State of the Art Report for

SimBest

An Innovate UK Project

Innovate UK
Technology Strategy Board

Delivered by

NAFEMS
KTN the Knowledge Transfer Network
ALSTOM

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SimBest Project Overview

Design is critical for the UK economy and reflects some of the most innovative and creative activities in business and other organisations. Engineering Design is one aspect of this, which addresses the engineering and technical aspects as well as the socio-technical factors of design.

Research in this area has the potential to revolutionise the way in which we approach design in the future as well as the opportunity to speed up innovation, enable new business models and technologies.

EPSRC's "Manufacturing the Future" theme [i] is looking to identify potential opportunities for fundamental computational methods to be integrated into novel or existing design approaches. This could be, for example, by the development of tools that could incorporate these methods into the design process.

Innovate UK's Modelling and Simulation – Best Practices Knowledge Transfer Project [ii] is looking to gather and disseminate best practice in the use of simulation and modelling tools for engineering design, and to encourage the take up and development of simulation tools by the UK manufacturing industry.

Innovate UK [iii] is funding a project to gather and disseminate best practice in the use of simulation and modelling tools for engineering design. The objective of this project, carried out in conjunction with NAFEMS [iv], Alstom Power [v] and the Knowledge Transfer Network [vi], is to encourage the take up and development of simulation tools by the UK manufacturing industry.

In particular, we hope to help SMEs that do not have the resources to develop their own procedures and practices make best use of these tools.

We are working with expert consultants to help evaluate the energy, automotive, built environment, health, aerospace, process and electronics sectors by evaluating how companies use simulation and how they maximise the benefits gained from the use of these tools.

The project has a very wide application but the scope has been reduced to focus on a few topics such as:

- Material technologies,
- Coupled/multi-phase simulations,
- Multi-scale modelling and
- Optimisation

Including important issues such as:

- High Performance Computing (HPC),
- Verification and Validation (V&V),
- Uncertainty Quantification (UQ) and
- Simulation Process and Data Management (SPDM).

This evaluation will involve interviewing many companies (please contact Gino Duffett - gino.duffett@nafems.org if you are interested in partaking and providing information) and holding presentation and discussion workshops to stimulate the flow of information and obtain a good understanding of the industrial knowledge and best practices. Particular focus is given to the following sectors:

- Automotive
- Aerospace
- Energy – generation to energy networks
- Built Environment
- Health (med care)
- Electronics - devices to systems
- Process Industry- specifically Chemicals and Food

Simulation users who are interviewed within this project will gain from their involvement in a number of ways. These include a range of channels for improvement in their use of simulation as well as the means to help their suppliers improve and integrate better with their methods. Benefits include:

- Review of the existing activities in the use of simulation**:** companies will receive a description of practices used to maximise benefits and overcome barriers in the use of simulation.
- Benchmarking: companies can benchmark themselves against other companies /

competitors.

- Information on 'world class methods': as explained in more detail below, KTN will be carrying out a parallel review of the state of the art in simulation and will ask leading academic researchers to identify potential avenues for addressing industry's key challenges in getting the most out of engineering simulation. As a participant, you will be able to input into the list of key challenges and will receive feedback on potential technical solutions.
- Gain an understanding of methods in other industry sectors and the potential for cross-sector exchange.

The project deliverables should facilitate users in their continual quest to achieve more efficiency savings and competitive advantages in their design and manufacturing activities by:

1. The definition of areas where new users to digital simulation can learn from experienced ones.
2. The definition of learning areas across sectors.
3. The definition of areas requiring further development to maintain the continual progress of experienced users.
4. The creation and presentation of material and training to encourage the learning process in using simulation.

Purpose of the Workshop

The intention of this workshop was to identify the state of the art and future developments in simulation and modelling for engineering design so that:

- Experienced users can progress in their use of new tools
- Key areas needing research and development can be identified

A diverse selection of end-users, developers and researchers in design, manufacturing and underpinning sciences will be brought together (Delegates in Appendix 2) to address the following questions:

- What are the latest research developments with the potential to have impact on the design and simulation user communities?
- How can these developments be better developed for exploitation by designers?
- What are the opportunities and barriers to uptake of these new design and simulation tools?
- What are the potential risks and benefits of uptake of these new design and simulation tools?

Delegates went through an expression of interest phase through EPSRC to take part in the workshop. This was to ensure that the right balance of experts in each of the four key areas; optimisation, materials, multi-scale and multiphysics were in attendance. The discussions which took place during the day took place in these four groups, and this is the way the remainder of the report is structured.

Breakout Session 1 – Challenges and Novel Approaches

The purpose of the first breakout session was to develop some of the industry challenges articulated in the morning talks. Additionally, a list of pre-compiled challenges was sent out to the delegates before the meeting (Appendix 3).

In the four discussion groups, delegates were asked to discuss the ones most relevant to their group, refine them and comment on where they had thoughts on novel approaches from the academic community.

Multi-scale

Multi-scale Validation

- Data Validation Through Scales: Stirred Tank reactor oxygen transfer CFD - Model + Experiment at several scales (10 L -> 10,000 L) in order to gain trust in simulation for larger and smaller scales outside of experimental range
- Aircraft surface tolerences: understanding effects of steps, gaps, surface waviness on lift and drag performance. Developing semi-empirical models within RANS CFD to trade-off manufacturing vs performance.
- Coupling between measurement experiments and modelling to improve understanding of the underlying physics
- Modelling to support parameter extraction from measurement data for validated input parameters, e.g. micro-indentation
- Hierachical Bayesian data assimiliation for hetrogenious multi-scale data (e.g. Reservoir Data)
- Full SD CFD with 2 way coupling to material properties (temperature dependence, shear dependance, flow dependance) in turbo machinery.
- Application of X-ray imaging for multiscale validation of models: in situ process / service
- Integration of modelling with experiment. How to use simulation to influence pilot plant scales & how to use pilot plant studies to influence simulation on a daily basis.

Understanding & Modeling Physics

- Stochastic multi-scale method for composite structural dynamics. Reduced order methods (ROM) across length & scales. Global sensitivity analysis across length scales.
- Multi-scale simulation of welding: a) CFD fluid flow & thermal 10^{-6} m b) Cellular automata for grain structure 10^{-3} m c) Crystal Plasticity finite element macro properties 10^{-2} m
- Multi-scale simulation of additive manufacturing - component analysis 10^{-1}m
- High speed, high temperature gas flow; plasma & arc welding
- Small an bis: semi-empirical models for small features such as vortex generators embedded in RANS CFD
- Predicting processing - structure - property relationships for polymer nanocomposites and blends - optimum formulation for enhanced performance
- Understanding and Modelling Physics: Solve one problem at a time for example - Liquid mixing - solve & validate velocity profile then freeze velocity to solve mixing time - accuracy compromise but big time saving.
- Increasing timescales of mesoscale modelling to obtain rheology & kinetics of structure forming that can be used in CFD. How does the rheology evolve in response to process.
- Incorporating field effects (eg electrical, magnetic etc) into models at different scales.
- Multi-scale Finite Element methods for dynamic crack porpagtion; Material Point Methods; Transient Analysis Schemes; Material Damage modelling
- Multi-scale models of particule process linking subparticle to particle to flow and unit operation behaviour; 1) 3D printing; 2) Spray dry; 3) pharma processes 4) digital/design of pharma
- Structural Identification model identification
- 1) Surface/interface effects; 2) describing, understanding; linking experiments and models
- Determining key physics affecting in service performance using synchrotron techniques
- Multi-scale methods for intensified process design
- Use of atomistic simulation to interpret high-res experimental characterisation of materials

Design Environment

- Design Environment: NPD as socio-technical systems
- Look at: -FEniCS - Firedrake
- Isogeomaterical based optimisation methods

Two-way Coupling

- Localisation -> Homogenisation FE2

Thermodynamic Constistency Across Scale

- Formulation of thermodynamically consistent diffusion models linking atomistic to bulk scales

Integration & Interpoerability

- Engineering information systems - Data exchange standards - STEPlike
- Represntative volume element (RVE) for cellular discreet structure - length scale bridiging; Non-local elasticity model; bottom-up multiscale - domain decomposition
- Mathematic and numerical homogenisation, volume averaging, up-scaling
- Inetgration-sequencing of CFD model of unit operation into a whole process
- Virtual reallity sructural modeling

Standard Data Structures

- Standard data structures; involved in developing an AP209 standard for DEM data (part of EU FP7 VELaSSCo project)

Big Data

- Big Data: Participating in EU FP7 VELaSSCo project - to develop a framework for analysis and visualisation of Big Data produced in enginerring simulations (e.g. CFD, DEM, FEM....)

Effect of Micro Behaviour to Improve Material Performance

- Embedding (in Design the Future) could be a tool for relating across scales
- Consistent multi-physics models for composite delamination / decohesion
- Consistent models for damage mechanics / crack propogation in quasi -brittle materials
- Manufacturing of nanocomposites thermoforming localisation - homogenity
- Probabilistic descripton of microsctructures to provide quantification of mechanical variation; application of model in integrated computational materials engineering approach - casting, forming, joining
- Incorperation of microstructure (crystalline and composites) into models to predict thermal and physical properties
- Structure characterisation - representation within models; distributed properties; stochastic approaches
- Developing open source 3 phase CFD codes for soldification processes, predicting defects and understanding underlying physics
- Two-phase floews in hot pipe / heat exchangers involving detailed boiling / condensation models
- Coupling of thermodynamic and thermodynamic models in bioheat problem
- Two-way upscaling and downscaling, homogenisation in soft tissue

Optimisation

Formulation of optimisation problems

- Problem formulation - avoid obsession with "perfect global optimum" - any design that meets / exceeds customer requirements is good enough?
- Formulation, object orientated definition of problems
- Optimisation of code to reduce run-time of applications. Don't depend on increased computer speed to overcome poor code writing
- Notation for uncertainty and noise
- Problem formulation - EXPRESS: "objective" as a balance of multiple product behaviours and attributes e.g. low weight, low cost, long lasting. Design space - list and foundationss of design factors that can be manipulated. Accept / reject criteria
- Hyper heuristics?
- Automatic model generation
- Models for discrete + continous variables coexistence
- Very large scale mathematical programming optimisation
- Mixed - integer. NLP -> MINLP. Dyn Opt -> MIDO
- Design + operational optimisation together
- Simplification of input requirements to run models. Ability for industry to use academic applications
- DV ranking selection of criertia vs constrainsts, selection of tools

Optimisation Under Uncertainty

- Stochastic otimisation
- Stochastic optimisation in industrial setting
- Integrating sampling and optimsation
- Access to data required to populate models at the right level of fidelity and cost

Optimising Noisy Systems

- Statistical ranking and selection techniques
- New optimisers tolerant to noise
- Derivative-free optimers
- User diversity / 'customer' priorities reactive
- Surrogate models
- Developing mid-rnage metamodel methods
- Integration in the design loop of "smart" systems that drive performance based on environment
- Noisy systems - coping with 'hyper sensitive' repsonse change: small perturbation in inputs result in significant reposnse change. Process stability: solver convergence mesh discretisation geometry
- Size of representative sample

Robust Optimisation

- Metamodels
- Robust optimisation using surrogates including operating and manufacturing uncertainties
- Interval analysis. Algebraic, dynamcic models
- Work on crashworthiness optimisation
- Worst case vs average case vs active robustness
- Iso-geometric analysis based shape otimisation
- Trade-off vs performance
- Worse-case optimisation

Discrete Optimisation

- Optimise parameter selection, physics-based models
- Various discrete structure optmisation formulation
- Flowsheet / design space superstructures
- Current development of metamodel based strategy for discrete optimisation

Highly-coupled Systems

- Dynamical vs steady state processes
- Metamodel based optimisation, development of MDO frameworks
- Quick and dirty tools for exploring space
- Multiphysics coupling / systems modeling
- Surrogate models
- Global optimisation

Interpretation During Process

- Data visualisation
- Graphical interfaces
- Use of gaming platfroms
- Optimisation of large multidiciplanry systems cost vs performance
- Learning user preference during interactive optimisation
- Interactive design software for comonents
- Innovization - automatic identification of design patterns
- Interactive modeling and visualisation

High Dimensional Optimisation

- Additive models
- Multi-level Monte Carlo
- Multi-point approximation methods (projects with Rolls-Royce)
- Adjoint methods
- Discipline specific trust region methods
- Commerical connectivity of different software packages. Standards required to make transfer of data easier. Avoid transfer via excel
- Hierachical models (automatic identification of building blocks)
- Reduced order modeling of high dimensaional systems
- Model reduction
- Global sensitity analysis

Early identification of dependnacy

- Parametric effectiveness
- Requirements capture
- Identification analysis
- *** ranking
- Multi level optimisation, concept, vs component vs detail

Multi-objective

- "Chip" thinking for built environment
- Mulit-objective training of Kriging models (surrogate models) liklihood versus ...
- Multi-objective evolutionary algorthms to identify trade-off frontier
- Multi-objective utility function
- Multi-level optimisation
- Bi-level optimisation
- Current work in SILOET-II project with Rolls-Royce
- Interactive (human) methods for exploring trade-off

Multi-discplinary

- Visualisation of multi-variable (more than 5) optimisation results
- Computing adjoints in multiphysics
- Slection of MDO startegy
- Human factors
- Multi-disciplinary adjoint methods

Failures + Dropouts of Model (handling of)

- Learning where the model fails during optimisation
- Explicit search for failure scenarios
- Adapting constriant handling techniues after simulation failtiure

Multi-fidelity Optimsation

- Learn which fidelity to use for which deisgn
- Maximising diversity of solutions on low-fidelity model so good chance of good solution on high-fidelity model
- What happens at transition between fidelities? How can we feedback this information?

Constraint Handling

- Problem formulation - dealing with constraint violation. fuzzy vs absolute constraints. Accounting for variation

Materials

Modelling Composites

- Micro-FEM/EFG, MESO/MACRO - FEM Modeling of damage, initiated and propagation
- Modeling impact damage compression adter impact / residual, strength / crush (FEM - Fracture / Damage Mech)
- QM Simulation of interface between layered materials (TMDC, graphene via LS-DFT)
- Microstructured, multi-plastic materials, strenagth, transport, multiscale
- Performance and failture of CMCs under complex thermo-mechanical cycles
- Direct methods of analysis for composite systems
- Modeling of composites failure with complex structure, macro-scale modeling is used. But it is hard to define the proper boundary conditions for the micro-scale modeling for the failure estimation. Failure mode of materials <> structure modeling <> failure estimation of material
- Combining thermal and mechanical damage via a hybrid FE / RUE methd
- Continuum damage - healing models
- Modeling of ceramic behaviour over a range of high strain rates
- Statistics - multi-type particularly systems with local interaction to explain global stratgey

Modelling Fatigue

- Modeling of ceramic behavior over a range of high strain rates
- Constitutive models from atomistics
- DVPT of user defined initiation criteria in fatigue, 3D crack propagation models
- Creep - fatigue interactions
- Dislocation creation and motion from atomistics
- Fatigue and fracture of concrete for infrastructure (from nano to macro) Organic-inorganic composite fracture (e.g. gas shale)
- Meso-scopic modeling of wear and material degredation
- Prediction of oxidisation assisted crach propogation in metal alloys

Complex Fluids & Solids

- Optimisation and mesoscale materials strcutures for additive manufacturing
- Linking atomistic to mesoscale models
- Modeling self-assembl behaviour and aggregation
- Soft materials at the liquid solid interface
- Fluid structure interaction, T-junction? Mixing zone, hot water, cold water ? temperature. Fatigue / crack - flow in fuel rods
- Hierarchical biomaterials and tissue (multiscale multiplastics) for personalised medicine
- Modeling at optical properties of polymers for photo? applications incoperating large - scale realistic?
- Poro-Visco plastic models for soft solids
- Fluid-solid interaction in the mesopores of cement, casuing issues of durability (? nuclear, reactors, infrastructure)
- Endoluminal stent & artery interaction
- Printing liquid drops with with high solid content > liquid solid interactions
- Printed materials & systems! (eg OLEDs)
- Robust, analytical theory of micellar, emulsion, liquid crystalline phases. Coupling of simulation ? & timescale atomiser<>mesoscopic<>CFD
- Complex ? flows in Random Heterogenous porous materials
- Rhelology of polymer nanocomposites and polymer blends
- Phase separation in multiphase polymeric systems
- 3D +time, in situ characterisation of complex fluids using x-ray & RM

Chemical mechanical material modeling

- Thermal degradation of phenolic risens
- Long time scale atomistic modelling - role of chemical effects
- Coupling between QM models and continuum models for cracks, defects? etc
- Cement formation as precipitation and aggregation of nanoparticles from ionic solution (soft matter)
- Chemical deterioration of cement
- Long timescales in nano scale sims
- Modelling (atomistic)/Experiment of stress corrosion cracking of zirconium alloys in fuel tubes
- Ultra high temperature ceramic behaviour under intense thermo-mechanical stress
- Drug delivery & tissue response biochemistry + mechanobiology
- Tribo Chemistry Modelling - chemo-mechanical interactions of lubricated contacts between different material systems. DLC/Steel/Polymer/Ceramic. Whole system approach
- Deformation modelling. Dislocation dynamics linked to macro plasticity

Residual Stress Modeling

- Coupled crystal plasticity modelling/Digital image correlation of complex plastic deformation
- Modelling thin film growth
- Modelling of phase transformation during welding process to predict residual stress
- Metamodel using ? data available can predict the residual stress quickly as well as can be calibrated by validation from experiment data
- Pressure Induced phase transformations in Nanomaterials e.g. Nanocrystals
- Residual stresses in cement paste formulation determine largely the subsequent failure but also creep and chemical stability

Materials in Aggressive Environments

- Creep and oxidation of ultra high temperature ceramics
- Modelling of materials (Atomistic) degradation/failure in nuclear industry - Irradiation damage/stress corrosion cracking/oxidation
- Graphite under oxidation and irradiation
- Modelling functional surfaces for catalysis in Gas to Liquids Conversion reactions via LS-DFT
- Hydrogen embrittlement
- Deformation, damage development and crack growth at elevated temperatures
- Erosian Modelling- predicting wear of different materials, wear maps
- Corrosion Modelling - To of Line (Pipelines), Artifical Joints (Hip etc), Bearing Failure/Lifetime
- Cement in aggressive environemtns - chemically, temperature & nucleation
- Modelling hydrogen transport, crystalline materials for hydrogen embrittlement
- Pif - to crack transition modelling in steel in underwater pipelines
- 3D + Time ? of material behavious in harsh environments
- Take a look at Livermore www.exmatex.org. Extreme Materials at Extreme Scale

Integration & Coupling

- Linking Atomistic to FEM
- Micromechanics - continuum mechanics
- Statistics - Micro-level models with interaction between particles. Macroscopic states parameter dependence
- Micromechanics & Continuum mechanics
- Look at - FENICS, Firedrake

Highly Non Linear & Highly Interactive Problems

- Fracture in composites at microscale using meshless methods
- Non linear problem - material behaviour (27 parameters ? ? Contact friction between graphite? Large ?
- Statistics - Micro-level models with interaction between particles. Macroscopic states parameter dependence
- Nano enhanced multifunctional composites
- Nonlinear mechanics in soft tissue for ? diagnosis
- Simulation of microstructural evolution under irradiation (and proton-irradiation experiments)
- Metamodel technique to convert highly non-linear problem into explicit mathematical problem, which could be easily solve
- Dynamic crack propogation
- Behaviour of microbubbles in an acoustic environment
- Secondary processing of polymer nanocomposites

Multi-physics

Interfaces & Geometry (meshing Geometry)

- Big data analytics & visualisation for scientific computations
- Robust & accurate FEM using implicitly represented geometries (level set)
- Object based simulation and interpretations of data

Move from single core processes to multi core. Processor architecture - software independent. Not enough computing power & to much data, big data.

- High order discontinuous Galerkin FEM - Good data locality, Non-conforming meshes, Accuracy ....
- Many core simulations GPGPU/Phi
- FEM modelling, development of new FEM elements (triangular, hexahedral, tetrahedral)
- LES/DES/CFD - Data Visualisation, efficient use of tools to develop quicker design solutions

Virtual verification & validation. What is the proper level of fidelity. End user wants to know limits.

- Vertical Engineering/V&V/Fidelity levels - Ongoing research for real-time simulations including fidelity level assessment - trying to answer how good is good enough?
- Goal orientated error estimates. Map of error contributions across component to the quantity of interest. A look up libary of pre-computed likely scenarios
- Collecting test cases and creating benchmarks

Standardisation between systems. Integration of different simulation environments

- Multi coupling
- Model based system engineering

Merging continuous & discrete systems. Integration of control system & its design. Intelligent selection method for portioning the model cheap simulation for part of the model. Reconfigureable, multi disciplinary design/analysis/opti. Model coupling, time and space.

- Multidisciplinary design, new design methods (set based design), Computational ?, Model based systems engineering
- Functional mock up interface (FMI) - co-simulation/Model exchange
- DES and continuous
- Multiphysics coupling over interfaces
- High resolution regularisation and stabilisation (less inverse problems)

Paramaterisation getting the data. Access to data from suppliers. Tracability of how results are produced. Explain & capture decision making process.

- Experimental design & parameter optimisation (energy storage)
- "Reverse enginerring - model to deliver optimised molecular properties etc

Multifield coupling, elctro, electro chem. Quantum molecules modelling. New theory & models

- Particle & fluid coupling, particle & electrical, dynamics electrochemicals, process design/engineering, suspension rheology/formulation
- Mechcanical & thermal props, Mathematical modelling, FEA/MM, Mateerial Modelling Fluid Flow team (Lattice Boltzmann), Gradient systems, Non C?, Non ?, ? systems
- Integration of molecular modelling to CFD
- Development of new theories/models e.g. polymers, gels, surfactants

Breakout Session 2 – Exploitation, Risks and Barriers

The second breakout session focussed on how these developments could be exploited by end-users, what opportunities they represent and where the risks, and barriers exist.

- How can these developments be better developed for exploitation by designers?
- What are the opportunities and barriers to uptake of these new design and simulation tools?
- What are the potential risks and benefits of uptake of these new design and simulation tools?

Multi-scale

How can these developments be better exploited by end users and researchers in design and manufacturing?

Software should be developed to be user friendly and of high quality. Software vendors should create solutions for users that - they want; they can use easily; and can afford. Training on how to use, what to expect and which modelling tool / level of model would be right for a particular job.

Interaction with academia could be improved to enable better and easier ways to share and progress developments. This includes support for moving developments from TRL 3 – 6, transfer of knowledge from universities to software vendors, and to help universities to transfer knowledge to SMEs so that larger companies can check out new software before making the large resource commitment required to take it on and train up staff in using it.

Make use of test cases and case studies, especially those that are well defined and can be used for demonstration of how to use the new developments and what can be achieved.

What are the opportunities and barriers to uptake of these new design and simulation and modelling techniques?

Computer / Software Issues

Opportunities:

- Opportunity to design software for use by people with lower skills

Barriers:

- IT system obsolescence means cant use old code
- Computing resources are expensive
- Unavailability of robust / reliable commercial codes across different scales
- Large companies often use bespoke tools – suppliers need access
- Open source software is usually abandoned

User Issues:

Barriers:

- Difficult to interpret results
- Difficulties to get acceptance by users (kudos of complexity and lack of understanding by managers)
- Many research results aren't reproducible so not trustworthy

Opportunities:

- Design innovative new materials
- Better, more competitive products with lower costs
- Reduced risk in product development
- In future, designers can design in different ways.

What are the potential risks and benefits of uptake of these new design and simulation and modelling techniques?

Benefits:

- Improved understanding of designs and how they might behave through life
- Think of innovations and designs never would have thought of
- Find most efficient designs / products
- Model based design is the future

Risks:

- Software over promises
- Unaffordable to most buy large corporates
- If we don't do it, the Chinese and Indians will – leading to loss of competitive advantage
- Users take results at face value
- Invalid assumptions give incorrect results, e.g. garbage in = garbage out
- Potential to miss failure mechanisms
- Data corruption across length scales.

Optimisation

How can these developments be better exploited by end users and researchers in design and manufacturing?

The ideas discussed were focussed around what an engaged community of industrialists and academics could do. The community would best approach this by focussing on industry pull problems; for example opportunities for industry to inform academics of what problems they are facing, and also conversely an opportunity for academics to keep industry apprised of what the new developments are.

One such mechanism which has worked well in the past have been university organised "optimisation surgeries" where problems are bought to a group who then work to solve, or explore approaches to solving. This is linked to the provision of open problems for the community to work on; for example Rolls-Royce have a problem involving UQ for blade and disk interaction which will provide macros and CAD files, to be released to the community. Methods sharing. AIMs

As well as open problems, a broad selection of case studies would be beneficial. Test cases e.g. NAFEMS. Independent bodies / platform providing challenges. Bite size booklets of industry problems. Success stories

This would also help to establish a common language. Skills Both way secondments, students and other levels

What are the opportunities and barriers to uptake of these new design and simulation and modelling techniques?

Opportunities

- Develop effective "grid" solutions to connect all computers in a company's LAN as resource for optimisation to significantly improve speed and quality of an optimisation
- Most systems can be optimised
- Exploiting UK science base
- Open source is an opportunity to build confidence in use
- Skills as an opportunity e.g. CPD

Barriers

- Interoperability between software and processes / work flows
- Education and skills
    - Problem formulation
    - Modeling optimisation techniques
    - Culture of maths within engineering
- Dependency on black box technology
- Attitude, risk adverse domain experts
- Confidentiality and legal
- Funding / time to make software open source
- HPC is inevitably architected in order to solve the biggest single physics problem imaginable – this is inevitably the wrong configuration for design exploration or optimisation: solve many problems simultaneously as possible

What are the potential risks and benefits of uptake of these new design and simulation and modelling techniques?

Risks

- Too many design variables being used
- Implicit trust in outcome (missing data)
- Risk of failure for industry
- Hard to demonstrate impact / effect of academics
- Academic time spent on non-academic progress
- Conflicting meaning of success e.g. KPI's of academics versus industry
- Over promising and under delivering
- Too much focus on too few open problems
- Over-reliance on optimisation

Benefits

- Reduced time to market
- Improvement of quality of life e.g. personalised healthcare
- Increased quality of product

- Reduced cost
- Increased knowledge from data for gaining insight into problem
- Better structure of data
- Elimination of safety factor
- Game change in competitiveness in industry
- Academics demonstrate impact
- Gain new ideas
- Serendipity and other benefits
- Both academic and industry can win from this
- How do small businesses benefit
- Moral satisfaction
- Potentially game changing
- Exploration tool
- Productivity
- Better decision support
- Customised / personalised products

Materials

How can these developments be better exploited by end users and researchers in design and manufacturing?

- Long partnership with Ind. Collaboration
- Relationship Building
- Consortia Building (cluster)
- Recognise the value of insight generation from new simulation technologies
- Innovate UK CR&D
- Skills Translation
- Direct exploit by partner
- Trade Association collaboration
- Short term problem solving
- Modelling & Simulation catapult

What are the opportunities and barriers to uptake of these new design and simulation and modelling techniques?

Opportunities

- Aerospace, Automotive, Energy (Nuclear, PV etc. – Nuclear UK competitive sectors)
- Defence – costs, injuries/staff protection
- Reduce time to market
- Cross sector technology transfer (Industry, clusters, collaborative)
- Silicon toxicology
- Standards & Regulations (competitions working together)
- Quantification of material specification

Barriers

- Validation and Certification
- Fundamental research underpins industry models
- ? compatibility

What are the potential risks and benefits of uptake of these new design and simulation and modelling techniques?

Risks

- Loose competitiveness due to lack of uptake of simulation
- Lack of data for model validation
- Limitations due to the lack of understanding of the model
- Lack of speciality
- Big data

Benefits

- Big data
- Design of end of life
- Ability to do through life ?

Multi-physics

What are the opportunities and barriers to uptake of these new design and simulation and modelling techniques?

Opportunities

- Provide funding covering a larger scope
- Standardisation (moving between meshes). Further research into geometry cycle and the design cycle. Aiming towards seamless flow between geometries and different models throughout the design cycle.
- To finding ways to meet verification and validation expectations of industry. This also includes looking for ways that allows the use of open source software
- Higher quality simulations needed with fewer assumptions. Also improving connecting scales and coupling different models at different scales
- Need co-design with a different multi-disciplinary approach. Identify single challenge for industry that could then stipulate the requirement to bring together different researchers from different research backgrounds
- Get better understanding between academic and industry. Can similar procedures be produced? Investment into collaboration required between academia, industry and software developers
- Options to explore how to reduce the conservatism in industrial R&D.

Barriers

- Funding for a solutions covering 'the bigger picture' are not available. Academia and research can be looking at a small/narrow research area
- Lack of consistent representation from beginning to end when moving through the design cycle
- Pre-processing and post processing can take longer then running the model
- Validation and verification requires the software to be kite marked and the results have to be validated through demonstration. Also old copies of software and models need to for future use e.g. auditing or having to return to recalculate values

- Number of assumptions needed to obtain high quality simulations. This includes assumptions needed to go between scales and different models
- Design is step-by-step and requires co-design utilising multiple disciplines
- Bigger gap between industry approach and research
- R&D in industry is to conservative
- Data is not available or has to be paid for
- Too much time spent on solvers. When it takes too long to mesh the model.

What are the potential risks and benefits of uptake of these new design and simulation and modelling techniques?

Risks

Benefits

- Problems / challenges closer to those encountered in industry may be solved.
- Important to numerous sectors: biomedical, automotive & energy storage, aerospace

Appendix One: Agenda

Time		Contribution	Speaker / Institution
09:30	10:00	Registration and Refreshments	
10:00	10:15	Introduction to Workshop	Lynne McGregor Innovate UK
10:15	10:30	Challenges by Industrialists [1]	Nadir Ince Alstom Power
10:30	10:45	Challenges by Industrialists [2]	Adam Kowalski, Massimo Noro Unilever PLC
10:45	11:00	Challenges by Industrialists [3]	Akin Keskin Rolls-Royce PLC
11:00	11:15	Interim SIG Update: UQ&M SIG	Jeremy Yates University College London
11:15	11:30	Interim SIG Update: HPC	Sondipon Adhikari University of Swansea
11:30	11:45	Explanation of Break-out	Paul Huggett The Knowledge Transfer Network
11:45	12:45	Break-out Session One	All
12:45	13:30	Lunch and Networking	
13:30	14:10	Summary Presentations from Groups	All
14:10	15:10	Break-out Session Two	All
15:10	15:30	Coffee and Networking	
15:30	16:00	Summary Presentations from Groups	All
16:00	16:10	UQ&M Capability Database	Matt Butchers The Knowledge Transfer

			Network
16:10	16:20	Activities of the Defence Science and Technology Laboratory	Jenny Decerbo Dstl
16:20	16:25	Innovate UK Activity	Lynne McGregor Innovate UK
16:25	16:30	EPSRC Activity	Rob Felstead EPSRC
16:30		Close and Networking	

Appendix Two: Delegates

	Surname	First Name	Institution
1.	Adhikari	Sondipon	University of Swansea
2.	Alderson	Andrew	Sheffield Hallam University
3.	Allen	Christian	University of Bristol
4.	Aston	Martin	Airbus UK
5.	Baty	Simon	Knowledge Transfer Network
6.	Bayly	Andrew	University of Leeds
7.	Branciforti	Valeria	Knowledge Transfer Network
8.	Branke	Juergen	University of Warwick
9.	Brettschneider	Julia	University of Warwick
10.	Brooks	Jeffery	University of Birmingham
11.	Burman	Erik	University College London
12.	Burnett	Michael	Knowledge Transfer Network
13.	Butchers	Matt	Knowledge Transfer Network
14.	Chen	Yuhang	Heriot-Watt University
15.	Chong	Seng	De Montfort University
16.	Cocks	Alan	University of Oxford
17.	Cooper	Jonathan	University of Bristol
18.	Correia	Tatiana	Knowledge Transfer Network
19.	DeCerbo	Jenny	DSTL
20.	Duffett	Gino	NAFEMS
21.	Evans	Ben	Swansea University
22.	Falzon	Brian	Queen's University Belfast
23.	Farid	Mohammad	Ford
24.	Farnsworth	Michael	Cranfield University
25.	Felstead	Robert	EPSRC
26.	Figiel	Lukasz	University of Warwick
27.	Fonseca	Joana	City University London
28.	Fraga	Eric	University College London
29.	Georgiorgis	Dimitrios	University of Edinburgh
30.	Gilbert	Matthew	University of Sheffield

31.	Grob	Ralph	Centre for Process Innovation
32.	Guenov	Marin	Cranfield University
33.	Hanley	Kevin	University of Edinburgh
34.	Hawe	Glenn	Ulster University
35.	Hine	Nicholas	University of Warwick
36.	Huggtt	Paul	Knowledge Transfer Network
37.	Icardi	Matteo	University of Warwick
38.	Ince	Nadir	Alstom Power
39.	Johnston	Jaimie	Bryden Wood
40.	Kenney	Richard	Siemens
41.	Kenny	Steven	Loughborough University
42.	Keskin	Akin	Rolls-Royce
43.	Knowles	Joshua	University of Birmingham
44.	Kowalski	Adam	Unilever
45.	Lee	Peter	University of Manchester
46.	Liu	Dianzi	University of East Anglia
47.	Mansfield	Neil	Imperial College London
48.	Marco	James	University of Warwick
49.	Marques	Simão	Queen's University Belfast
50.	Masoero	Enrico	Newcastle University
51.	Masters	Andrew	University of Manchester
52.	May	Gordon	Rolls-Royce PLC
53.	McGough	Stephen	Durham University
54.	McGregor	Lynne	Innovate UK
55.	McKay	Alison	University of Leeds
56.	Morris	Tim	NAFEMS
57.	Noro	Massimo	Unilever
58.	Palacios	Rafael	Imperial College London
59.	Papanicolopulos	Stefanos	University of Edinburgh
60.	Race	Chris	University of Manchester
61.	Rix	Nigel	Knowledge Transfer Network
62.	Shah	Nilay	Imperial College London
63.	Shaw	Simon	Brunel University
64.	Shires	Andrew	University of Leeds

65.	Sun	Jin	University of Edinburgh
66.	Toropov	Vassili	QMUL
67.	Tran	Van-Xuan	EDF Energy
68.	Triantafyllou	Savvas	University of Nottingham
69.	Visavadia	Rhia	EPSRC
70.	White	Mark	University of Liverpool
71.	Wilson	Mark	University of Leeds
72.	Wright	Louise	National Physical Laboratory
73.	Wrobel	Luiz	Brunel University
74.	Xia	Yuying	University of the West of England
75.	Yan	Joseph	University of Liverpool
76.	Yates	Jeremy	University College London

Appendix Three: Key Industrial Challenges

Challenge	Description
CAD - CAE link	Pre-CAD design space representation and compatible link to CAD for manufacturing
Integration and coupling	Integration and coupling is technically challenging and often requires compromise on either scalability or precision
Mix of high order with simple models	Flow control needing high order modelling like LES linked to lower fidelity models like RANS
Incorporating metal forming micro behaviours	Effect of micro behaviour to improve metal forming, forging, etc. for large (all sectors) and small (e.g. heart pumps) components
Incorporating composite micro behaviour	Effect of micro behaviour on cracking and composite delamination.
Large noisy, discontinuous models	Challenges arise with working with large (order of 1000 design parameters) and simulation outputs that are noisy and discontinuous.
Inclusion of highly non-linear or highly interactive behaviour	How to include highly non linear models and/or high levels of interaction
Identifying dependent parameters	How can we tell which objectives share design parameters – i.e which are independent and which ones are dependent?
Small sets vs monolithic optimisation	Risks and benefits of using small sets vs monolithic optimisation
Real, complex problems	Usefulness of new techniques on real, complex problems
Modelling of composite failures	Detailed modelling of composite failure within complex structures (e.g. aircraft and/or automotive components).
Mathematics of fatigue calculations	Faster fatigue calculations, possibly mathematics of fatigue calculations
Complex fluid and solids material models for health sector	Complex fluid and solid material models for the health sector (bone, blood, tendons, etc.)
Composite materials modelling for health sector	Complex material composite
Prediction of residual stress	Calculation and predictions of residual stress in formed and machined parts based on grain structure
	Methods for material model for FE based on the microstructure and chemical constituents of the raw material
Parameterisation	Parameterisation - easier solutions required to access and transfer parameters from one type of model (e.g. CAD) for use in another
System modelling	Tools and methods to enable better multidisciplinary and systems based modelling in the built environment
V&V	Validation & Verification is a challenge in the health sector
Inverse Mapping	Use of Inverse mapping to understand the key uncertain contributors to the resulting output

Affect of regulations	Regulations do not allow to embrace new techniques easily (aero and medical for example) and slow down the deployment of
Automated meshing	Improved automated meshing.
Hex meshing	Automatic meshing for complex geometry using all Hex meshing (needing automatic blocking in 3D)
	Intrusive stochastic solvers for non linear equations
Visualisation of results	Improved tools and methods for visualisation of data, making results more intuitive and easier to understand, especially for non-modelling personnel e.g. managers needing the information.
Visualisation of design space	Tools for visualisation of design space.
Visualisation of optimisation results	Visual tools would be of benefit to demonstrate the optimised solution
Accuracy of surrogate models	Surrogate models often required to reduce simulation time but difficult to tolerate reduced accuracy inherent in this approach
Reduction of solution time	How can we reduce the design (optimisation) time where surrogate models cannot accurately be generated?
Improvements in surrogate models	Improvements in use of surrogate models to deliver value

References

i https://www.epsrc.ac.uk/research/ourportfolio/themes/manufacturingthefuture/

ii http://www.nafems.org/about/projects/simbest/

iii https://www.gov.uk/government/organisations/innovate-uk

iv http://www.nafems.org

v http://www.alstom.com

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