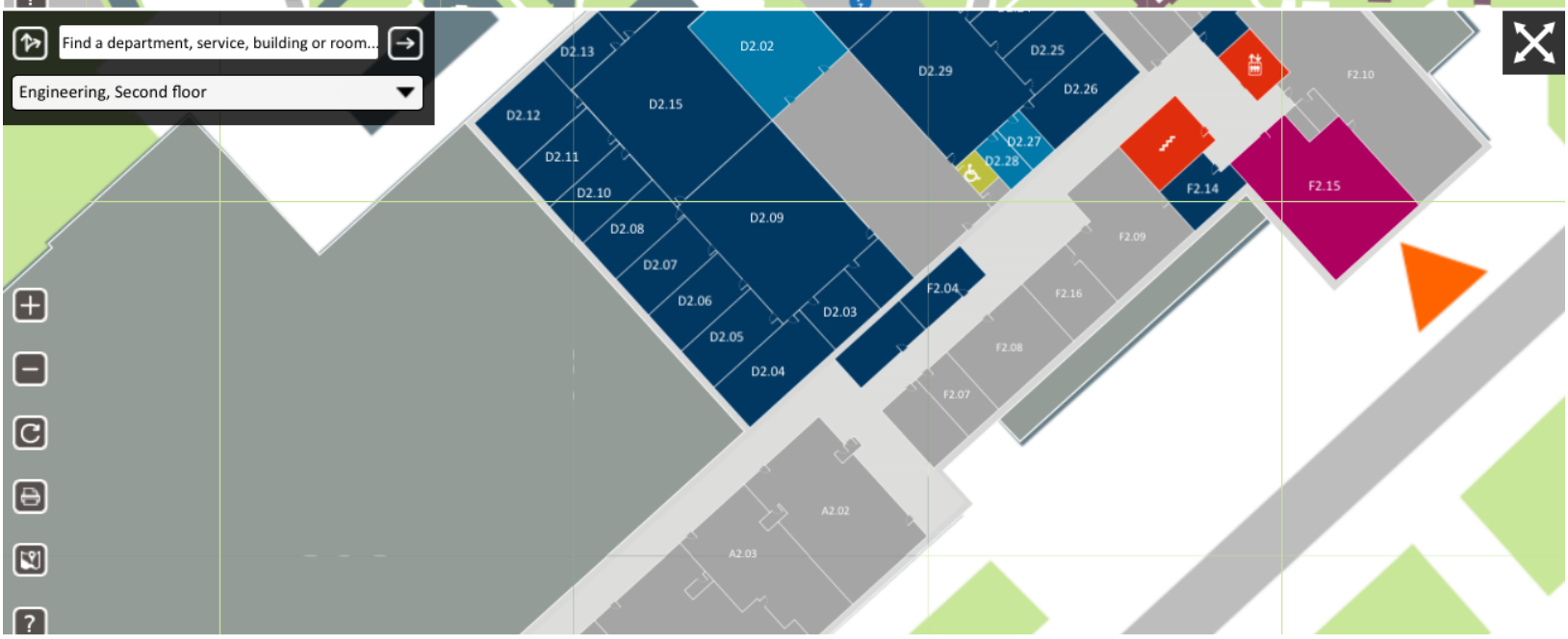
Directions of how to reach the campus can be found: https://warwick.ac.uk/about/visiting/

5 Campus Map

The Study Group will take place in the Warwick Centre for Predictive Modelling (in the **Engineering Block** on the Campus Map below). The Centre is located in the D-block extension on the 2nd floor of the main Engineering building at Warwick.

There is an interactive campus map available to help visitors find their way around. Registration will be outside D2.02. https://warwick.ac.uk/about/visiting/maps/interactive/





5.1 Wi-Fi for Guests

Who can connect to the wireless network at Warwick?

Full information https://warwick.ac.uk/services/its/servicessupport/networkservices/wifi

There are several wireless network services available across the University. Choose the appropriate service depending upon who you are:

- Warwick Staff and Students (hotspot-secure)
- Residents in campus accommodation (resnet-secure)
- Academic visitors (eduroam)
- Conference guests and campus visitors (Warwick Guest)

6 Supporting Organisations

6.1 Knowledge Transfer Network

Innovate UK
Knowledge Transfer Network

KTN Connects people. To speed up innovation, solve problems and find markets for new ideas. Established to foster better collaboration between science, creativity and business, KTN has specialist teams covering all sectors of the economy - from defence and aerospace to the creative industries, the built environment to biotechnology and robotics. KTN has helped thousands of businesses secure funding to drive innovation. And we support them through their business cycle to see that investment through to success.

Website: http://www.ktn-uk.co.uk

6.2 Warwick Centre for Predictive Modelling, University of Warwick

The Warwick Centre for Predictive Modelling (WCPM) is an interdisciplinary research centre focussed on providing a framework for the application of predictive modelling and uncertainty quantification (UQ) tools in science and engineering research. These mathematical tools provide a powerful new way of thinking about how to model complex systems and how to translate research outcomes into improved technology & design.

Website: https://www2.warwick.ac.uk/fac/sci/wcpm/

6.3 Instiute for Risk and Uncertainty, University of Liverpool

A centre for research and education. The University's Institute for Risk and Uncertainty is dedicated to helping people and organisations create a safer world. Large scale funding totalling £ 21 m has been secured to establish an EPSRC and ESRC Centre for Doctoral Training (CDT) on Quantification and Management of Risk & Uncertainty in Complex Systems & Environments within the Institute for Risk and Uncertainty.

Website: https://www.liverpool.ac.uk/risk-and-uncertainty/