A productive year is ending

NEW RESULTS, COLLABORATIONS AND RECRUITMENT







ACOUSTIC SCATTERING T. KHAJAH, X. ANTOINE

IntuiSIM

FNR PROOF OF CONCEPT FUNDED

LEGATO & Z. TEAM NEWS

This newsletter was produced by the teams of Prof. S. P. A. Bordas and Prof. A. Zilian at the University of Luxembourg, *Department of Computational Engineering and Sciences*.

Main results

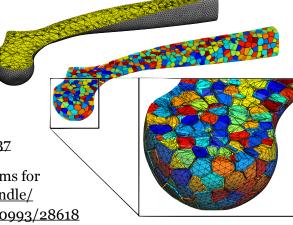
This year was very productive in terms of new results. The Team contributed to four major directions:

- Real-time error estimation for strong topological changes in surgical simulation
 Paper1 http://orbilu.uni.lu/handle/10993/30937
- Uncertainty Quantification and inverse problems for soft tissue biomechanics http://orbilu.uni.lu/handle/10993/28618
 10993/30946 and http://orbilu.uni.lu/handle/10993/28618
- Energy-minimal fracture http://hdl.handle.net/10993/29414
- **Bayesian** identification methods in mechanics: http://orbilu.uni.lu/bitstream/10993/29561/3/template.pdf http://orbilu.uni.lu/bitstream/10993/28631/1/1606.02422v4.pdf
- **CISM Udine** Short Course notes on CAD to Analysis Transition: http://hdl.handle.net/10993/31585

Selected New Collaborations

Year 2017 is ending and it is time to reflect on our achievements and what we could have done better. 2017 was particularly prolific in terms of collaborations. We developed new productive links with:

 The Mathematics laboratory in Besançon (Franz Chouly and Alexei Lozinski) where Stéphane Bordas was visiting professor in 2017.
 Together, they developed a posteriori error estimates for soft tissue The Department of
Computational
Engineering and
Sciences is being
created at the
University of
Luxembourg.



simulation https://hal.archives-ouvertes.fr/hal-01616322/document

- Alexander Tkatchenko (Physics, University of Luxembourg) on quantum-continuum coupling for adhesive and cohesive systems which led to exciting results.
- Giuseppe Sciumè on tumour growth. A PhD student (cofunded by France and Luxembourg through our matchfunding scheme will start within 2018 on cut-FEM approaches to tumour growth simulations.
- The Polish Academy of Sciences (**IPPT**), in particular Jakub Lengiewicz in the field of programmable and reconfigurable matter. A Marie Curie Fellowship is under review.
- Bruno Lévy at Inria with Natarajan Sundararajan IIT
 Madras on polyhedral finite element formulations (top)
 http://onlinelibrary.wiley.com/doi/10.1002/nme.4965/full
 https://arxiv.org/pdf/1407.1909
- TU **Prague**, with Dr. Jan Novak who will visit the lab for 2 years to work on multi-scale simulation of materials.
- Thasin Khajaj at the University of **Texas** at Tyler and Xavier Antoine (Nancy) on **acoustic** and electromagnetic **scattering**. This work will be continued in collaboration with Elena Atroshchenko from the University of Chile. https://arxiv.org/pdf/1610.01694 https://orbilu.uni.lu/bitstream/10993/28982/1/Wave_2017 paper.pdf
- The US Army Research Development and Engineering Command (RDECOM): the International Technology Center – Southern Europe (ITC-SE) located at the American Embassy
- The group of **Christophe Ley** at the University of Ghent. See our new paper "What makes Data Science Different" http://hdl.handle.net/10993/30235

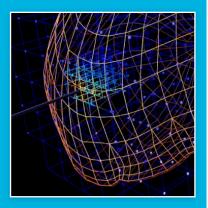
New Colleagues

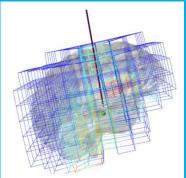
To support the creation of the Department of Computational Engineering and Sciences (DCES) at the University of Luxembourg, which will be led by Prof. Andreas Zilian, a professor of Data-Driven Modelling and Simulation will be recruited early in 2018. Negotiations are ongoing with the chosen candidate. DCES is also investigating:

 An FNR ATTRACT application in the field of analytical, experimental and computational approaches to smart soft materials.

Error-controlled real-time biomechanics







Top: ITN Rainbow project on breast cancer, with Anatoscope

Middle: Real-time error estimation for needle insertion.

Bottom: Deep-brain stimulation simulation with real-time quality control.

http://orbilu.uni.lu/handle/10993/29846 http://orbilu.uni.lu/handle/10993/30937

- An FNR PEARL application which will be discussed within the first quarter of 2018.
- An ERC Advanced Grant Transfer to the Department.

New Ph.D. Students

- Raphaël Bulle on error estimation for stochastic PDEs.
- Michal Habera joined on a FEDER-funded project and works on modeling and prediction of concrete degradation using FEniCS.
- Soumianarayanan Vijayaraghavan on FNRS-FNR-INTER Project on stochastic modelling of additive manufactured structures.

New projects

• Marie-Curie ITN Rainbow started on rapid biomechanics simulations for treatment optimisation (See **Jobs** below).

- FNR Proof-of-Concept IntuiSIM will investigate commercialisation routes for the novel CAD to Analysis pipelines developed at Legato.
- FNR OPEN with Alexander Tkatchenko on the multi-scale simulation of adhesive systems in collaboration with Thanh-Tung Nguyen and Paul Hauseux.
- FNR Public-Private-Partnership with Goodyear (SLIPEX) in collaboration with Physics and Materials Science at the

University of Luxembourg. The aim is to investigate the rheology of non-Newtonian fluids during tire manufacture. The Legato lead Investigator is Jack Hale and <u>Martin Řehoř</u> is the post-doctoral fellow in charge of the simulations.

• DFG-FNR-INTER Project led by Lars Beex on statistical modelling of foam structures for energy absorption, in collaboration with Saarbrücken Materials Science will start within 2018.

Outputs

Main publications emanating from the permanent team members in the team available here:

- Stéphane P. A. Bordas https://www.scopus.com/authid/detail.uri?authorId=23033088300
- Andreas Zilian https://www.scopus.com/authid/detail.uri?authorId=24485714700
- Lars Beex https://www.scopus.com/authid/detail.uri?authorId=35101441400
- Jack Hale https://www.scopus.com/authid/detail.uri?authorId=24331647800





This year, we published in new journals we had never contributed to: PlosOne, Mechanics of Time-Dependent Materials, IEEE Transactions on Biomedical Engineering and Probabilistic Engineering Mechanics.

Institution building proposals

This year was marked by the submission of 4 major institution-building proposals aimed at addressing

structural research gaps at the University of Luxembourg.

- H2020 ERA Chair in Applied Mathematical Modelling with applications to Free Boundary Problems (2.5M)
- H2020 ERA Chair in Applied Statistics for BigData (2.5M)
- H2020 TWINNING with Inria (France), ICES Texas,
- FNR PRIDE Proposal on Data-Driven Modelling and Simulation across the fields (Fig. p3). This was the first all-UL proposal and assembled collaborators from the LIST, LISER, LCSB and all the faculties at UL (2.5M).

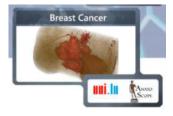


4 PhD Graduates

Congratulations! Four PhD students graduated this year: Danas Sutula (energy-minimal crack propagation); Mohammed Al-Saad: (SPH simulations of blood flow); Srivathsan Ravi (energy harvesting) and Amalya Khurshudyan (model order reduction).

Alumni news

- Nguyen-Xuan Hung is for one more year an ISI Highly Cited Researcher in Computer Science.
- Danas Sutula is now post-doctoral researcher at FEMTO ST in Besançon.
- Huu-Phuoc Bui is now post-doctoral researcher at the Laboratoire de Mathématiques de Besançon.
- Davide Baroli continues his work on model order reduction in FEniCS with Prof. Zilian with applications to FSI for energy harvesting.



Awards

Stéphane P. A. Bordas is for the second consecutive year a **ISI Highly Cited** Researcher in Computer Science. In 2017, he is also a highly cited researcher in the field of Engineering.

This is not only a personal award and would never have been possible without the contribution of close colleagues, in particular Pierre Kerfriden, Timon Rabczuk, Sundararajan Natarajan, Nguyen-Vinh Phu and Nguyen-Xuan Hung.

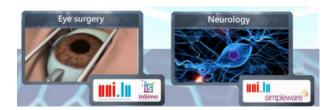
Events

The Legato and Z. Teams organised the 2nd Exploratory Workshop on Model Order Reduction in Luxembourg with roughly 50 participants. http://eumornetlux.weebly.com/ as well as a number of distinguished Computational Sciences seminars.

Dr. Jack HALE and the Legato and Z. Teams organised a FEniCS conference https://fenicsproject.org/fenics17/ which was a great success with 82 participants, 39 presentations and 16 posters: proceedings are found here https://dx.doi.org/10.6084/m9.figshare.508636 and a NUMFOCUS report can be downloaded here: https://www.numfocus.org/blog/fenics-conference-2017-in-review/

Jobs

We are looking for 5 PhD students for the RAINBOW Marie Curie Network led by Kenny Erleben in Copenhagen, both in Luxembourg and at Cardiff University.





Teaching and Doctoral Programme

The team continued teaching within the Engineering Curriculum, both at the Bachelor and Master's level, taking on significant courses from basic mathematics in the first year to engineering mechanics and MATLAB.

Some post-doctoral fellows in the team as well as all PhD students are contributing to teaching.

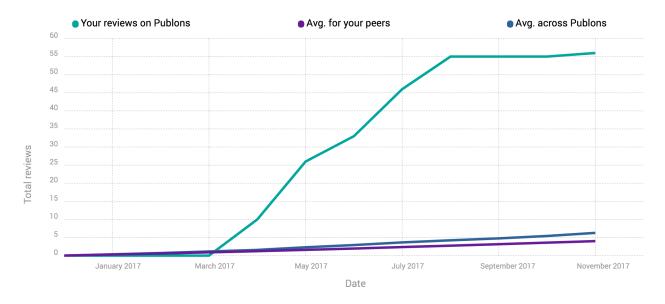
Since year 2017, we have been contributing to the courses in Industrial Mathematics, part of the Master in Mathematics of the University of Luxembourg. We have been actively involved in organising CISM Courses, in Udine *CAD to Analysis Transition*: http://hdl.handle.net/10993/31585

We have created a new Programme in Computational Sciences across the Faculty and are aiming to make this programme the home to all PhD students at the University of Luxembourg doing research in the field of Computational Sciences. As shown in the DRIVEN PRIDE proposal submitted in 2017, this will involve all faculties in the University.

Contribution to the Community

In addition to the events described above, the team has increased its contribution to the community through Editorial responsibilities and the organisation of a number of mini-symposia at various conferences, participation in recruitment committees and panels at various funding agencies worldwide. In 2018, S. Bordas will be the vice president of the Jury responsible for the recruitment of Chargés de Recherche at Inria (France).

See, for example, a Year in Peer Review https://publons.com/year-in-review-2017/659621/





In the name of all researchers in our teams at UL, we wish you the best for 2018 and a happy festive season. May 2018 be a year for meaningful contributions and respect amongst researchers.