COMPUTATIONAL AND DATA SCIENCES IN LUXEMBOURG

LUXEMBOURG, AN EMERGING KNOWLEDGE ECONOMY

Luxembourg is one of the wealthiest countries in the world in terms of gross domestic product (GDP) per capita. The country has successively and successfully transitioned from an agricultural to a service-driven economy, through the heavy industry characteristic of the industrial revolution. In spite of these undeniable successes, driven in the recent past by the financial sector, Luxembourg has still not achieved the status of world-leading marketplace.

In 2003, the University of Luxembourg was created, with the aim to diversify the country's economy and facilitate its transition to a Knowledge Economy. Yet, in 2012, Luxembourg spent only 1.51% of its GDP on Research and Development, complemented by as much as 1% of its GDP provided by large companies such as ArcelorMittal, GoodYear (who is today the second employer in the country) and Delphi. The University, along with most of the research, development and innovation actors, including start-up incubators are now collocated in the exciting Belval Campus in the south of the country Figure 1.

Luxembourg has developed a Smart Specialisation Strategy (S3), focusing on Information and Communication Technology (ICT), Ecotechnology and Biotechnology. The materials, space and ecotechnology sectors are already somewhat consolidated and host a number of competitive companies, from metallurgy to high-performance composites (ArcelorMittal, Eurocomposites, e-Xstream, GoodYear and many others).

The health/biomedical sector was created ex nihilo from a 140M euro government investment in 2008 and reinforced by the creation within the University of the Luxembourg (Interdisciplinary) Centre for Systems Biomedicine (LCSB), which led to the creation of various spin-offs supported by fundamental research in Systems Biology. The ICT sector is supported by the Interdisciplinary Centre for Security and Trust (SnT) at the University of Luxembourg, and benefits from world-class interconnect infrastructure, providing the country with a clear competitive edge which attracted the likes of Google, Paypal and Amazon to the Grand Duchy.

This research and innovation landscape includes recent initiatives ranging from additive layer manufacturing to space and asteroid mining and may, at first, appear disparate in focus. Over the last 5 years, Computational and Data Science has been emerging as a

Figure 1. Belval Campus in the South of Luxembourg where the government, the funding council (FNR), the national research institutes and the University of Luxembourg, along with incubators are collocated

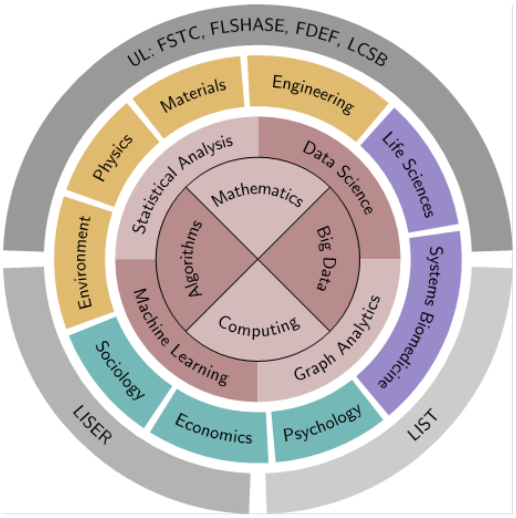

Figure 2. The methodological approach for computational and data sciences in Luxembourg. The methodological core relies on mathematical and computer science constructs which is used for a wide variety of applications, in collaboration with research centres and the industrial sector

unifying discipline. In 2013, the University of Luxembourg has made the field one of its core priorities. This unifying multi-disciplinary focus area relies on a strong mathematical, computational and methodological core (Figure 2) and has convinced policy makers, funding councils and the private sector through its ability to drive education, research and innovation across a wide range of sectors of central importance to Luxembourg.

We review in the following the key concepts underlying computational and data sciences in Luxembourg and focus on one particular application area: Computational Engineering Sciences, particularly relevant to ECCOMAS.

WHAT IS COMPUTATIONAL AND DATA SCIENCE (CODES) AND WHY IS IT IMPORTANT TO LUXEMBOURG?

Computational Sciences are fundamental to all fields: Translating complex real-world processes into mathematical models and simulations in the virtual world has been a key aspect of scientific advancement since the 1940's. The upcoming challenge is to build on the undeniable successes of Computational Sciences in Engineering and Technology to ethically and efficiently harness and exploit the soaring amounts of data and address open problems in medicine, social sciences and finance and build a smart, resilient, future-proof society (Bordas and Ley, 2018).

With powerful computers and robust algorithms, we are now able to simulate increasingly complex systems on the computer, and thus gain valuable insights without performing elaborate and costly experiments. Computations underpin disciplines as varied as biology, biomedicine, transportation, materials science, engineering, social sciences and even art.

Computations are pervading all disciplines. Modelling techniques are relevant to all technical and scientific areas. CoDeS aims to leverage this methodological commonality to increase the research and innovation productivity. Computational and Data Sciences researchers act as translators by using mathematical language as a common communication means to bridge gaps between disciplines and make research and innovation more effective.

At the University of Luxembourg, the CoDeS Community unites 10 core Faculty and 40 application Faculty members (including 5 ERC grants) who submitted third party projects for a total approximate cost of 240 million euros (20% of the total number of projects submitted at UL), produced half of the highly cited publications in Luxembourg at large.

- In years 2015-2016: 2,152 journal papers were published in Luxembourg. A third of those publications are in the field of Computational Sciences, including 8 highly cited articles, of which half were published by UL. The UL hosts a ISI Highly Cited Researcher in Computer Science (2015, 2016) and in Engineering (2017) [Link]
- A Doctoral Programme in Computational and Data Science was created.
- A Data Driven Computational Modelling Doctoral Training Centre application (DRIVEN - 22 PhD students) was funded by the Fonds National de la Recherche (FNR) funding council. The proposal bridges across all faculties and inter-disciplinary centres as well as two of the Luxembourg Public Research Institutes.

The Computational and Data DRIVEN Science Doctoral Training Unit (DTU) will train a cohort of Doctoral Candidates (DCs) who will develop data-driven modelling approaches common to a number of applications strategic to the Luxembourgish Research Area and Luxembourg's Smart Specialisation Strategies.

We propose to create this bridge between a methodological core and application domains by training each DC both in state-of-the-art data-driven approaches, and in the particular application domain in

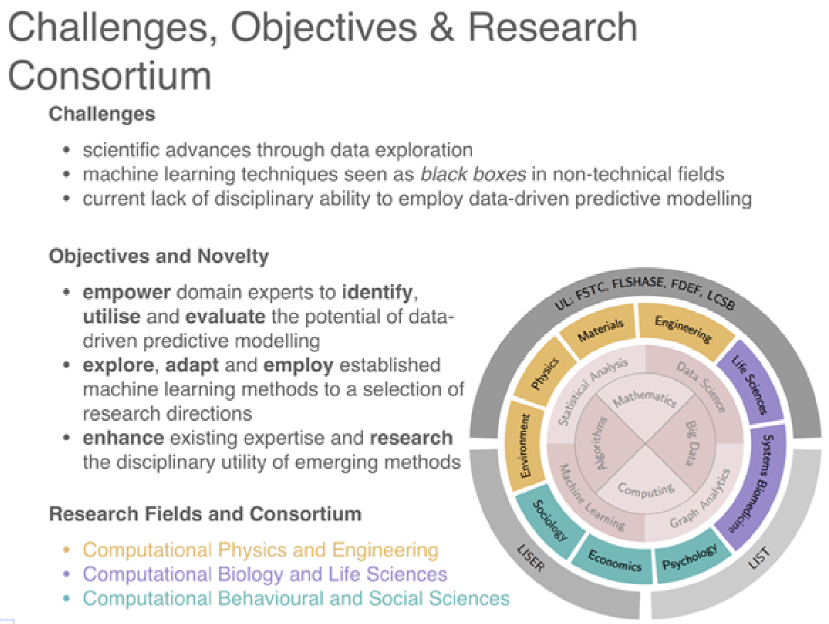

Figure 3. Concept behind the DRIVEN Data-Driven Modelling and Simulation Doctoral Training Unit (19 PhD students) funded by the FNR (2018-2023), led by Prof. Andreas Zilian (Computational Engineering) and supported by the University of Luxembourg Computational and Data Science Priority (CoDeS)

which these approaches are expected to lead to new discoveries: Computational Physics and Engineering Sciences, Computational Biology and Life Sciences, and Computational Behavioural and Social Sciences (Figure 3). In six years, DRIVEN will result in a group of scholars that enriches Luxembourg's socio-economic landscape not only with expertise in data-driven discovery and machine learning, but also with a fundamental understanding of how these approaches can be of most use to a wide range of focus areas.

We will strengthen the data-driven repertoire in areas already benefiting from these techniques, and will strive to establish similar techniques in areas where these approaches are only nascent. By embedding the DRIVEN DTU in the existing Doctoral School (DS) structure of the University of Luxembourg (UL), we will create its first transversal Doctoral Programme (DP), spanning all three Faculties and reaching out to the Interdisciplinary Centres, the LIST and LISER. DRIVEN will benefit from the already established doctoral education framework and best practices gleaned from previous DTUs, allowing our DTU to focus on innovative doctoral training strategies for its highly interdisciplinary research directions.

DRIVEN will contribute, in conjunction with strong national and European initiatives such as Digital Lëtzebuerg and the Important Project of Common European Interest on HPC and Big Data Enabled Applications, to boosting Luxembourg's competitiveness thanks to an increased ability to make use of the vast amount of data generated worldwide on a daily basis.

COMPUTATIONAL ENGINEERING

The Department of Computational Engineering Sciences (DCES) will provide a means to link and rationalise research and education efforts across a wide range of disciplines by tackling common fundamental methodological hurdles involved in modelling, simulating, controlling and understanding the physical world. Built around an open-source, open-data and collaborative approach, DCES will inspire and foster innovation and collaborative opportunities to ensure Luxembourg's international competitiveness and economic growth.

The aim of DCES is to become an internationally renowned institute, dealing with methodological research in Computational Engineering Sciences. By focusing on fundamental research while keeping a link to different applied science domains, we will continue to foster a nimble and adaptive economy and provide general methodologies on which to strengthen existing and build future priority application areas of National Importance.

The Department aims at building intuitive and interactive platforms for computational engineering problems that allow the users not only to understand and predict the behaviour of real systems but also to better capture the interaction between models and data and hence gain insights into unconventional and counter-intuitive phenomena.

We target the data-driven modelling, simulation, control and quality assurance of complex (dynamical) systems governed by partial differential equations applied among others to glacier, energy harvesting, medicine and surgery research, through the multi-scale design of lighter, stronger tunable, adaptive functional and reconfigurable matter (with Marie Curie Fellow Jakub Lengiewicz, IPPT Poland) as well as the modelling of organisms and diseases progression. As a second research strand, we target complex networks and their interaction with human behaviour, such as those arising in logistics, traffic, communication, energy, biological and social systems.

To achieve this goal, several challenges must be overcome, which are the core research directions of the Department.

- **Data** Acquire, process and fuse data sets for phenomena and systems of interest;
- **Model** Select the proper mathematical models capturing the problem dynamics and identify the most relevant parameters, given experimental evidence. This includes adopting multi-scale and single-scale approaches, multi- or single-field problems and solving large-scale instances;
- **Simulate and Control** Discretise and control the computational complexity of the models and of the predictive simulations. This will require working hand-in-hand with HPC developers, through co-design to optimise hardware for given computational needs, e.g. for (machine) learning algorithms and neural networks;
- **Assure quality** Quantify, measure and control the effects of uncertainties and errors on quantities of interest to the modeller;
- **Visualize** Provide tools for interpreting and visualising phenomena in order to develop decision support systems for different application domains.

The Department focuses on general methodological developments which are as application independent as possible in order to streamline research and optimise open innovation and productivity.

The research done at DCES is primarily data-driven modelling. We work in close synergy with (applied) mathematicians to ensure the mathematical rigour of the numerical methods we develop. We collaborate with computer scientists to create robust computational techniques required for reliable analysis and control of complex systems. Finally, we include in the Department an engineering flavour to guarantee that the theories and models developed are proven to provide societal and economic impacts.

DCES is instrumental in building powerful and impactful interdisciplinary connections between engineering, computer science, mathematics, physics and other priority application areas in Luxembourg. Areas where we have already had impact include in particular: Space Science, Advanced Manufacturing and Materials, Robotics, Automotive, Transport and Logistics as well as Neuro-degenerative Diseases.

The Department is organised within three subgroups:

- Data acquisition and analysis;
- Computational Modelling and Simulation for Networks and PDEs;
- Control.

In the following, we provide a few ongoing research directions of the Computational Modelling and Simulation subgroup as it is most relevant to ECCOMAS. The subgroup is led by three professors (Bordas, Peters, Zilian) working alongside three experienced postdoctoral researchers (Beex, Besseron, Hale). The team deals with advanced discretisation techniques for partial differential equations and particulate systems aiming at understanding the effects of variability, ambiguity, uncertainty in the selection of the most adequate models and their discretisations. Another key research direction deals with simulation quality control and acceleration, through model order reduction, error estimation and adaptivity. The team deals with problems ranging from real-time simulations (for image-based surgical guidance) to large multi-scale scale simulations. Through specific research examples, we provide below an overview of the work done in this subgroup.

MULTI-SCALE ANALYSIS OF MECHANICAL IMPACT OF GRANULAR MATERIAL ON STRUCTURES THROUGH EXTENDED DISCRETE ELEMENT METHOD (XDEM)

Handling of granular media e.g. transport and storage generates severe mechanical loads on walls or structures in contact. The latter may be static or moving in an arbitrary mode. In particular devices such as conveyors, chutes, truck bodies, grain elevators, hoppers or tyres are important examples of structures that experience a strong mechanical impact from moving granular material. Forces exerted may be predominantly static as during storage or may have a highly dynamic character as observed during discharge operations. It is essential for both design and operation to assess these evolving loads and to avoid major failure.

In order to estimate these forces acting on structures a coupling between the Finite Element Method (FEM) and the Discrete Element Method (DEM) is applied in the LuXDEM team. Contrary to approaches involving overlapping domains, the current concept employs non-overlapping computational domains. Thus, deformable structures and their stresses are represented by the Finite Element Method (FEM) while the granular material is described by the Discrete Element Method (DEM). The coupling technique identifies contact between discrete elements and the FEM mesh i.e. its surface elements. Contacts between the surface elements of the mesh and discrete elements generate forces due to impact that determine motion of individual particles

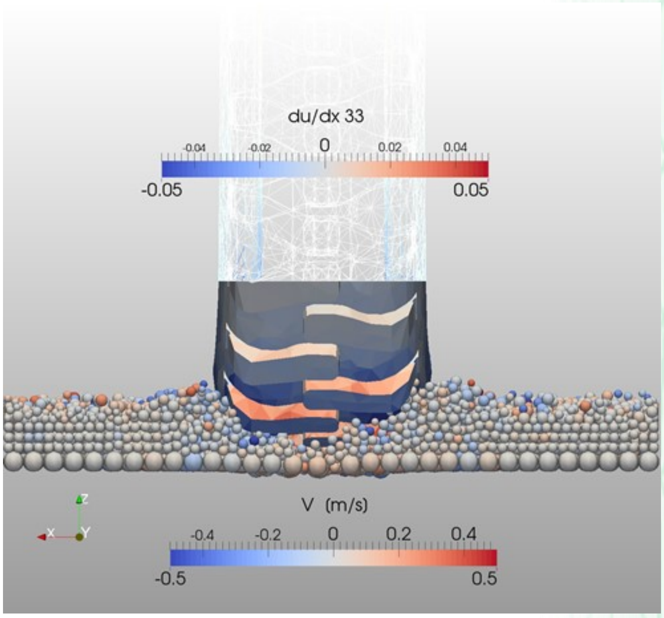

Figure 4. Deformation of a tyre and displacement of granular underground during rolling motion

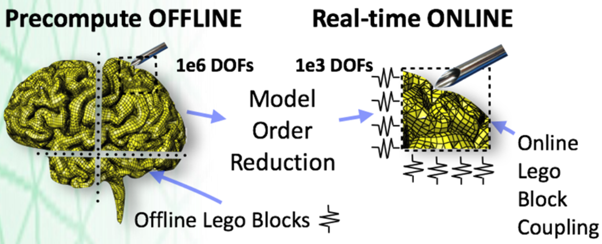

Figure 5. The principle of our domain-based model order reduction approach. Only the reducible subdomains are reduced (precomputed), whilst the subdomain where the needle is inserted or the tissue is cut cannot be reduced and is fully assembled into the system matrix. This work was done in collaboration with Pierre Kerfriden (Cardiff) and published in a series of papers

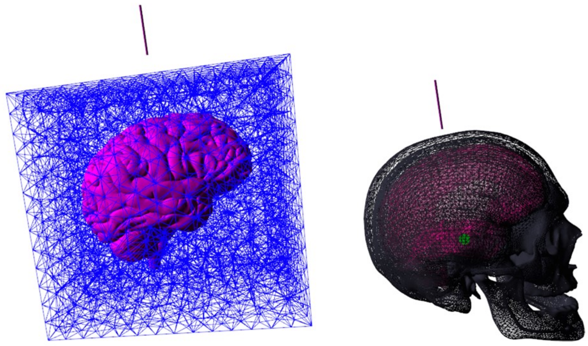

Figure 6. Implicit boundary definition and adaptive XFEM (CutFEM) approach to needle insertion for deep-brain stimulation. This work by Bui Huu Phuoc and Satyendra Tomar was submitted for publication in March 2018 (CMAME)

according to Newton´s second law for translation and rotation.

Similarly, forces generated exert a mechanical load on structures that consequently deform and respond with an internal stress distribution as shown in the following fig. X. The tyre supports the weight of the vehicle and thus, generates forces between the tread and the loose underground. It responds with a compaction and a displacement of individual particles. Integrating these individual contacts yields the total traction forces of the tyre that has a strong influence on load-carrying ability, steering stability and driveability.

REAL-TIME ERROR-CONTROLLED SIMULATIONS FOR SURGICAL TRAINING AND GUIDANCE

The team of S. Bordas has been working since 2012 (ERC RealTCut) on the development of real-time simulation tools for surgical training and guidance. This work has been done in collaboration with Dr. Pierre Kerfriden (Cardiff), Dr. Jack Hale and Dr. Lars Beex as well as strong collaborations with colleagues in computer science (Stéphane Cotin and Christian Duriez) and mathematics (Profs. Franz Chouly and Alexei Lozinski) as well as with neurosurgeons (Dr. Pierre Robe and Dr. Frank Hertel).

The work has focused mainly on the acceleration of non-linear computational mechanics of soft tissue deformation undergoing severe strains, cutting or topological changes. The main difficulty lies in the fact that model order reduction such as the proper orthogonal decomposition fails in regions where localisation takes place (Figure 5). To circumvent such problems, we developed adaptive reduced order modelling based on domain decomposition techniques. To further control the computational cost, we investigated the use of a posteriori error estimates, which we employed successfully for needle insertion problems with applications to deep brain stimulation.

To address the difficulties associated with dealing with complex geometries and topological changes, we developed enriched finite element methods (CutFEM approaches) where the boundary of the domain and that of the cuts or material interfaces (tumour/tissue) are not meshed conformally.

Finally, we realised that some of the most difficult questions in surgical simulation arise because of the difficulties associated with identifying the optimal material model, and associated parameters for a given patient. These requirements for patient-specific simulations led us to investigate model selection and model parameter identification using Bayesian inference, which is the focus of the team of Dr. Jack Hale and of part of the endeavours of Dr. Lars Beex, presented next.

EFFICIENT SCALABLE METHODS FOR UNDERSTANDING UNCERTAINTY AND IDENTIFYING OPTIMAL MODELS IN PHYSICAL SYSTEMS

The work described within this section is carried out by experienced researcher Dr Jack Hale whose team deals with large scale stochastic inverse problems and uncertainty quantification alongside advanced discretisation techniques for problems involving small parameters (e.g. locking).

Uncertainty quantification is an area of recognised importance in the computational sciences, and is receiving an ever-increasing amount of attention from the ECCOMAS community. In Luxembourg, we are developing new techniques and methodologies to tackle the next generation of uncertainty quantification problems.

We have recently looked at the question of how to calculate derivatives of systems with respect to their underlying stochastic parameters [Hauseux et al. 2017a]. We apply the Malliavin Calculus, a powerful tool of mathematical analysis, which extends the more classical notions of a derivative (e.g. Fréchet, Gâteaux) to stochastic processes. We have developed a computational method based on Monte-Carlo sampling to efficiently and accurately calculate this Malliavin derivative. In a hyperelastic beam buckling problem (Figure 7) we have shown that the classical notion of a derivative taken about the mean parameter is insufficient to quantify the sensitivity of the system. The Malliavin derivative gives a far more complete picture, taking rigorously into account the stochastic nature of buckling processes. Other interesting examples in fluid mechanics, viscoelasticity and elasticity are shown in the paper.

In another paper we looked at using classical (Fréchet) derivatives as a control variate method to reduce the sampling error of a classical Monte-Carlo estimator (Figure 8). In low to moderate-variance regimes, the proposed estimator is orders of magnitude more efficient than a standard Monte Carlo approach. We automatically compute derivatives of high-level finite element models using the FEniCS Project, making the approach broadly applicable to many different numerical models.

Ongoing work in the group includes the extension of the estimator in [Hauseux et al. 2017b] to random field problems [Hale et al. 2018].

MULTISCALE MECHANICS OF FIBROUS AND DISCRETE MATERIALS

The research conducted and supervised by experienced researcher Dr Lars Beex, whose team deals with the computational modeling of materials with some form of small-scale discreteness. Examples are paper materials, fabrics, foams and printed lattices. His efforts focus on

(i) the development of appropriate discrete models at the small-scale
(ii) the development of multiscale and model order reduction techniques to allow their use at the engineering scale.
For some time, Beex' group also targets (iii) the identification and propagation of the small-scale randomness of fibrous materials.

i) The development of discrete models for metal printed lattices and fabrics currently takes place thanks to the financial support of the Luxembourg National Research Fund and the University of Luxembourg, respectively. Issues of special interest are model-order-reduction with hyperreduction and volume-to-volume contact approaches for beams.
ii) Beex is mostly experienced with the quasicontinuum (QC) method as the multiscale method to allow discrete micromodels in engineering-scale computations. Advantages of the QC method compared to other nested multiscale approaches are its intrinsic concurrent character and the lack of scale separation (top in Figure 9). Originally developed for atomistic lattices, Beex et al. have widened its application domain towards elastoplastic, damageable spring and beam lattices [Beex et al., 2011, 2014a,b,c]. He has also advised in the efforts of Dr Ondrej Rokos and Dr Jan Zeman to include adaptivity in the QC method [Rokos et al, 2016, 2017]. His own efforts currently focus on the enhancement to treat random networks instead of lattices (top in Figure 9).
iii) The randomness in discrete materials such as random fiber networks is assumed to originate from two issues. First, each fiber has its own set of material parameters. This set is assumed to be a realisation from a probability distribution [Rappel et al., 2017]. Second, geometrical randomness is present. Current efforts focus on identifying the

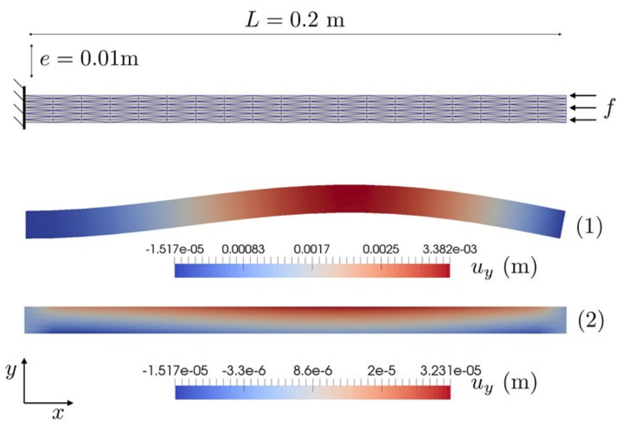

Figure 7. Two realisations of the solution of a geometrically non-linear hyperelastic beam problem with stochastic Young's modulus. Source: https://doi.org/10.1371/journal.pone.0189994.g006 Creative Commons Attribution License

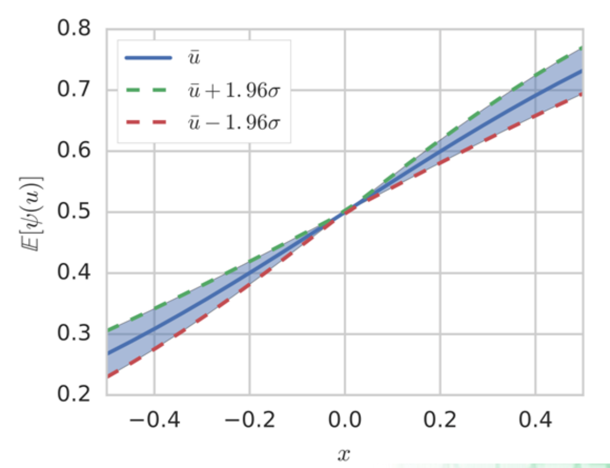

Figure 8. Solution of a stochastic non-linear Burgers equation using the proposed sensitivity control variate method. Mean and 95% predictive envelope shown. Source: https://dx.doi.org/10.6084/m9.figshare.3561306.v2. License: GNU LGPLv3 or later.

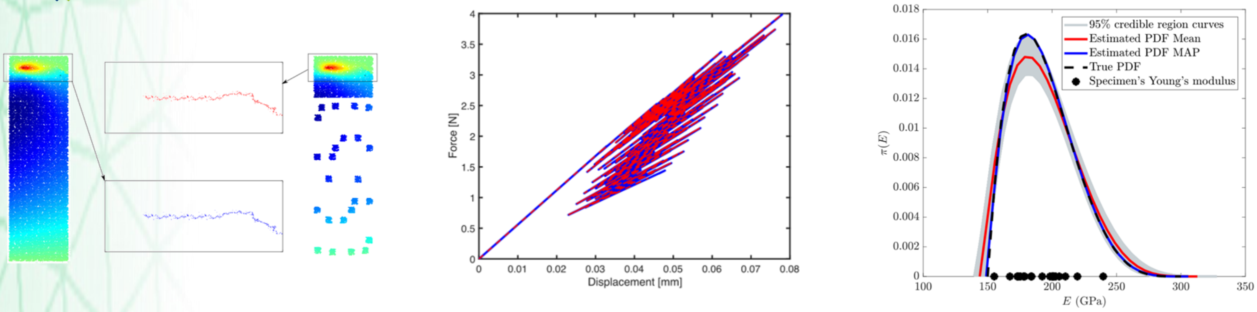

Figure 9. LEFT: Results of the DNS (blue) and a QC simulation for a model of 35x10 unit cells. Each unit cell consists of 100 fibers, discretized by 2001 linear elastic-perfectly brittle beams. Shown are broken beams and force-displacement responses. RIGHT: 15 Young's moduli (black dots) are generated from a beta-distribution ('True PDF'). Based on these 15 'measurements', the parameters of the beta-distribution are to be identified. These identified parameters are distributions themselves, and some realisations are shown in grey, whilst the mean is shown in red (a result of the PhD of Mr. Hussein Rappel)

parameters of the material parameter distribution, if only a small number of fibers are tested (bottom in Figure 9). Bayes' theorem is used to incorporate additional assumptions and to regularise the identification problem. The question currently being investigated is how precise we need to know the material parameter distribution, if geometrical randomness of the network itself will also be of influence.

SELECTION OF RECENTLY ACQUIRED PROJECTS BY THE COMPUTATIONAL AND DATA SCIENCE TEAM AT THE UNIVERSITY OF LUXEMBOURG

4 million euros for a doctoral training centre funded by the FNR for 20 PhD students

ERA chair funded by H2020 in Data Science and Mathematical Statistics for 2.5 million euros

Several grants funded by the FNR including

- a proof of concept grant to create a start-up from our research in CAD analysis transition for 250k
- a private public partnership with GOODYEAR for 700k euros
- a fundamental OPEN FNR grant for 350k from FNR on quantum continuum coupling using many body approaches

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