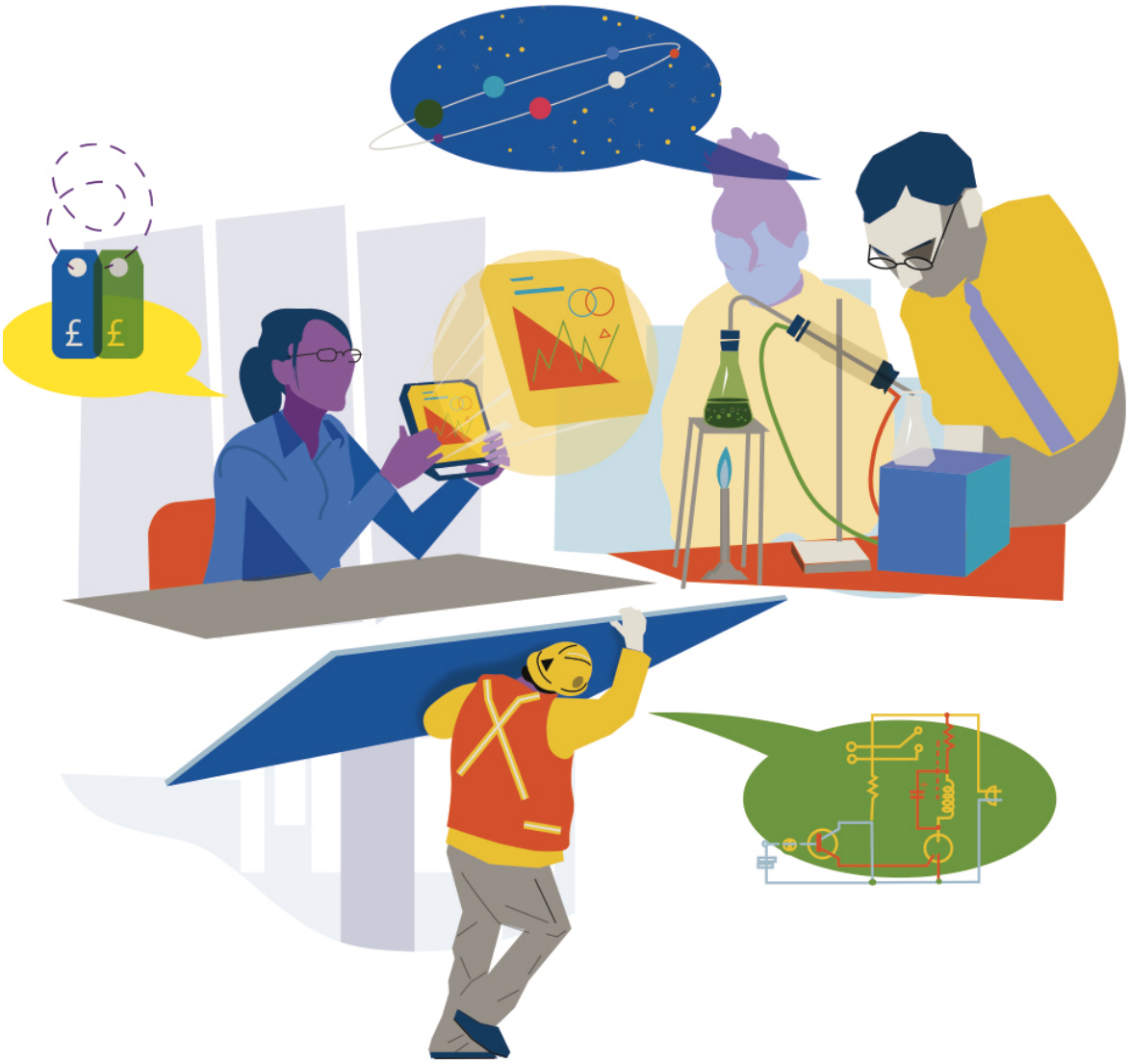

Third Uncertainty Quantification & Management Study Group with Industry

13th - 15th December 2017

Innovate UK
Knowledge Transfer Network

WARWICK
THE UNIVERSITY OF WARWICK

WCPM

Innovate UK
Knowledge Transfer Network

WCPM

Contents

Problems posed by:

AWE

ZENOTECH
SIMULATION UNLIMITED

hs2 engine for growth

AstraZeneca

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). In the KTN, the Uncertainty Quantification and Management (UQ&M) Special Interest Group (SIG) looks to draw together a UQ&M community and provide a structured meeting space where all the players can share their aspirations, knowledge and expertise.

The SIG was founded in 2014 by the late Prof. Tony Hutton at Airbus and continues to be chaired by Sanjiv Sharma, also at Airbus. The SIG is a joint venture between KTN, Innovate UK, Government, industry, and academia. Our First Year Report highlights progress to date. It is expected that much tangible value will be created, such as:

- Collaborative groupings that identify real benefit in working together,
- The development and refinement of challenges and aspirations,
- The emergence of a clutch of industry pulled projects that make significant advances against the wider challenges within given industrial High Value Manufacturing (HVM) sectors,
- An increasingly statistics-savvy engineering design and assessment community,
- A highly visible joined up and holistic UK based UQ&M capability that can respond positively to end-user aspirations and requirements.

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.

Use cases gathered and worked on can be found here.

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 (10 - 15 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 afternoon 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 March 2018.

After review from the industrialist, we wish for this report to be made public as the sponsoring parties have a responsibility to distribute good practice to the wider community. Thus, it is important for the industrialists to check for sensitive outcomes to be redacted within a month of receiving their report.

1.4 Agenda

<table>
<tr><th></th><th>Tuesday 12</th><th>Wednesday 13</th><th>Thursday 14</th><th>Friday 15</th></tr>
<tr><td>09:00 onwards</td><td rowspan="9"></td><td>Registration
(D2.02 WCPM)</td><td rowspan="2">Group Work</td><td rowspan="2">Group Work</td></tr>
<tr><td>10:00</td><td rowspan="2">Welcome, Introductions and Problem Presentations
(D2.02 WCPM)</td></tr>
<tr><td>11:00</td><td>Tea and Coffee</td><td>Tea and Coffee</td></tr>
<tr><td>11:30</td><td>Group Work
Individual Rooms</td><td>Group Work</td><td>Group Work</td></tr>
<tr><td>13:00</td><td>Lunch</td><td>Lunch</td><td>Lunch</td></tr>
<tr><td>14:00</td><td>Group Work</td><td>Group Work</td><td>Final Presentations
(D2.02 WCPM)</td></tr>
<tr><td>15:30</td><td>Tea and Coffee</td><td>Tea and Coffee</td><td>Tea and Coffee</td></tr>
<tr><td>16:00</td><td rowspan="2">Group Work</td><td>Group Work</td><td rowspan="3">FINISH</td></tr>
<tr><td>17:00</td><td rowspan="2"></td></tr>
<tr><td>18:30 onwards</td><td>Drinks Reception
Varsity Pub
(On Campus)</td><td>Dinner
Buffett at WCPM</td><td>Dinner
Scarman House</td></tr>
</table>

1.5 Do I need to pay?

The sponsoring parties are grateful to Innovate UK who have sponsored the Study Group through the KTN, as such we are pleased to cover for **all** delegates accommodation on the 13th - 15th December, including breakfast and lunches. We do however ask for a nominal payment of between £ 15 - 60 depending on the length of your stay. Additionally, we do ask that researchers and industrialists cover their own costs for travel to and from the venue.

1.6 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.

1.7 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, where drinks and light snacks will be available. It will also be a good opportunity to discuss research ideas and how problems may be addressed in an informal manner.

1.8 Conference Dinner

The dinner on Thursday will be held at Scarman Conference Centre o the main Warwick Campus. There is no dress code, and no cost associated with the dinner. We would ask that people arrive promptly by 18:00 (for a 18:30 start). 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 Problems

2.1 Developing a Surrogate Model for Predicting Metallic Corrosion Events

Presenting Institution: AWE plc, Materials and Analytical Science Division

Problem Presenter: Phil Monks

Abstract (Technical Topics and Desired Outcomes): The corrosion of uranium during long-term storage presents a challenge to the safe operation of nuclear facilities and equipment. The formation of uranium hydride is of particular interest, since it can lead to embrittlement of the metal (potentially leading to structural failure), and the resulting hydride powder is pyrophoric (potentially igniting upon exposure to air). Predicting the occurrence of hydride corrosion is therefore an important challenge for materials research.

AWE have developed a conceptual model of the key physical processes leading to hydride formation [1], namely: i) the oxidation of uranium metal by humid air, which leads to the formation of hydrogen as a by-product, ii) once the oxidation source is depleted, diffusion of hydrogen through the protective oxide over-layer is enhanced through local defects and thinned regions, whilst also being hindered by the presence of trap sites in the oxide, iii) accumulation of hydrogen in the metal approaches its terminal solubility limit, leading to the nucleation of a hydride site, iv) the hydride site breaches the surface of the material, is no longer protected by the oxide over-layer, and subsequently grows rapidly to form discrete corrosion "pits" on the sample surface (see Fig. 1).

There are many factors which influence the rate at which the hydriding reaction proceeds, e.g. the temperature, extent of oxidation, availability of hydrogen, sample production route (which determines the levels of impurities), and sample microstructure and mechanical properties (such as grain size, work-hardening, and residual stresses). The hydriding model must be capable of predicting, among other things, the "initiation time", which is the time at which the first hydride site ruptures the surface. A numerical diffusion model has been developed which estimates the initiation time by simulating the transport of hydrogen through the oxide over-layer and metal substrate. The operating range of the model is wide, since the relevant model parameters (diffusion coefficients, microstructure, etc.) are notoriously difficult to measure experimentally and are therefore subjected to a high degree of uncertainty. The model is also expensive computationally, and so global sensitivity and risk analyses remain a challenge.

Objectives: This use case is aimed at developing a surrogate model of a simplified case which can be sampled much more frequently and efficiently, allowing for extensive sensitivity analysis and quantification of risk, which is required in system-level assurance assessments. It is anticipated that the existing numerical code could be run numerous times to sample an adequate range of model inputs, building a suitable response surface which can be used as an emulator. It may prove beneficial, however, to approach the problem at a more fundamental level and examine the underlying governing equations and variables. The key output of interest is the initiation time, though it would also be desirable to apply the chosen technique more generally to other model predictions such as the hydrogen concentration at the oxide / metal surface.

An additional aspect of interest relates to the use of the surrogate model to design an efficient set of validation experiments. We measure validation performance via the use of a Validation

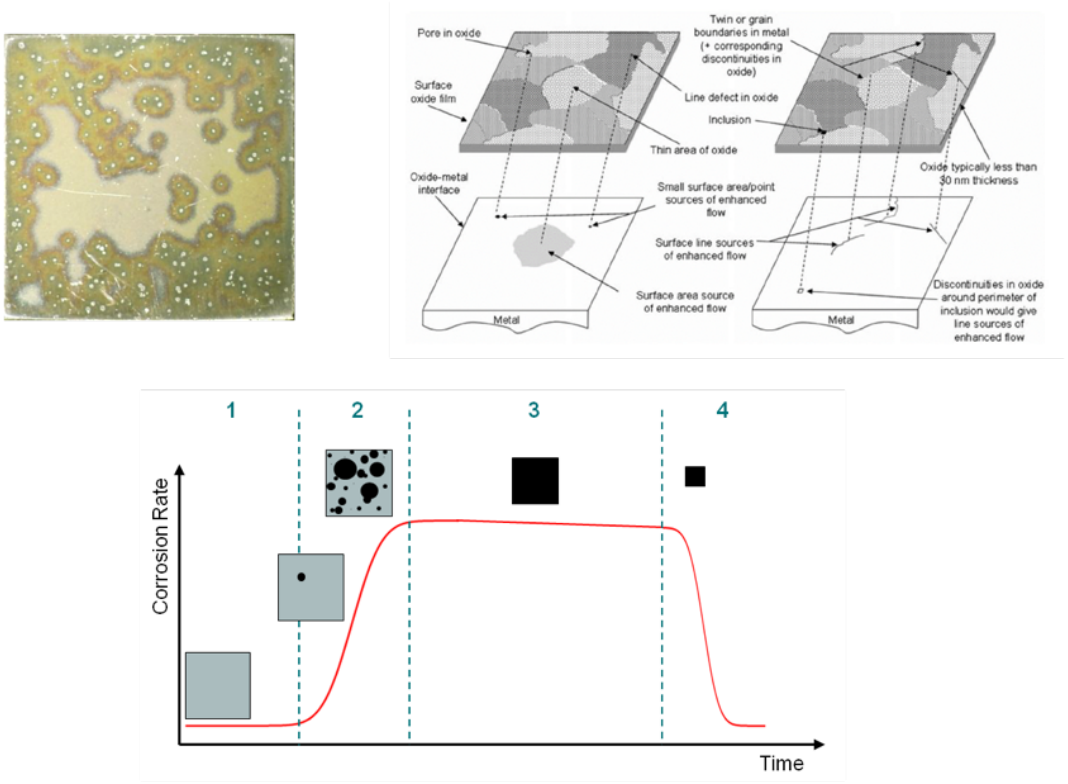

Figure 1: Schematics depicting the four stages of uranium hydride corrosion: 1) Induction, 2) Initiation, 3) Propagation, 4) Bulk Corrosion, 5) Termination. We are interested in the Induction and Initiation stages, which involve the diffusion of hydrogen through the protect oxide over-layer, and are functions of the reaction conditions and micro-structural properties of the material.

Metric [2], which provides a useful level of objectivity to the assessment of a given model across a range of experimentally-controlled variables (e.g. temperature and pressure), as well as tracking its performance as a function of time. Validation experiments can be expensive, both in terms of material resources and research time, and so it would be beneficial to optimise the experimental programme by determining i) the most important variables to test (which may be highlighted by a suitable model sensitivity analysis), ii) the number of experiments and variable values to use, iii) the length of time an experiment should be conducted for. The latter point is important since ageing experiments could continue for months in some cases, and model accuracy tends to degrade over this period as the prediction extends far beyond the original timescales involved in the training datasets. The key question arising is therefore: given a set of uncertainties in the model input parameters and a desired operational timescale, when can the experiment be stopped without premature estimation of the Validation Metric and subsequent loss of confidence (or over-confidence) in the model?

UQ&M Considerations: The major model inputs which will be used as part of the analysis are:

- Diffusion coefficient in the oxide
- Various trapping rate constants in the oxide
- Diffusion coefficient in the metal
- Surface concentration of hydrogen
- Terminal solubility of hydrogen in the metal
- Oxide thickness distribution
- Temperature
- Pressure

The uncertainties in these parameters have been partially characterized either through experimental measurement (which in some cases involves significant extrapolation from high temperature data), through assumption, or else according to the operational experimental range. The uncertainty ranges cover multiple orders of magnitude in most cases, and correspond to a variety of distributions (i.e. normal distributions arising from regression, uniform distributions where detailed knowledge is lacking). The manner in which the model parameter values may be interdependent is understood only to a first level of approximation.

The numerical code has been developed in-house in *Mathematica*. There exists the functionality for reading and writing of inputs / outputs to file, which provides a basic ability for interrogating the model. Computational times per simulation vary according to the input parameters, however timescales of seconds are typical (depending on the degree of coarseness of the numerical mesh). The model being used here is also simple enough that participants could code up their own versions in a reasonably short period of time using whatever numerical methods they wish. The main output would be a set of polynomials, a reference / lookup table or algorithm that acts as the surrogate. This should be independent of the main numerical code, allowing it to be interrogated separately during other dependent assessments.

Otherwise, there are no restrictions on the visualisation of the UQ analysis. Top-level summaries of key uncertainties and risk factors would be desirable to aid communication across various levels of our business (e.g. modelling, engineering analysis, programme management, and leadership teams).

To date, UQ techniques adopted have involved "brute force" Monte Carlo sampling of the input distributions in order to apply a global sensitivity analysis technique (which involves the crude assumption of linear relationships between the inputs and output). Lengthy computation times have limited the usefulness of this technique. Limited investigations into developing a response surface using the PSUADE UQ package [3] have also been carried out, however irregularities in the output surface have resulted in unreliable results, and so more in-depth experience of applying these types of tools to problems of this type is sought.

References:

1. J. Glascott: "A model for the initiation of reaction sites during the uranium-hydrogen reaction assuming enhanced hydrogen transport through thin areas of surface oxide"; Philos. Mag., 94(3), 221-241 (2014).
2. W. Li, W. Chen, Z. Jiang, Z. Lu, and Y. Liu; New validation metrics for models with multiple correlated responses; Reliability Engineering and System Safety, 127, 1-11 (2014).
3. PSUADE - Problem Solving environment for Uncertainty Analysis and Design Exploration;

2.2 Improved Drug Discovery Through Better Machine Learning Models

Presenting Institution: AstraZeneca

Problem Presenter: Stan Lazic, Ola Engkvist

Abstract (Technical Topics and Desired Outcomes): As has been widely published, there is a renewed interest in machine learning. There has been remarkable progress with new innovative methods creating a step change in image analysis and very recently in developing a program that beat the world champion in GO. A feat that only a few years ago was thought of as close to impossible.

It is therefore natural that also in drug discovery there is a renewed interest in machine learning methods. While proven very useful in QSPR (Quantitative Structure Property Relationships) modeling to predict physicochemical properties like lipophilicity, there is a renewed interest to both increase the application domain of machine learning as well as take a fresh look at classical machine learning tasks to predict the bioactivity of a compound and the ADME (Adsorption, Distribution, Metabolism and Excretion) of a compound. This is not only driven by progress in machine learning, but also by the increased automation of drug discovery generating more data than has been done historically.

A lot of decisions within AstraZeneca are based on predicting various properties of molecules. In many instances, we are using substructure based descriptions as an approximation of the molecular graph and combine it with support vector machines (SVM) as machine learning tool. [1] In the early phases of discovery, we experimentally test tens of thousands of molecules and use this knowledge as a base for predictive modeling of the corresponding properties.

We are interested to investigate different methods that could increase our predictive accuracy and make a comparison to our current standard approach. We do not see any limitations to what can be tried if it is related to small-molecule drug discovery. One approach we are interested to pursue is to investigate advances in deep learning and molecular graph convolution. Participants are encouraged to build models either with scikit-learn [2] or for deep learning within the DeepChem [3] framework; however, participants can also use other frameworks. Several interesting and inspiring articles have recently been published using molecular graph convolution, that might be of interest for the participants. [4]

Resources Available for this Problem: AstraZeneca will for the project bring data sets that can be used by the participants. There will be some sets for bioactivity prediction downloaded from PubChem. A second type of data is ADME datasets that have been generated internally. The training set is in the public domain. The external training set are compounds that are in the public domain while the test set results are not. For this set the participants will do predictions and we will feedback the accuracy achieved.

References:

1. http://pubs.acs.org/doi/abs/10.1021/ci500361u
2. http://scikit-learn.org/stable/
3. https://deepchem.io/
4. https://arxiv.org/pdf/1603.00856.pdf
5. http://pubs.acs.org/doi/abs/10.1021%2Facscentsci.6b00367
6. http://pubs.acs.org/doi/abs/10.1021/acs.jcim.6b00601
7. https://arxiv.org/abs/1709.03741

2.3 Visualising, Communicating and Managing Risk in Large Infrastructure Projects

Presenting Institution: High Speed Two Ltd.

Problem Presenter: Darryl Stephenson

Abstract (Technical Topics and Desired Outcomes): The primary objective of this challenges is to developed improved communication and transparency of risk information in a succinct manner but with highly flexible, easy to use, interactive drill-down (and / or alternative views) to promote engagement and understanding of the risk "big picture" and offer the prospect of gaining greater strategic insights.

Background: HS2 is a huge undertaking; Britain's first new intercity railway north of London in 100 years; Europe's largest infrastructure project. It will be the new backbone of our rail network. Once fully completed, around 345 miles of new high speed track will connect the city centres of London, Birmingham, Manchester and Leeds. The new line will include stops at Old Oak Common in West London, Birmingham and Manchester Airports and at Toton in the East Midlands between Derby and Nottingham. HS2 will also be integrated into the East and West Coast Main Lines, so HS2 trains will cross over to the existing network and serve towns and cities in the North of England and Scotland. This will open up access to the high speed network to around half the population of Britain and cut journey times between the North and the South.

HS2 is more than a transport project, it's an economic, and social project too. Our overarching vision is to be a catalyst for growth across Britain.

Capacity: As a new line, HS2 will provide a step change in capacity. It will create more seats for passengers, and more space on the rail network as a whole, allowing operators to run new, more frequent regional, local and commuter services.

Connectivity: By providing faster and easier travel between Britain's major cities and economic hubs, HS2 will help bridge the North-South divide and drive economic growth. It will open up local and regional markets, attract investment and improve job opportunities for hundreds of thousands of people across the whole country.

Risk Management System (RMS): Phase 2a and Phase 2b (Fig. 2) can each be considered as mega projects in their own right. The volume of identified risks is significant, however maturity of quantification is

Figure 2: HS2 planned route

variable, primarily based on design maturity and project lifecycle stage. Note, the term risk is used to describe both threats and opportunities.

The RMS includes qualitative assessments for all active threats and opportunities

- Current risk rating: probability and impact (cost; schedule; environment; reputation; health, safety & security; people; operational performance; benefit realisation)
- Response actions (threat mitigation / opportunity exploitation)
- "Target" risk rating i.e. post mitigation

Risk relationship mapping to establish dependencies, however correlation coefficients have not been identified at this stage. Approach for this is currently under investigation.

Xactium	HS2's Enterprise RMS is Xactium. All risks are recorded and assessed (qualitatively) in this system.
Both qualitative and quantitative assessment are made.	Qualitative assessments are made in HS2's risk management system, Xactium. Quantitative assessment and modelling uses *@Risk* for cost and *PRA* for schedule risks. The output of the schedule risks is used to model prolongation risk in the cost model.

Current risk reporting practice: Risk is reported from Xactium in a number of ways:

Conga reports	A tool that allows for extract of RMS information and merge with pre-defined templates (Excel, PowerPoint, Word etc.)
Xactium reports, Dashboards, and Heatmaps	Reports are text based with limited formatting, however they can be exported to Excel/CSV. Dashboards are better but do not provide great flexibility
Tableau	Tableau reporting is in the relatively early stages of development. It provides more visually appealing reporting / visualisations based on monthly data dumps from Xactium.

Risk Visualisation Aspirations: Several visualisation options would be beneficial to communicating risk and developing more holistic risk insight. Some examples might be:

Risk clustering on geographic maps	• Plotting risks in specific locations within a defined area based on, for example, community area, chainage range, contract, etc • Ability to print large format maps for static display in project room spaces or for workshops • Interactive selection and drill-down / expansion on geographic maps (including on GViewer)

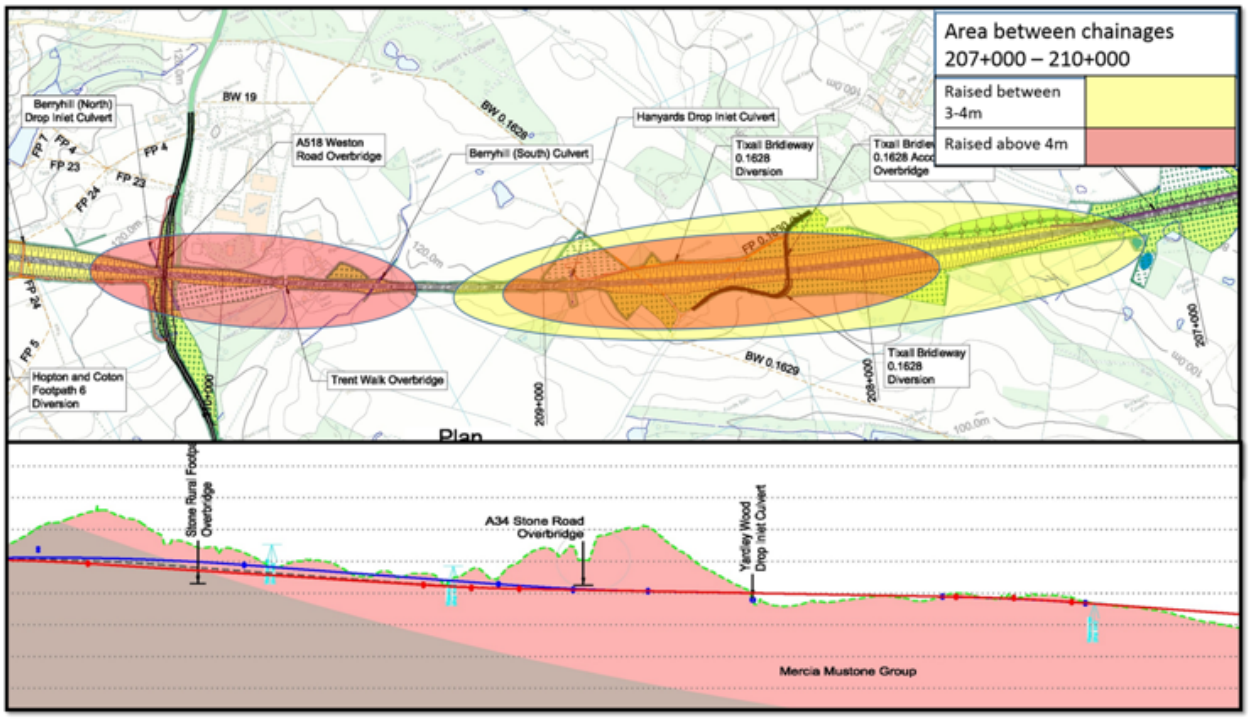

Figure 3: Example of risk heat map used in HS2 to highlight risk associated with raising parts of the track.

Risk relationship and dependency mapping with interactive what-if scenarios e.g.	• **Simple risk relationships:** Parent-Child, Peer (two-way) - ability to visualise critical risk dependencies. Example shown in Fig. 3. • **What-if:** For example, show the impact of deciding to approve a costly risk mitigation by changing the values for a risk and seeing how this affects related risks • **Effect of correlations:** e.g. pick a risk, adjust values and see impact on correlated risks i.e. not necessarily those with direct relationships
Risk Bow-Ties	

Resources Available for this Problem:

- Value Engineer experts from HS2
- Access to past project plan. Examples could include; SG: P6 programme, Plans & Profiles / models (G Viewer), Risk Register, Opportunities Log

References:

1. http://www.xactium.com
2. http://www.palisade.com/risk/

2.4 Machine Learning for Wind Energy Modelling

Presenting Institution: Zenotech Ltd.

Problem Presenter: David Standingford

Abstract (Technical Topics and Desired Outcomes):
Background: The United Kingdom is one of the best locations for wind power in the world, and is considered to be the best in Europe. Wind power contributed 11% of UK electricity generation in 2015, and 17% in December 2015.

Allowing for the costs of pollution, onshore wind power is the cheapest form of energy in the United Kingdom. The use of computational fluid dynamics (CFD) to assess the wind energy resource for a prospective new site is an established method that has been used for many years, however the inclusion of wake interaction effects - particularly for larger arrays of turbines - is less mature.

The SWEPT2 consortium (led by DNV-GL, with SSE, ORE Catapult, STFC, CFMS, Zenotech and the universities of Surrey, Strathclyde, Bristol and Imperial College) has been developing new tools to improve the utility and accuracy of CFD-based wake interaction modelling. Large amounts of data can now be generated and consolidated to inform engineering and investment decisions.

Objectives: The consortium is interested to know how well machine learning methods might be able to infer the interaction patterns and consequent power production from sites, given sufficient training data.

Resources Available for this Problem: The datasets include a range of wind directions, terrain maps (including roughness parameters and tree canopies) and full CFD fields (millions of datapoints, including velocity, pressure, temperature and turbulence quantities of interest). We will provide CFD data for a wind farm site in a Python notebook, with links to supporting datasets as needed.

If the study group wants to run additional simulations then the software can be made available - either on a local HPC cluster or on ARCHER. We will challenge the study group to reconstruct the wind data for a wind direction that is not part of the original dataset. This will requires the machine learning system to develop a an internal representation of the principal wake interaction modes as a function of wind direction, including nonlinear fluid dynamics effects and terrain!

3 Participants

First Name	Surname	Institution	Capabilities
Justin	Allen		I am doing a maters in statistics, with my dissertation on 'particle filters'
Alexandre	Andrey	University of Warwick	Postgraduate statistics: - modelling- data analysis also have about 2 years of work experience in industry trend research/forecasting for clients across finance, government and industry.
Stephanie	Ashenden	AstraZeneca	
Faheem	Ashraf	University of Warwick	Statistics
Ian	Atkinson	University of Warwick	Machine Learning
Martine	Barons	University of Warwick	Graphical models for decision support
Thomas	Blaschke	AstraZeneca	Computational chemistry: de novo design deep learning property predictions
Peter	Brommer	University of Warwick	Host
Angela	Busse	University of Glasgow	Computational Fluid Dynamics. Turbulent flows. Surface simulation and characterisation. High performance computing
Matt	Butchers	Knowledge Transfer Network	Organiser
Jonathan	Carter	Uncertainty Quantification Ltd.	UQ Analysis & Bayesian Statistics
Bhavan	Chahal	University of Warwick	My research involves using Python and inferring house prices via elastic nets, and I am sufficient with maps. I also know Data Mining techniques.
Hongming	Chen	AstraZeneca	Machine learning
Antoine	Choffrut	University of Warwick	Mathematical Analysis, Partial Differential Equations.
Andrei	Cimpoeru	CFMS	Computational Fluid Dynamics
Gabor	Csanyi	University of Cambridge	Machine learning, molecular modelling
Marco	de Angelis	University of Liverpool	sampling techniques on projected probabilities; interval statistics
Alez	Diaz	University of Liverpool	Bayesian methods, calibration, reliability analysis, metamodelling.
Geneviève	Dusson	University of Warwick	Mathematics - Numerical analysis - A posteriori error estimation.
Ola	Engkvist	AstraZeneca	Machine Learning, Informatics, Drug Discovery
Simon	Etter	University of Warwick	Approximation TheoryNumerical linear algebraScientific Computing
Maryam	Farsi	University of Cranfield	Decision Making Under Uncertainty
Simon	French	University of Warwick	Statistical, Risk and Decision analysis
Alfredo	Garbuno	University of Liverpool	Research
Stuart	Gatley	Bechtel	Civil engineering

First Name	Surname	Institution	Capabilities
Kathryn	Giblin	AstraZeneca	
Alex	Grenyer	University of Cranfield	Focussed on the mathematical quantification of uncertainties relevant for industrial maintenance.
Petr	Grigorev	University of Warwick	Scientific software development, atomistic modelling
Matteo	Icardi	University of Warwick	Deterministic and Monte-Carlo sampling for PDE-based continuum models, Fluid Dynamics, Multiscale problems
Andre	Jesus	University of Warwick	Bayesian model identification, Gaussian process surrogate modeling, measurement system design.
James	Kermode	University of Warwick	UQ + materials modelling
Timoleon	Kipouros	University of Cambridge	Multidimensional data visualisation and interactive analysis. Change propagation and risk analysis.
Joe	Loxham	University of Cranfield	Probabilistic Modelling
Robert	MacKay	University of Warwick	Dynamical systems
Andrew	Marsh	University of Warwick	Cheminformatics, synthesis, chemical biology
Reinhard	Maurer	University of Warwick	Electronic structure theory of surface photochemistry and materials structure prediction
Phil	Monks	AWE Plc.	System modelling and assessment
Matt	Moores	University of Warwick	statistical computing and Bayesian inference
Anthony	O'Hagan	Professor A O'Hagan Ltd	Statistics; Bayesian methods; Gaussian process emulation; model discrepancy; elicitation
Berk	Onat	University of Warwick	Materials modelling using first principle, molecular dynamics, and machine learning approaches as well as force field development based on neural networks
Edoardo	Patelli	University of Liverpool	Rare event simulation, Imprecise probability, HPC, System reliability and Bayesian methods
Lorenzo	Pellis	University of Manchester	Area: Epidemic modellingTools and methods: Stochastic models, statistical methods, uncertainty quantification
Karolis	Petruskevicius	University of Manchester	Uncertainty quantification. Dimensional reduction. Convex optimisation
Jonathan	Sadeghi	University of Liverpool	Structural Reliability Analysis, Metamodelling, Interval predictor Models, Epistemic Uncertainty (Imprecise Probability)
Enrico	Scalas	University of Sussex	Probability theory, Stochastic processes, Econophysics, Monte Carlo simulations
Pranay	Seshadri	Cambridge University	My methods for the PhD include dynamic stochastic programming for solving optimal control problems
Chris	Son	New Providence Consulting	UQ&M Approach in Financial Industry

First Name	Surname	Institution	Capabilities
Muhammed	Sogut	University of Warwick	My area of expertise is sustainable energy technologies.
Gabriele Cesare	Sosso	University of Warwick	My main area of expertise is computational physical chemistry. I have some experience with machine learning-based interatomic potentials (particularly neural networks-based), and I am quite interested in developing order parameters for computer simulations and descriptors for machine learning algorithms.
David	Standingford	Zenotech	Machine Learning for Wind Energy Modelling
Darryl	Stephenson	High Speed Two	Value Engineering
Luke	Stephenson	High Speed Two	Value Engineering
Ekaterina	Svetlova	University of Leicester	Decision-making under uncertainty/Qualitative empirical research
Inara	Watson	London South Bank University	Sustainability of High-Speed railways
Jan	Wildenhain	AstraZeneca	

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

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

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.

Contact(s): Matt Butchers
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 and design.

Contact(s): James Kermode, and Peter Brommer
Website: https://www2.warwick.ac.uk/fac/sci/wcpm/