

Computational Sciences Luxembourg



2016 ACTIVITY REPORT

Digital Lëtzebuerg

CoSc are the backbone of Digital Lëtzebuerg by stimulating multi-disciplinary research and innovation across Luxembourg and contributing to the diversification of its economy.

What are CoSc?

Scientific computing is a key enabling technology to address technological and scientific challenges. It has become the third pillar of research and innovation. Traditionally, CoSc have been key to engineering applications. A challenge is to impact other disciplines such as social sciences, finance and medicine.

Computational Sciences (CoSc)

CoSc is a crucible that brews brains with computers to distill multi-disciplinary innovation. Computations are pervading all disciplines and modelling techniques are relevant to all researchers. CoSc will leverage this methodological commonality to increase the research and innovation productivity in Luxembourg.



Luxembourg Computational Sciences for Medicine Workshop 2016 Dec <https://csworkshop2016.uni.lu/> 60 computational science researchers and clinicians discuss the future of virtual medicine. <http://wwwen.uni.lu/fstc/actualites/computational-sciences-conclude-a-flourishing-year>

From FSTC to Luxembourg

Born from a bottom-up initiative of Mathematics, Computer Science, Physics and Computational Engineering, Computational Sciences (CoSc) have contributed to create at UL a positive and symbiotic research environment relying on a strong fundamental scientific research core. CoSc will continue to rationalize research efforts across a range of strategic innovation domains by centralizing research and development tools and building upon the existing strengths of the



Translators

CoSc researchers act as translators by using mathematical language as a common communication means to bridge gaps between disciplines.

Building bridges

We have the dual aim to strengthen UL's theoretical and computational core and building bridges between strategic priorities. Our **objectives** are to:

- deliver nimble computational researchers and computation-aware application scientists;
- drive research and innovation at the interface between Data and Computational Sciences;
- increase research productivity by mutualising resources and talent;
- help diversify the Luxembourgish economy by building on existing strengths in data security and IT.

Strategy

Focus on academic excellence in the core methodological building blocks common to a number of identified strategic application domains ranging from FinTech and logistics to biology, materials and cognitive psychology.

An active community

Today, the CoSc Community unites 10 core faculty and 40 application faculty (including 4 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.

Luxembourgish research and socio-economic landscape.

Challenges

The challenge for Europe at large is to leverage the "data revolution", educate specialized experts able to follow the ever-increasing complexity of the application domains and to harness the power of extreme computing architectures (High Performance Computing). Our CoSc strategy aims at providing Luxembourg with a head-start to lead Europe into this challenging and exciting future.

A digital revolution in teaching, learning and research

By enabling Digitalisation at all levels within the Luxembourgish socio-economic context, CoSc will help make UL a model University of the 21st century, at the heart of Europe. Through an integrated teaching, learning and continuing education programme from early age to professional life, CoSc will train the actors of the 3rd Industrial Revolution and make Luxembourg one of its forerunners. CoSc will strengthen education and training of the Luxembourgish population, attract talent from abroad and train a local and nimble skilled workforce able to embrace the challenges of the Digital Revolution.

Table I.

Faculty/ Centre	CoSc projects submitted* in 2015-2016
FLSHASE	6
FSTC	68
LCSB	26
SNT	89
DEIS	1
Grand Total	190
% of all UL submissions	19%

Critical mass

To support its strategy, CoSc foresees the recruitment in 2017 of core professors in computational applied mathematics and statistics.

Third party funding

Data retrieved from the electronic Project Announcement Sheet (e-PAS) shows that 19% of all submitted projects (approx. 1000) in 2015 and 2016 are classified as "Computational Sciences" (Table 1). SNT and FSTC have the largest portions of CoSc-related submissions, followed by LCSB, FLSHASE, and DEIS (Fig. 1).

These project proposals amount to 240 million euros.

Publications

In the last two years (2015-2016), 2152 journal papers were published in Luxembourg. **A third of those are in the field of Computational Sciences**, including 8 highly cited articles, of which half were published by UL.

2015-2016 activities

With the nomination of Prof. Stéphane P.A. Bordas as Head of the Computational Sciences Priority in 2014, an intensive round of bilateral and group talks was kicked off between him and researchers from all UL Faculties and Centres. After many personal exchanges with highly motivated colleagues, Stéphane created the Monthly CoSc Group Meetings.

Invitations were sent very broadly across the University in the hopes that each interested unit or group would send a representative. The attendance varied from one meeting to the next but generally included at least one representative from: Mathematics Research Unit (RMATH); Institute for Computational Engineering (ICE); Computer Science and Communications Research Unit/Centre for Reliability, Security and Trust (CSC/SnT); Physics and Materials Science Research Unit (PhyMS); Luxembourg

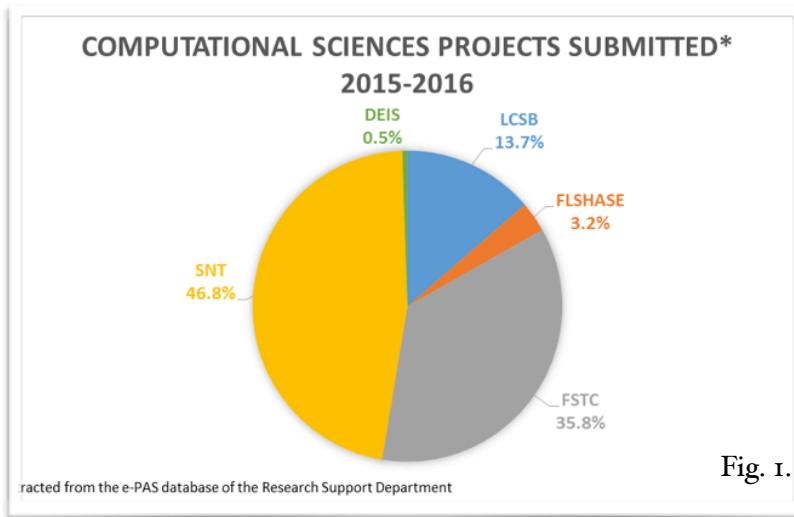


Fig. 1.

	2016 only	Luxembourg	UL	% UL
Articles published (cf. WoS)	1105	496	45%	
CoSc articles	152	96	63%	
Highly cited articles	10	5	50%	
CoSc Highly cited articles	2	2	100%	

Socio-economic impact

CoSc are already key to local industry development. To further strengthen socio-economic impact, we will:

- create a "Luxembourg Modelling Week" for Industry. To increase international collaborations;
- create a Distinguished Visiting Fellowship programme will be created for high-quality foreign PhD students, post-docs and faculty. We will aim at the creation of Industrial chairs and to a funding programme similar to the French CIFRE;
- encourage staff (in particular professor) secondments to the local industry.

2018 Crucible in a box

We will run in 2018 the first Crucible in continental Europe based on the CrucibleInABox model from NESTA. This innovative approach helps "researchers, who face demanding challenges in their own fields, to network and look to solve more complex challenges across several disciplines. By bringing bright thinkers together, Crucible was designed to help people see the bigger picture [...] how evidence-based policy is made, how to communicate with the media and public, skills and attitudes likely to make their research more innovative, how thinking creatively can really make a difference to their work and career."

School of Finance (LSF); Integrative Research Unit on Social and Individual Development (INSIDE); Life Sciences Research Unit (LSRU); Luxembourg Centre for Systems Biomedicine (LCSB).

These meetings showcased two important features of the CoSc priority initiative: its extremely open interdisciplinarity, and its "bottom-up" character.

Core mathematics and application scientists

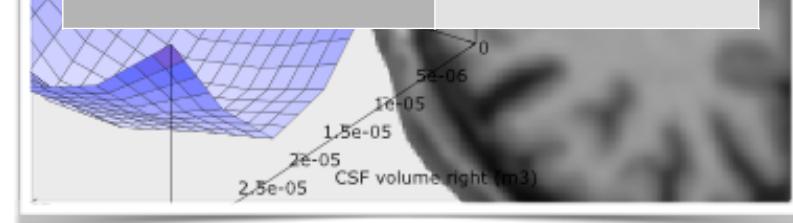
Monthly discussions within such a diverse group of researchers always proved fascinating and often proved challenging. It was clear to see that the relation of each represented domain to Computational Sciences could be classified according to:

- The researchers advance the mathematical foundations of CoSc.
- CoSc is more like a "tool" to perform more applied research.

Such a differentiation yields what can be described as a

Table II.

Funding source	CoSc Projects submitted* in 2015-2016
EC	46
FNR	115
Others (foundations, etc.)	11
UL	18
Grand Total	190



Milestones

- 14 CoSc seminars (2015/16)
- CoSc workshop in Computational Sciences for Medicine (Dec. 2016)
- 2016 June Creation of "computational sciences" category in orbi.lu to track publication output
- Creation of http://wwwen.uni.lu/recherche/fstc/computational_sciences
- Identification of interested UL researchers (2015/16)
- ScienceRELATIONS collaboration (2016)
- Multi-disciplinary computational office @LCSB
- 12 CoSc flagship projects
- Maths-Engineering-Industry co-supervision of Master students
- New teaching and PhD programme in CoSc (CSC, RUES, RMATH)
- New master programme in industrial mathematics
- Professor in data-driven computational engineering (50 applications received)
- Monthly multi-disciplinary seminar driven by CoSc Post-docs
- Monthly multi-disciplinary PhD seminar
- Over 30 CoSc visiting scholars and 14 seminars

reduced "mathematical core" of researchers (around 10) pushing the frontier of mathematical knowledge, with help from computer sciences, to enable the study of new, more complex systems or the exploitation of (often large amounts of) information.

The remainder (around 40) of the researchers find themselves rather in the category of "advanced application scientists" of those developments. The **particularity of UL** on this matter is that the "application scientists" are very mathematically and algorithmically advanced: they themselves publish methodological papers on the analysis of complex systems or big data within their disciplines.

Computational Sciences in the next P4

CoSc have been successfully implemented over the first 3 years of the 2014-17 P4, with one year left of that P4. Much of the work accomplished until now has dealt with assessing the level of CoSc activity already present at UL, increasing its visibility, and creating scientific exchange fora for interdisciplinary research. The main takeaway from this first P4 of the CoSc priority, and from the 2016 external evaluation, is that UL needs to strengthen its "computational core" by hiring five new computationally-oriented professors: one in numerical modelling (PR1 with RMATH), in data analysis and statistical modelling (PR2 with RMATH), in artificial intelligence and dimensionality reduction (PR3 with CSC), in optimisation (PR4) and in multi-level and parallel methods (PR5). Their expertise, together with the existing professors in computer science and HPC, will solidify the core mathematical competences needed to advance the state of the art in Computational Sciences which, in turn, will enable outstanding research in other priority fields requiring CoSc (e.g. materials, systems biology, Logistics, FinTech, etc.).

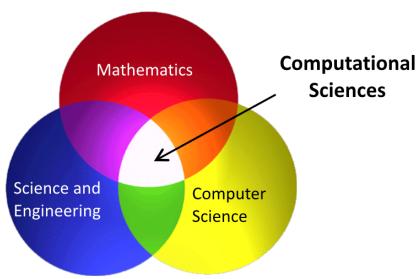
Goals for 2017

- 2017-01 S. Bordas visits IWR in Heidelberg to discuss best practice
- 2017-01 S.Bordas & P. Souza: Luxembourg CoSc road show
- 2017-01-27 Amis de L'Université: CoSc meets Industry networking cocktail (>30 confirmed) at UL
- 2017-03 Interviews for Data-driven computational engineering professor
- 2017-04 ERC Proof-of-concept with CHL on Surgical Simulation
- 2017-06-12/14 FEniCS Open-Source Scientific Computing Conference in Luxembourg
- 2017-06 Distinguished CoSc Workshop
- 2017 ERC Advanced Grant transfer in the field of "mesh generation"
- 2017-10 Widening participation H2020 proposals: TWINNING, TEAMING
- 2017-10 ERA Chair application for PR
- 2017 Recruitment of Computational Mathematics and Data Analysis and Statistical Modelling Professors (PR1, PR2)
- 2017 first steps towards an ERC Synergy grant

We propose that PR1-3 be recruited as early as 2017 or, at the latest, early in the next P4. These recruitments are urgent as opportunities are currently being missed for industrial projects at the interface with mathematical modelling, statistics and artificial intelligence/model reduction. Importantly, PR1-3 will consolidate multi-disciplinary CoSc teaching across RMATH, CSC, PhyMS and Computational Engineering. PR4-5 should be recruited within the next P4. For this, we will leverage ATTRACT, PEARL, ERA Chairs, ERC and industrially-sponsored chairs.

Closely following the strengthening of the CoSc core, bridging professors at the interface between modelling and Luxembourg's strategic priorities will be recruited. This will create "bridging" positions between the mathematical foundations and high-impact fields for Luxembourg and UL.

- Medical Imaging with application to surgery simulation (with LCSB and CHL)
- Complex systems in biophysics (with LCSB and PhyMS)
- Artificial Intelligence with data-driven application (with Computer Science RU, SnT and LCSB)
- Active and programmable matter (with LIST, LCSB and PhyMS)
- Computational finance (with LSF)
- Modeling interfaces with applications in microfluidics and organoids (with LCSB and PhyMS)



Philosophy

Research in CoSc, at the confluence between Science and Engineering, Mathematics and Computer science, focuses on the development of new computational tools driven by application areas in science, engineering and technology, but also emerging areas where simulations are gaining importance such as the humanities and medicine/surgery.

Computational Sciences are therefore transversal to all areas of the university, and priority areas of the Smart Specialisation Strategy of Luxembourg and of the FNR.

Our research strategy is to focus on developing a continuum methodology, from real-time, data-driven simulation to predictive, multi-scale models, connecting these two by statistical modelling and dimensional reduction enabling users to make decisions in uncertain conditions.

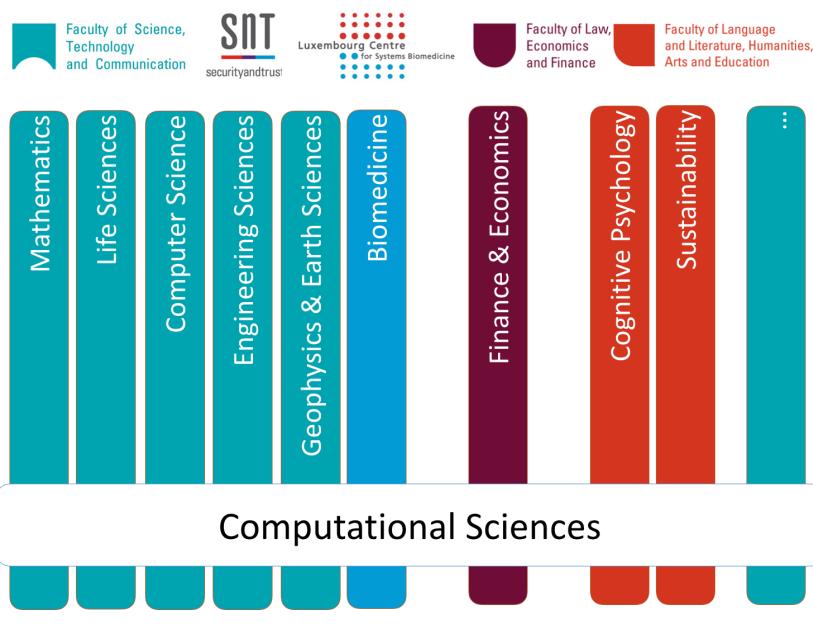
This strategy is expected to be particularly strong in Luxembourg where the abundance of data, IT firms, high-end engineering companies, insurance and reinsurance are flourishing.

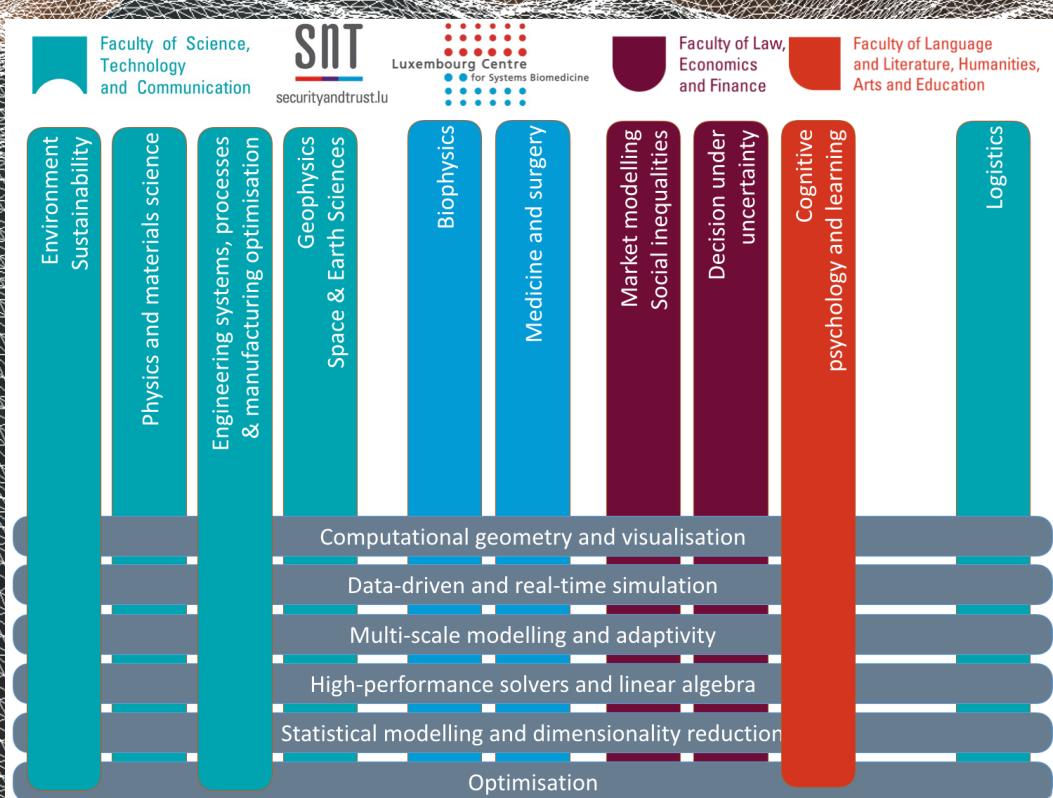
Conclusions

Computational Sciences are a key enabling technology for all strategical domains in Luxembourg. It relies on core mathematical building blocks to streamline research efforts, accelerate innovation, diversify its economy and prepare the country for the 3rd industrial revolution. A nation's success will depend on its ability to harness computational methods and Luxembourg stands today at a turning point.

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Multi-grid generation of random fields (Jack Hale and Paul Hauseux, Legato team)