

Colloquium Final Report

N. 618 – Uncertainty quantification in computational mechanics

Dates and location: 13/12/2021 - 14/12/2021, Luxemburg

Chairperson **Lars Beex**

Co-Chairperson **Eleni Chatzi**

Conference fees

- registration fee **0.0 €**

What other funding was obtained? **Thanks to the virtual nature of the colloquium, no funding was necessary. This involved the financial support offered by EUROMECH (which was kindly waived as communicated with Prof. Magnaudet). Consequently, we also did not ask for any registration fees from the participants, but kindly asked all participants to register via the colloquium website. Because the colloquium was free and virtual, scientists from all over the world have attended the colloquium - as the registration list demonstrates. Although most participants have indeed registered, most presenters did not. For completeness therefore, the list of presenters reads:**

KEYNOTES: * Bruno Sudret (ETH Zurich) * Mark Girolami (Alan Turing/Cambridge) * Phaedon-Stelios Koutsourelakis (Munich) **STANDARD PRESENTATIONS:** * Alice Cicirello (TU Delft) * Feras Alkam (Bauhaus University Weimar) * Ludovic Noels (Liege) * Konstantinos Agathos (Exeter) * Sid Kumar (TU Delft) * Elizabeth Cross (Sheffield) * Yupeng Zhang (Texas A&M) * Rudy Geelen (Oden Institute) * Keith Worden (Sheffield) * Jack Hale (Luxembourg) * Pierre Kerfriden (MinesParisTech/Cardiff) * Costas Papadimitriou (Thessaly) * Hussein Rappel (Alan Turing/Cambridge/Exeter) * Johann Guilleminot (Duke) * Ethan Pickering (MIT) **LAST MINUTE CANCELLATIONS:** * Lori Brady (KEYNOTE, Johns Hopkins) * Bojana Rosic (Twente)

What were the participants offered? * **The abstracts of all presentations can still be found on the colloquium website (<https://618.euromech.org/programme/>)** * **The slides of 11 of the 18 presentations can still be downloaded via colloquium website (<https://618.euromech.org/slides/>).** The remaining presenters did not wish for their slides to be openly shared.

Number of members of Euromech (reduced registration fee) **54**

Number of non-members of Euromech (full registration fee) **9**

Applicants (members)

- Azam Abdollahi

PRESIDENT

Professor Marc Geers
m.g.d.geers@tue.nl

VICE PRESIDENT

Professor GertJan van Heijst
g.j.f.v.heijst@tue.nl

SECRETARY GENERAL

Professor Jacques Magnaudet
jacques.magnaudet@imft.fr

MANAGEMENT ADVISOR

Sara Guttilla
sara.guttilla@euromech.org

TREASURER

Stefanie Reese
euromech@ifam.rwth-aachen.de

- Feras Alkam
- Giacomo Arcieri
- George Burke
- Luis Celorrio
- Eleni Chatzi
- Li Chen
- Gonçalo Cruz
- Saranika Das
- SAURABH DESHPANDE
- Selamatit Dires
- Davi Matias Dutra da Silva
- Mahmoud Eltayieb
- Pravinkumar Ghodake
- Rainer Groh
- Phyo Wae Hein
- Cyprien Hoelzl
- Md Nurtaf Hossain
- Diego Hurtado Cathalifaud
- Gil Jacot-Descombes
- Colette Jost
- Inho Kim
- Artem Kulachenko
- Jyrki Kullaa
- Abhijeet Kumar
- Pulkit Kumar
- Zhenkun Li
- HyeongUk Lim
- Marcela Machado
- Muhammad Mohsan
- Jonas Nitzler
- Shashank Pandey
- Arjen Poot
- Matthias Preisig
- Laura Rahm
- Chiranthan Ramesh
- Mahindra Rautela
- YVES REULAND
- Gil Robalo Rei
- Annika Robens-Radermacher
- Nefize Shaban
- Gourav Sharma
- Anay Shembekar
- Joep Storm
- Zhaojie Sun
- Alessandro Tognan
- Matteo Torzoni
- Jörg F. Unger
- Ton van den Boogaard
- Manish Vasoya
- Kartik Venkatraman
- Kiran Vijayan
- Qianhui Yu
- Jie Yuan

Applicants (non members)

- Ali Amini
- Sharan Balasubramanian
- Manoj Kumar Dhadwal
- Suzana Ereiz
- Fotis Kopsaftopoulos
- Ning Li
- Yuriy Marykovskiy
- Ketson Roberto Maximiano dos Santos
- Mathias Peirlinck

Scientific Report

Uncertainty quantification in the virtual world of predictive modelling is the discipline of both characterising uncertain features and discrepancies of a model and propagating these uncertainties, in order to assess their effect on quantities of interest. Probability theory forms a quintessential corner stone of uncertainty propagation, as it provides the mathematical foundation to quantify uncertainties. Surrogate modelling, which generally only emulates a model's relevant input-output relations, and reduced-order-models, which incorporate the physics of the full model at reduced computation, are also further main ingredients. This is mandated from the complex, often non-linear and time-varying (and hence, time-consuming) nature of models that describe actual engineered systems.

The presentations in this colloquium all focus on one or more of the aforementioned foundations of uncertainty quantification: (A) probabilistic modelling and identification, (B) surrogate/reduced order modeling. Although not all presentations employ these concepts for uncertainty quantification, the diversity in themes and use cases bestowed the colloquium a liveliness that was well appreciated by the participants due to the colloquium's virtual nature.

Uncertainty quantification forms the foundation of numerous engineering fields, including reliability analysis and structural health monitoring and is well formulated, understood, studied and exploited by researchers working in such domains. In the field of computational mechanics however, uncertainty quantification is relatively new. The colloquium aimed at exchanging knowledge on uncertainty quantification across different research fields, with the physics of interest being, thus, highly diversified. The talks touched on both static and dynamic analysis, as well as both mechanics of solids and fluids. Depending on the target use case, certain presentations heavily relied on the treatment of experimental data, whereas others focused on development of novel numerical methods and their mathematical foundations. Again, this element of diversity was well appreciated by the participants.

Since each abstract can still be accessed online, the remainder of this section clusters the presentations in the three aforementioned topics: (A) Probabilistic models, (B) Surrogate/Reduced-order-models, albeit it may be clear that some would fall in more than one category.

(A) PROBABILISTIC MODELS

A fair portion of presented works dealt with probability theory. This group may be subdivided in two sub-clusters: those that dealt with efficiently probabilistically modelling and propagating uncertainties and those that focused on probabilistically identifying model features and their uncertainties.

Prof. Guillemot's presentation lied on the side of probabilistic modelling, focusing on fractional finite elements (FE) to effectively and efficiently sample parameter

inputs from random fields. Compared to commonly sampling from a high-dimensional probability density function, fractional FE models render the advantage of (1) being faster, and (2) ease of exploitation for complex geometries. Other presenters who focused on probabilistic modelling were Prof. Girolami and Prof. Worden who constructed finite element frameworks to efficiently and accurately incorporate uncertain model features such as uncertain model parameters. Such frameworks were demonstrated to work well in the context of non-linear problems. Prof. Worden presented a framework that evaluates the accuracy of a stochastic FE framework and, when this is deemed insufficient, the approach fuses the framework with use of a data-driven ML model. The last presenter incorporated probability theory in mechanical simulations was Dr. Hale, who used the Malliavin derivative to quantify the sensitivity of stochastic mechanical problems - in analogy to its use in econometrics. Prof. Cicirello, presented a non-intrusive framework for propagation of uncertainties through expensive-to-evaluate models. Bayesian optimization is employed to reduce the number of simulations to be evaluated and simultaneously quantify the uncertainty in the resulting response bounds estimates.

On the other hand, five presentations considered Bayesian inference to probabilistically identify model aspects such as model parameters and cracks. Bayesian inference unifies measurement data with a-priori knowledge of the physical system of interest and can even be used when the data has a high degree of sparsity. Dr. Alkam employed Bayesian theory for the probabilistic identification of cracks in catenary columns and validated his results with measurements from columns still in service. Prof. Noels on the other hand used the framework to identify orthotropic elastoplastic parameters of short-fiber-reinforced polymers in combination with a neural network to rapidly emulate the model's forward runs. Dr. Zhang on the other hand exploited Bayes' theorem to identify the parameters of elastoviscoplasticity using force-displacement curves and plastic surface deformation of nano-indentation. Dr. Rappel first presented a inter-correlated, bounded random fields model and then used Bayesian inference to identify the random fields' parameters for a sparse data set. Finally, Prof. Papadimitriou presented a design-of-experiments framework based on Bayes' theorem in the context of structural health monitoring where the aim is not to identify damage, but to identify what sensor locations have the highest probability to identify damage if it occurs.

(B) SURROGATE- /REDUCED ORDER MODELS

In this class of methods, we are concerned with models which substitute physics-based simulators. One approach to this end, is to rely on Full Order simulations from expensive numerical models. In this regard, Dr. Agathos presented a Reduced order Modeling (ROM) approach, where low-dimensional spaces are constructed from appropriately selected columns of the flexibility matrix of the system. In a similar spirit, Dr. Geelen presents a localized reduction approach that can be applied non-intrusively for nonlinear systems. The proposed reduced model is constructed entirely from snapshot data and does not require access to high-fidelity discretized operators. Prof. Kerfriden presents a Bayesian approach for reducing computation in multiscale simulations, by replacing the local microscale solution by an Encoder-Decoder Convolutional Neural Network that generates fine-scale stress correctors to coarse predictors. Dr. Pickering presented a Neural Network surrogate approach for nonlinear systems experiencing extreme events. The framework is demonstrated on prediction of extreme events related to deep-water waves.

On the other hand, surrogate models may be developed by means of data-driven inference. Prof. Kumar suggests such an approach, the EUCLID framework for

data-driven discovery of hyperelastic material constitutive laws, via either (i) a hierarchical-Bayesian sparse regression framework drawing from a large catalogue of candidate functions, or (ii) an ensemble of physics-consistent neural networks with higher generalization capabilities.

Finally, the possibility exists to combine physics-based models with data (grey-box modeling), as presented by Prof. Cross, who demonstrated a grey-box approach to physics-informed machine learning, where ML algorithms are adapted to account for physical engineering insights for improving predictive capabilities in Structural Health Monitoring (SHM). Prof. Koutsourelakis, further presented an integrative methodological framework, relying on both a black and grey-box approach for inverting the Process-Structure-Property chain in order to identify those variables which result in designs that satisfy property-related objectives.

Number of participants from each country

COUNTRY	PARTICIPANTS
Finland	2
India	12
Switzerland	10
Canada	1
Netherlands	7
Brazil	2
United Kingdom	2
Belgium	2
Ireland	1
United States	3
Iran	2
Luxembourg	3
Germany	6
Croatia	1
China	1
Italy	2
South Korea	2
Sweden	1
Spain	1
Japan	1
Turkey	1
TOTAL	63

Please send this report in electronic form to the Secretary General of EUROMECH, within one month after your Colloquium.