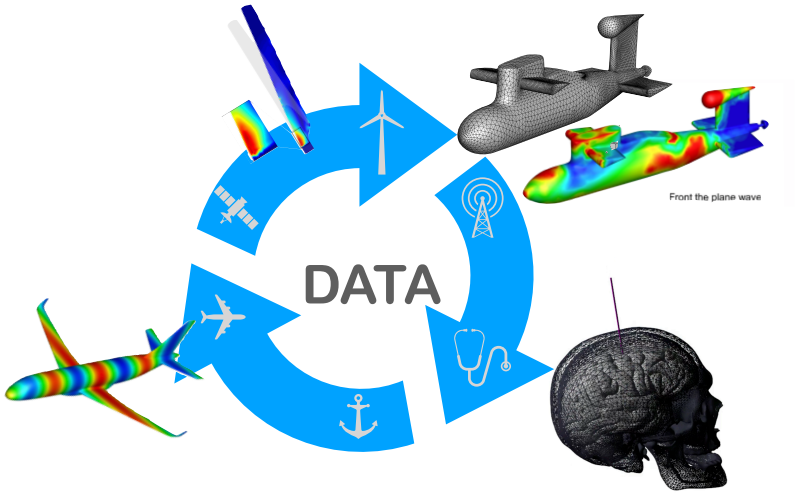
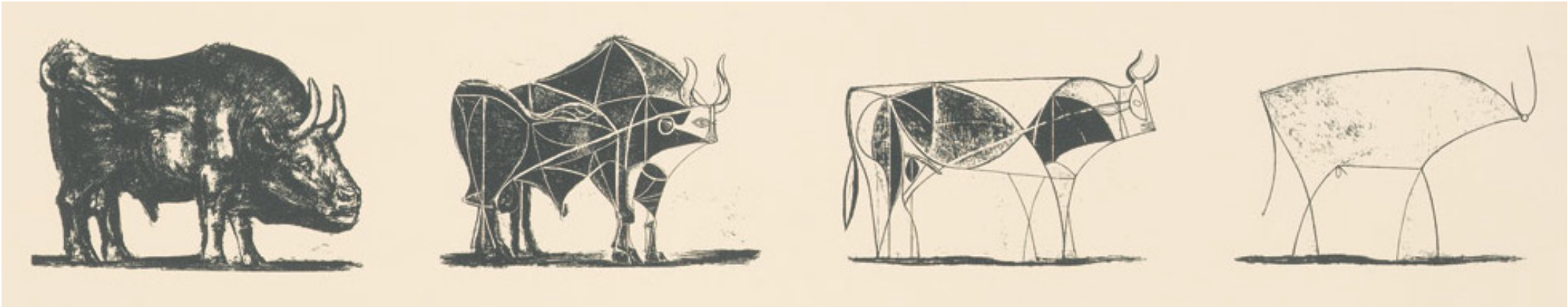
Data-driven computational engineering sciences in Luxembourg



Bordas, Peters, Viti, Zilian

Biomedicine & programmable matter



DTU DRIVEN | DRIVEN | stephane.bordas@alum.northwestern.edu | legato-team.eu | http://twitter.com/stephanebordas | UNIVERSITÉ DU LUXEMBOURG |

New journal!

DATA-CENTRIC ENGINEERING

Transforming engineering science and practice

A peer-reviewed **open access journal** at the intersection of data science and engineering, now **open for submissions**.

Publishing:

- **Original research** exploring the potential of data-driven models for engineering
- **Case studies** showcasing downstream applications
- **Position papers** on new data standards, ethics and policy

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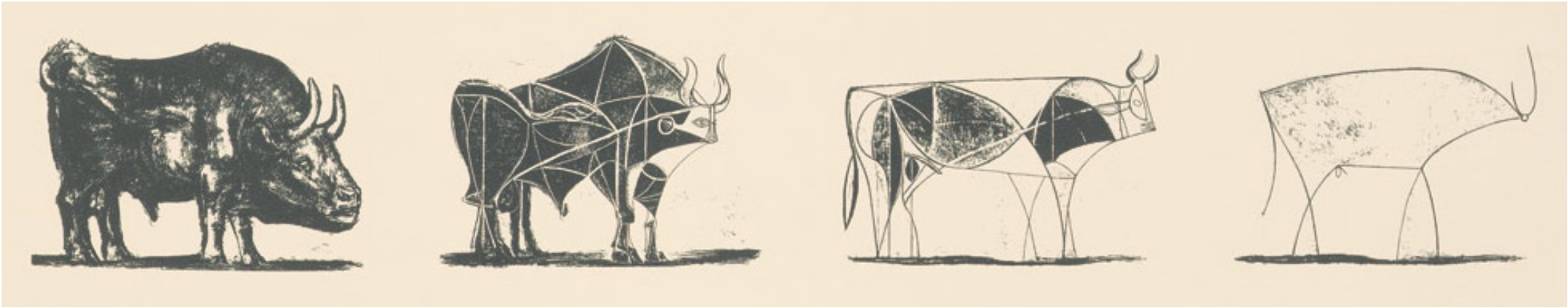
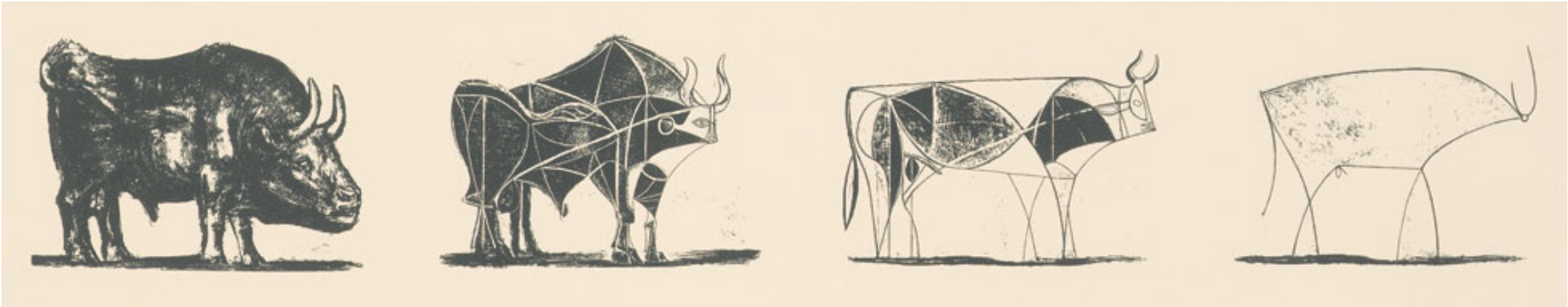
RESEARCH LUXEMBOURG



RESEARCH & INNOVATION
in Luxembourg

EIB CONFERENCE 2019



European Investment Bank Conference 2019

The institute of computational engineering sciences supported the organisation of the TECH Fair at the EIB conference, 2019.

Arnaud MAZIER and Saurabh DESPHANDE demonstrate real-time photogrammetric acquisition for medical simulations - check out twitter.com/stephanebordas for details

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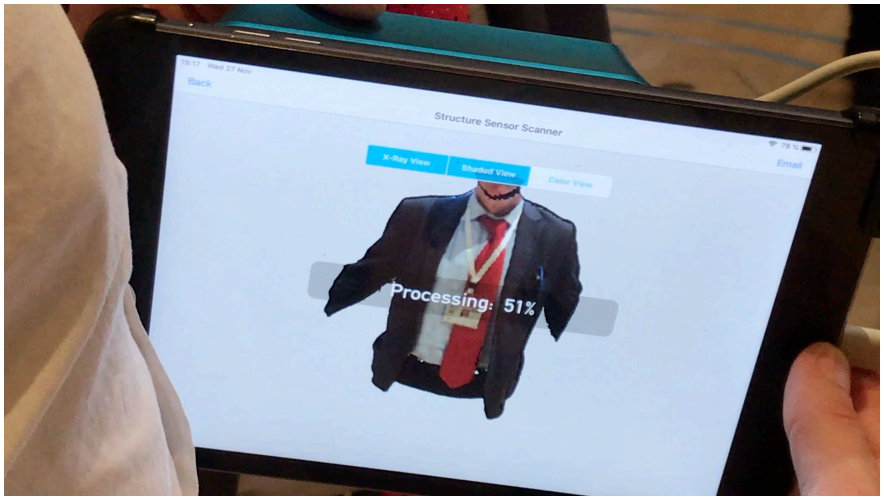

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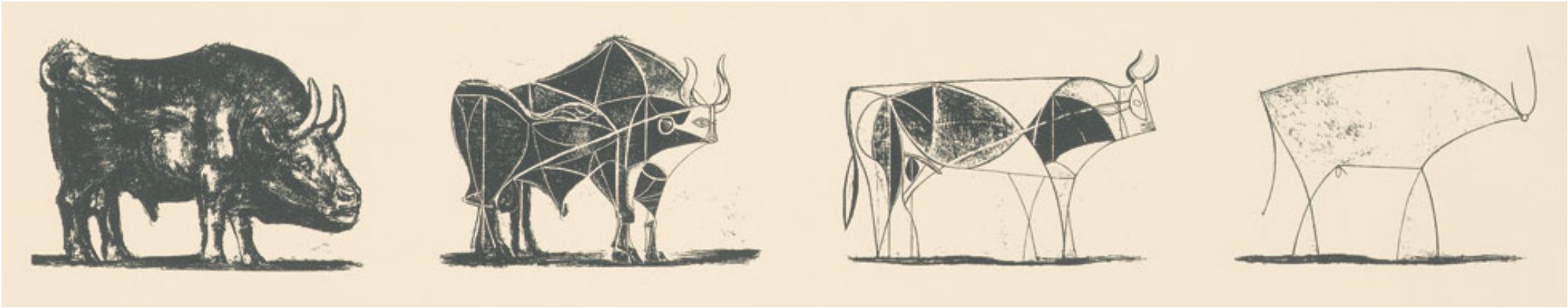
COMPUTATIONAL ENGINEERING SCIENCES LUXEMBOURG IN NUMBERS



Key facts for 2019

PhD graduates 2019

Claudia	BANDIERA
Carolina	CISTERNA
Saurabh	DESPHANDE
Amrita	FRANCIS
Qingyuan	HU
Haiqin	HUANG (creating a startup in Luxembourg!)
Georgios	LASKARIS
Hussein	RAPPEL - now at Turing Institute/Cambridge
Bogdan	TOADER
Piergiorgio	VITELLO

Welcoming 11 new PhD students: 9 nationalities!

Juan	AGUILAR
Saurabh	DESPHANDE
Aflah	ELOUNEG
Chintan	JANSARI
Diego	KOZLOWSKI
Vasilis	KROKOS
Arnaud	MAZIER
Antoine	PERNEY
Camilo	SUAREZ
Milad	ZERAATPISHEH
Fa	ZHU

Key facts for 2019

WELCOMING POST-DOCTORAL FELLOWS

Olga BARRERA
MSCA Fellow www.metabiomec.com

Anina SARCIC
FNR Funded CORE JUNIOR DATA4WIND

Eleni KORONAKI
FNR BRIDGES CERATIZIT Data-driven optimisation of Chemical Vapour Deposition (with Yannis KEVREKIDIS) https://en.wikipedia.org/wiki/Yann%C3%ADs_G._Kevrekidis

Georgios LASKARIS
Richard CONNORS

Hamidreza DEHGHANI
Christophe HOAREAU

2019 MEETINGS

- ERCIM Workshop 2019 (LUX)
- DRIVEN Workshop 2019 (LUX)
- DATA-CENTRIC Engineering Workshop 2019 (MIT)
- Data-Science introduction to the European Commission
- ITN RAINBOW WORKSHOPS
- 9 PhD trainings in DTU DRIVEN
- EIB Tech Fair
- 12 distinguished multi-disciplinary seminars

Key facts for 2019

GRANT SUCCESSES (2.5 million)

- Stephan RUDYKH ERC StG (Trento)
- FNR BRIDGES Automobile Club Luxembourg
- FNR BRIDGES Goodyear
- FNR BRIDGES CERATIZIT
- FNR BRIDGES Kiswire
- FNR CORE JUNIOR Anina SARCIC
- 1 RDI funded project with ExaMotive/Oply (via SnT in collaboration with Prof. BOUVRY). New partnership with the company and SnT created
- Computational and Data Engineering Hub - CDE-HUB / funded by the Luxembourg Ministry of Economy (FEDER 2018-04-024)

STRATEGIC GRANTS

- Lars A.A. BEEX submits his ERC StG
- Marco RINALDI submits his ERC StG
- ERA Chair in Applied Mathematical Modelling submitted to H2020

OUTPUTS

- Over 60 papers in ISI international journals
- Over 3000 citations

Prof. BORDAS ISI Highly Cited for the 5th consecutive year

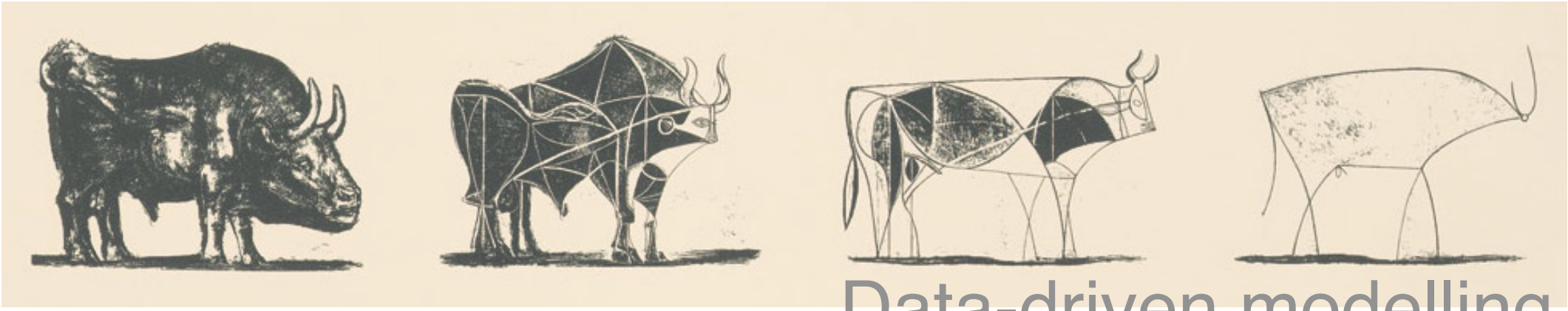
Cambridge University Press launches DATA-CENTRIC ENGINEERING Journal https://www.cambridge.org/core/journals/data-centric-engineering
Prof. Bordas - Executive Editor

2020 stay tuned!

NEWS FOR 2020

- Multi-disciplinary workshop at UL (2020 April 29)
- First Multi-disciplinary European Crucible in Luxembourg (NESTA Crucible in a Box) funded by the Scottish Research Funding Council (2020 May)
- WCCM2020 SYMPOSIA https://www.wccm-eccomas2020.org/frontal/MSList.asp
- SCIENCE OF SCIENCE & BIBLIOMETRICS LECTURE SERIES
- EUROMECH Symposium organised by Lars A. A. BEEX and Eleni CHATZI https://euromech.org/colloquia/colloquia-2020/618
- Data-Science introduction to the European Commission DIGICONNECT with the Competence Centre

Data-Driven Computational Engineering Sciences in Luxembourg

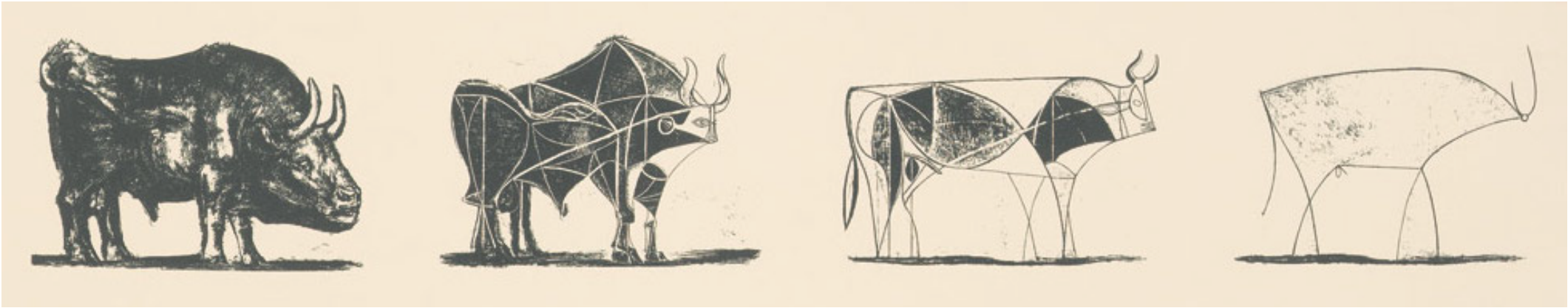


Data-driven modelling

- Quantum-continuum coupling
- Shape optimisation
- Chemical Vapour Deposition
- Plasma flow (space propulsion)
- Astrocyte/ neuron
- Urban comfort and wind energy
- Science of science
- Fracture across scales
- Digital archeology
- Programmable matter
- Surgical planning, training and assistance
- Meniscal replacement
- Gaming addiction

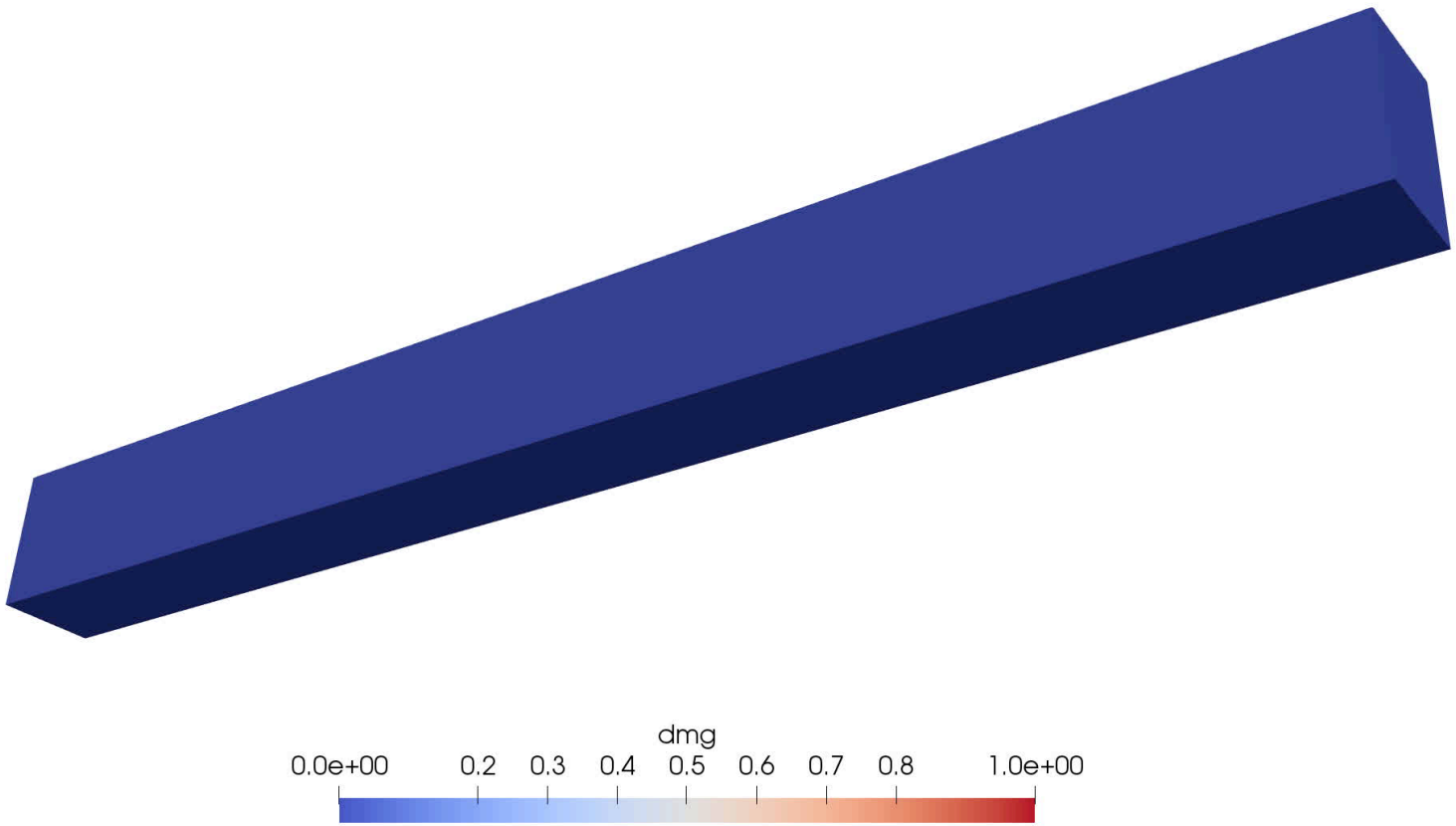
Small Data → Big Data

FRESH CONCRETE!



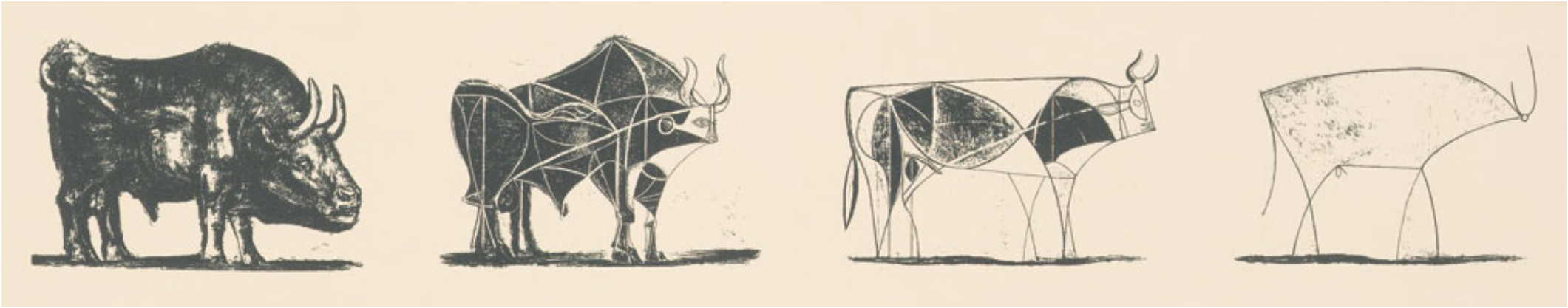
Fresh concrete modelling and simulation

Time: 0.0 days

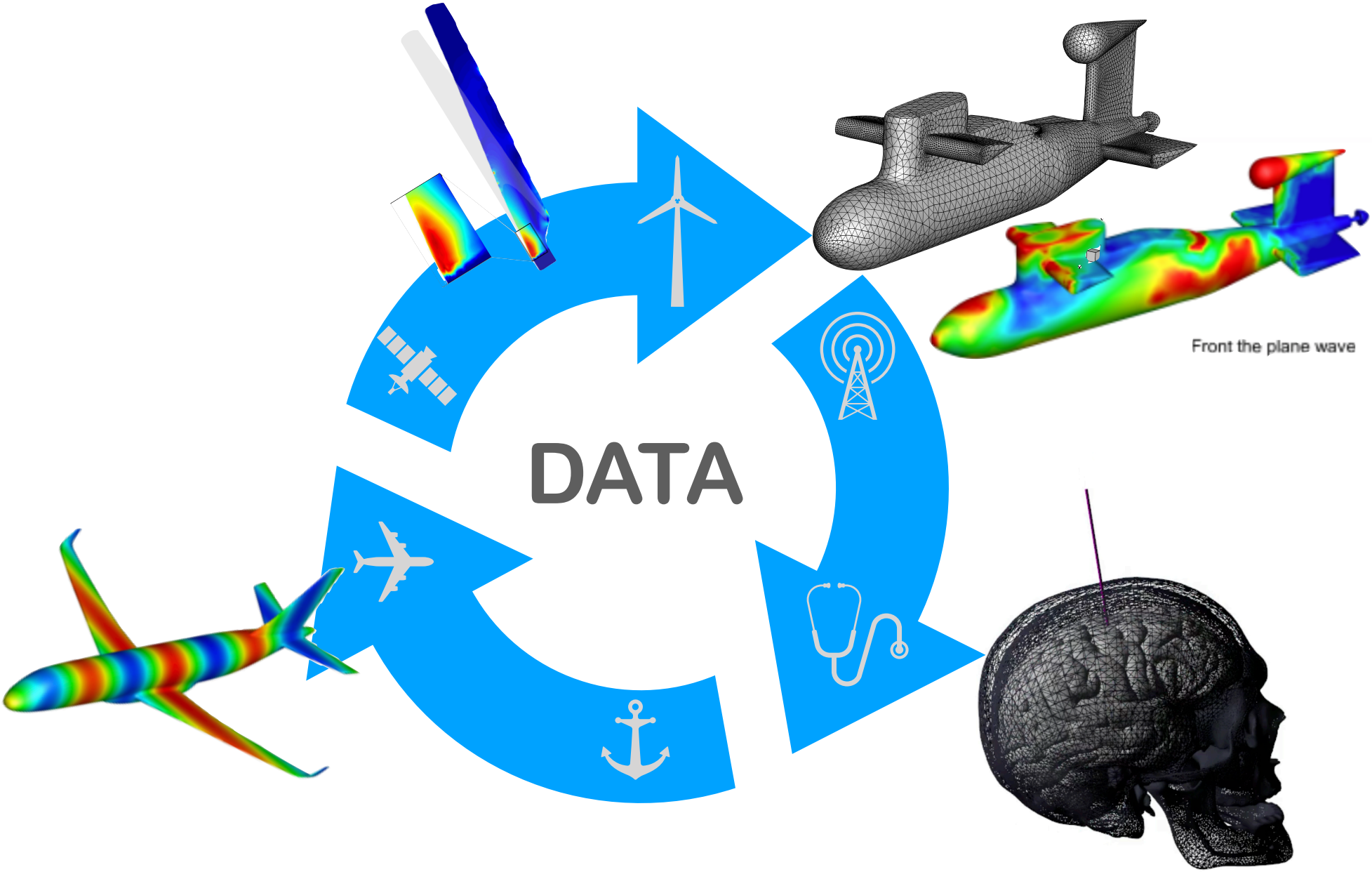


Michal Habera and Andreas Zilian

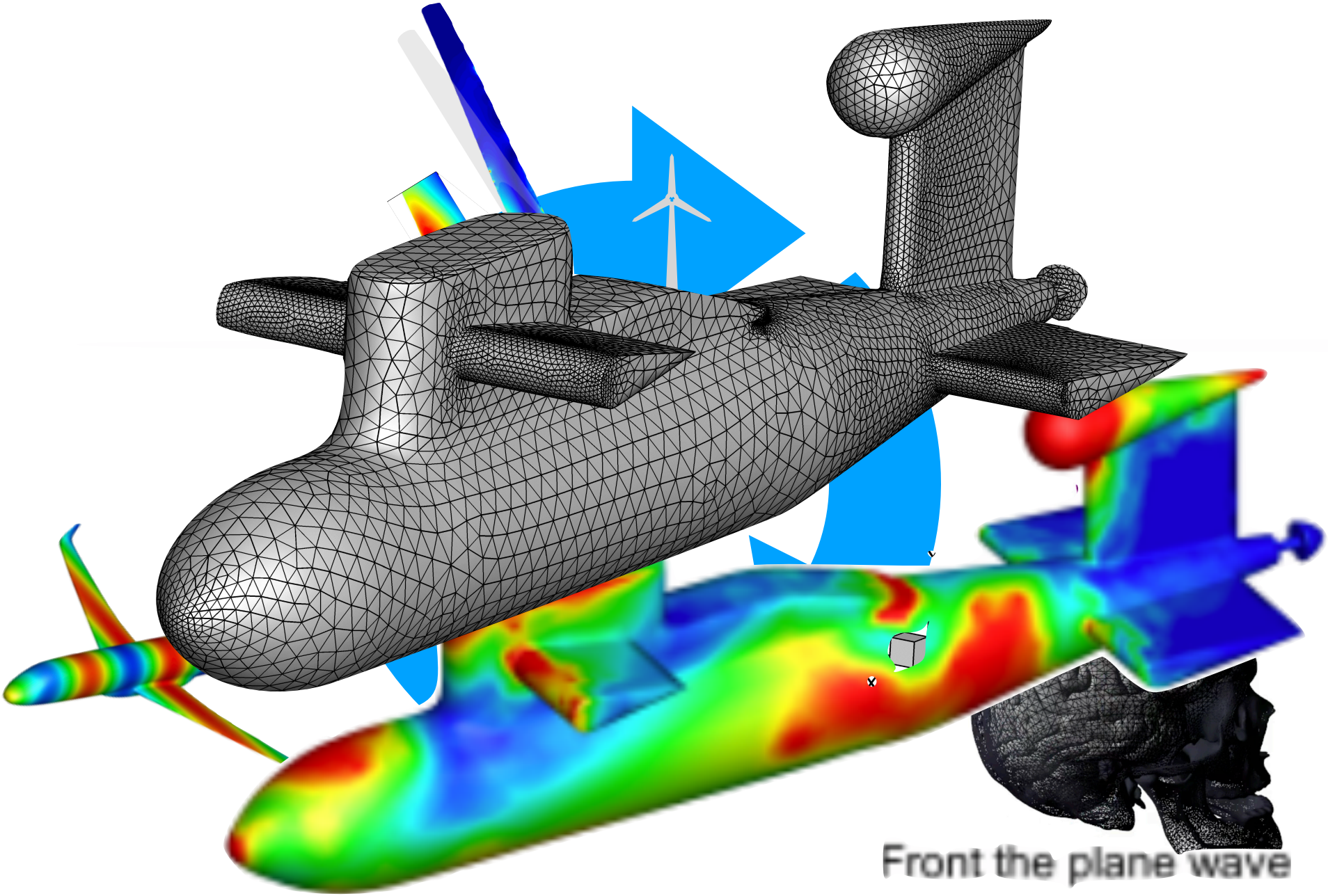
DATA-DRIVEN & DATA CENTRIC ENGINEERING, MODELLING & SIMULATION



Data-centric Engineering in Luxembourg

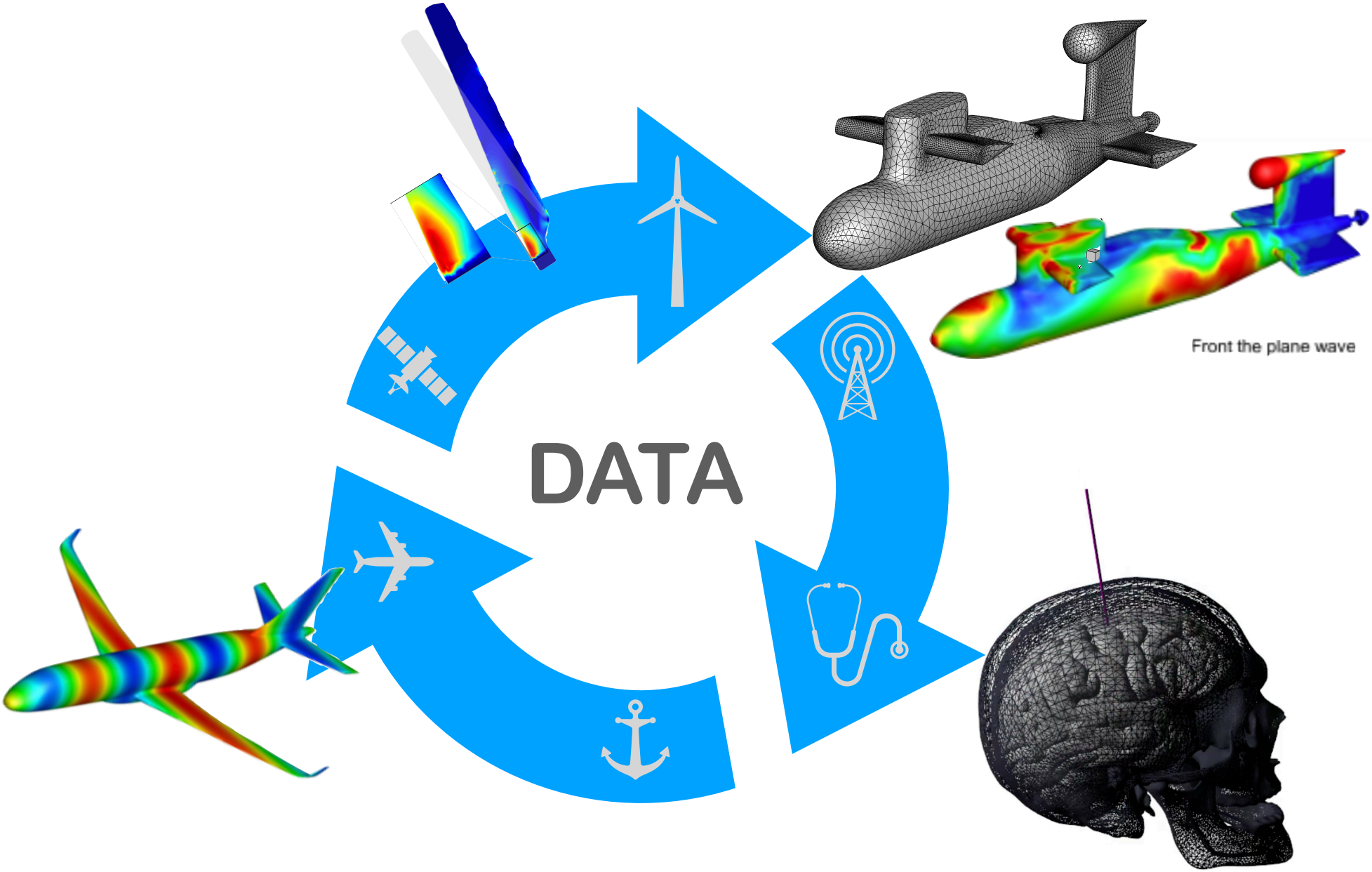


Acoustics optimisation with isogeometric BEM

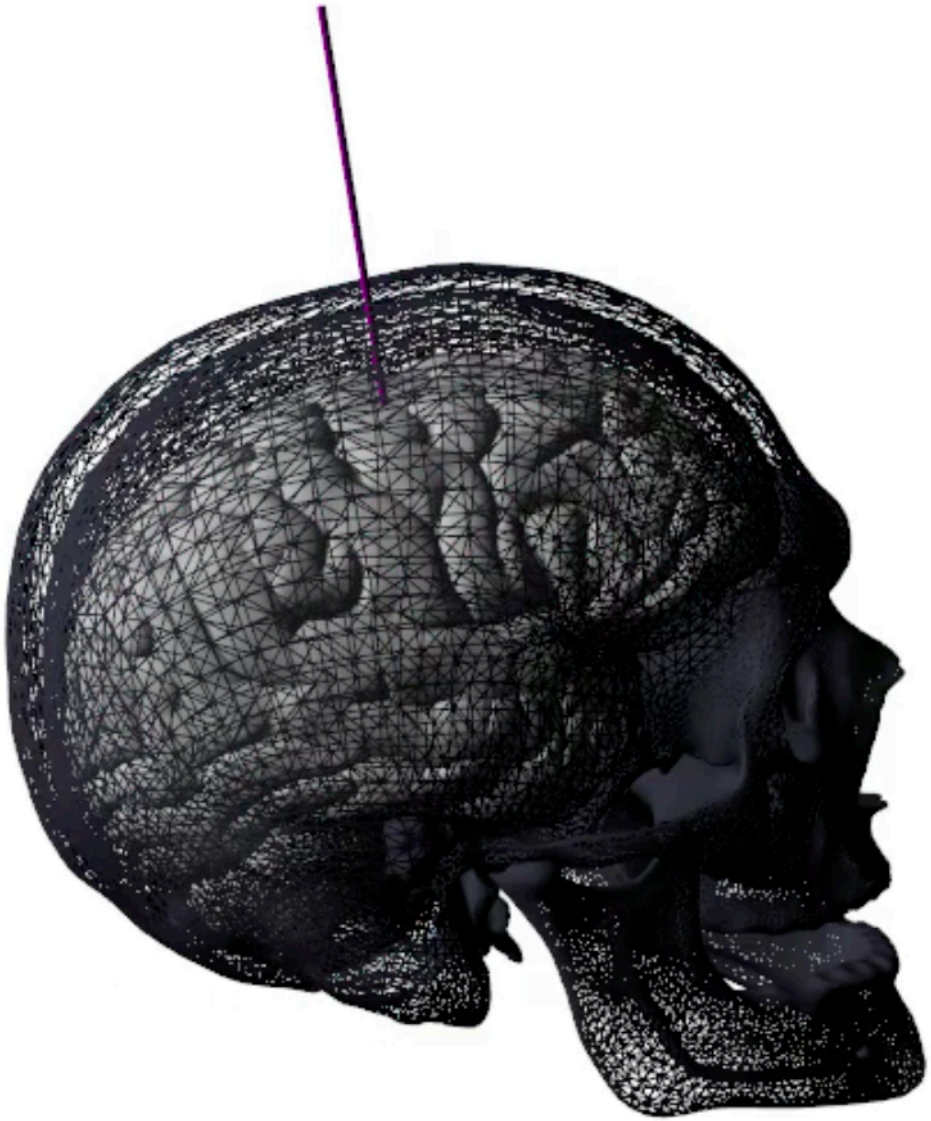


Structural shape optimization of three dimensional acoustic problems with isogeometric boundary element methods (CMAME2020)

Data-centric Engineering in Luxembourg



Deep brain stimulation simulation in real time



Quantifying discretization errors for soft tissue simulation in computer assisted surgery: A preliminary study (AMM2020)

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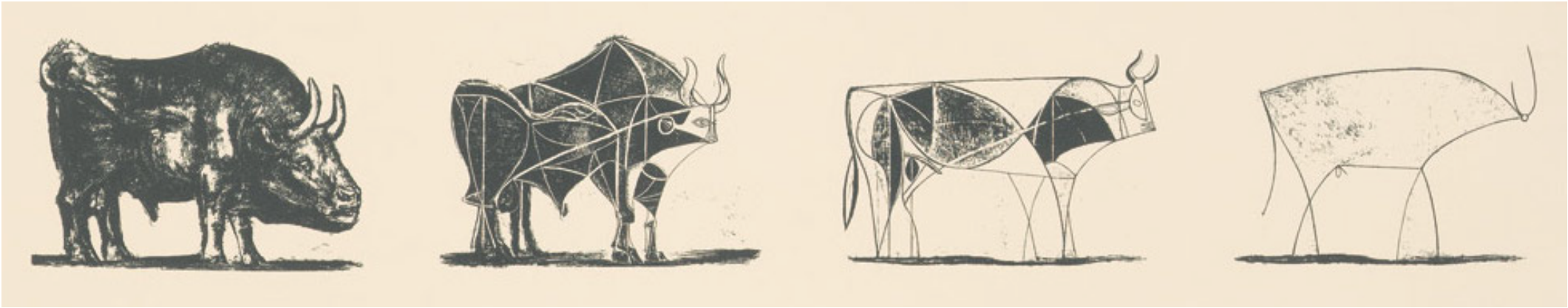
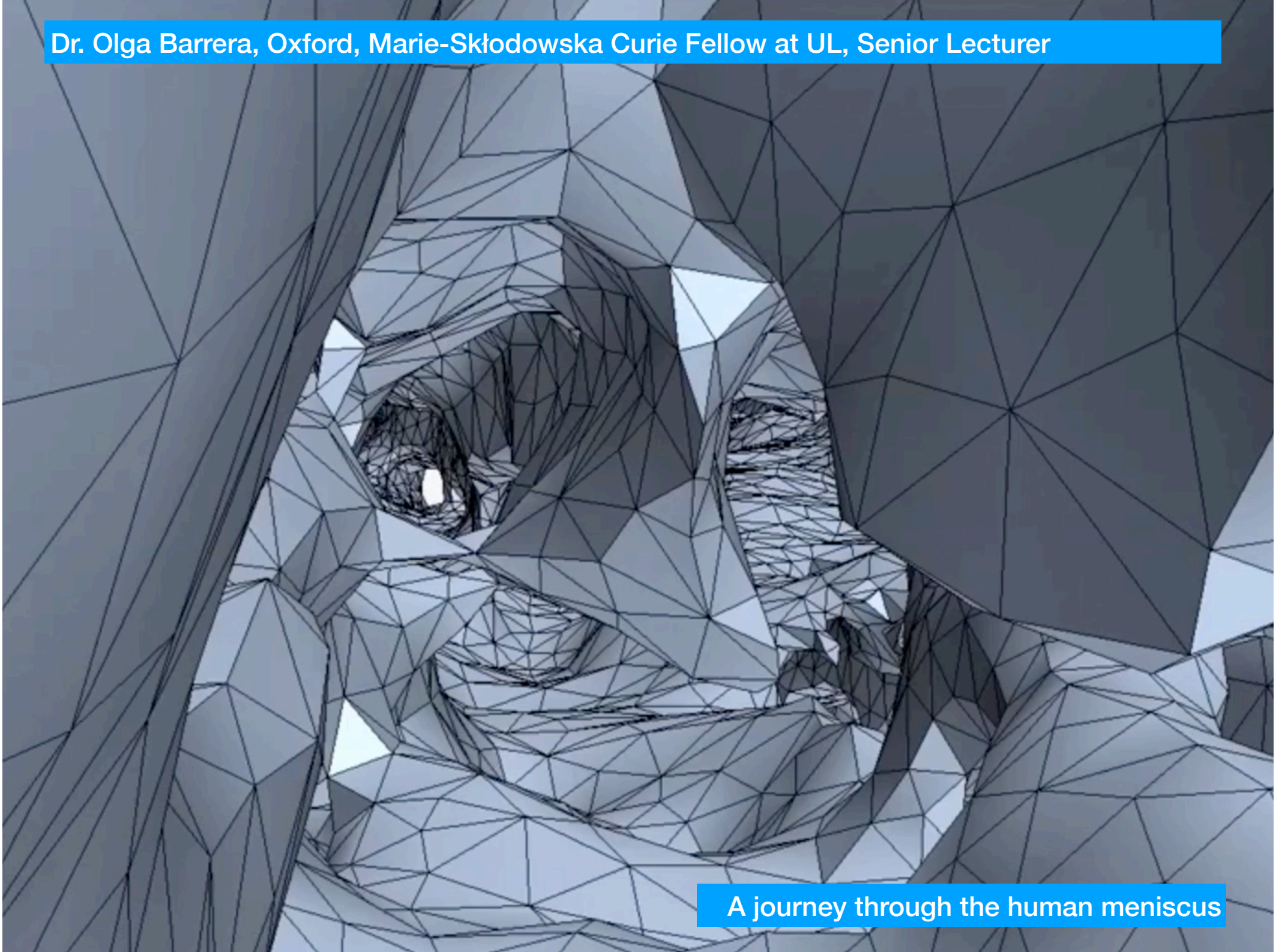
DIVE IN THE HUMAN MENISCUS



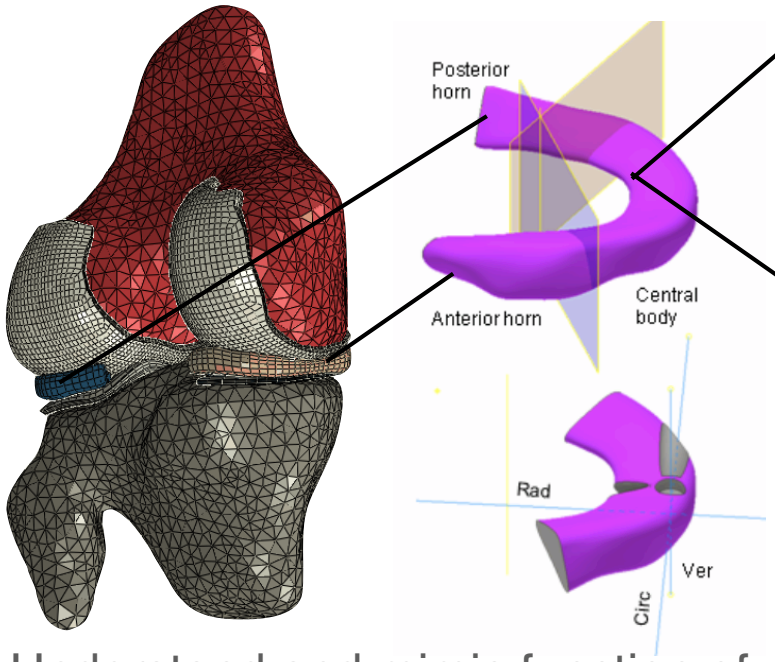
Dr. Olga Barrera, Oxford, Marie-Skłodowska Curie Fellow at UL, Senior Lecturer



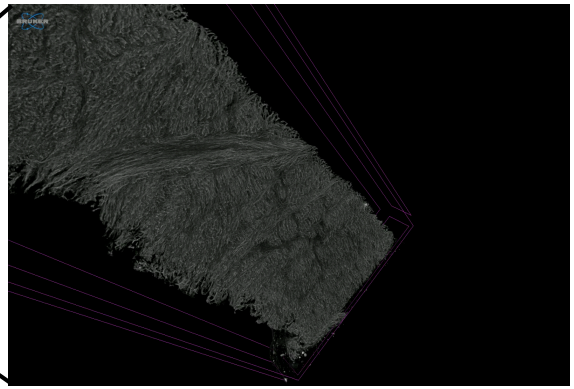
A journey through the human meniscus

Journey through data-driven engineering

data

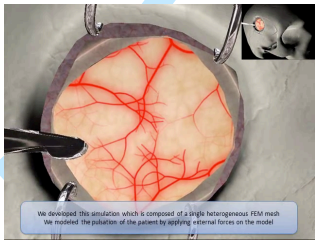


Understand and mimic function of human meniscus (Olga Barrera, Oxford)

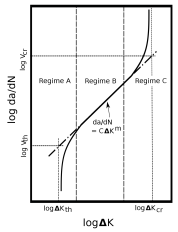


Microscopy 1 pixel = 0.6μm

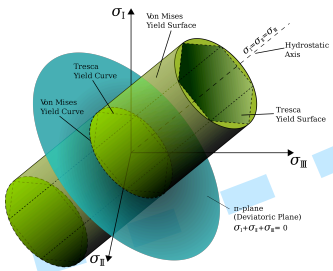
Channels 50-100μm in diameter



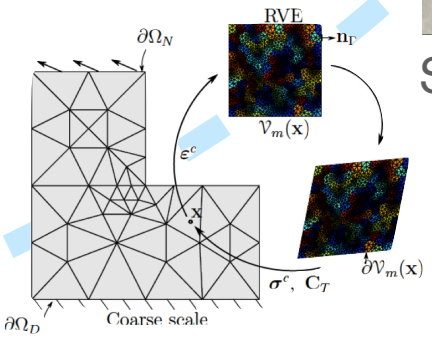
Surgical simulation



Fracture mechanics



Non-linear fracture

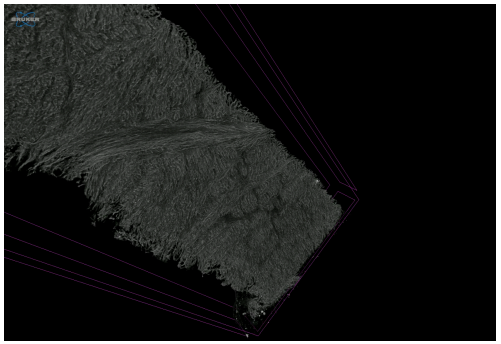


Multi-scale fracture

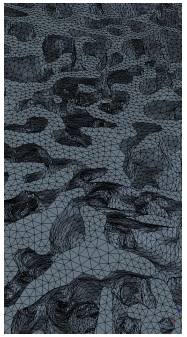
2003 2006 2009 2013 Today

Journey through data-driven engineering

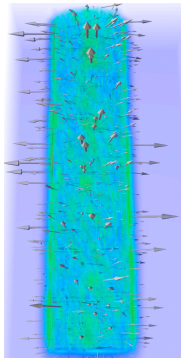
data



Real microstructure

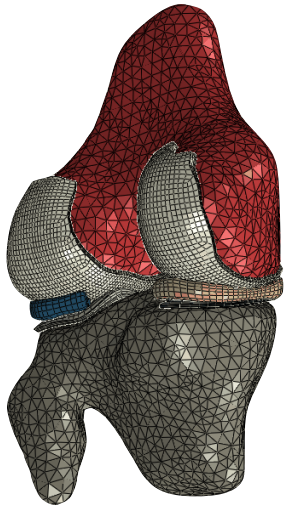


Simplified Microstructure



Physical Response

Homogenise



Model (PDEs) Parameters

…

Improve microstructure

Manufacture and test artificial meniscus

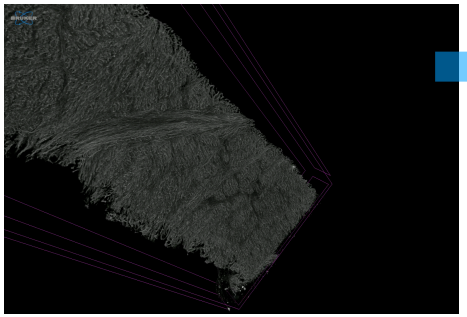
Olga Barrera, Oxford, Marie-Skłodowska Curie Fellow at University of Luxembourg

2003 ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE 2006 University of Glasgow 2009 CARDIFF UNIVERSITY PRIFYSGOL CAERDYDD 2013 UNIVERSITÉ DU LUXEMBOURG Today

Journey

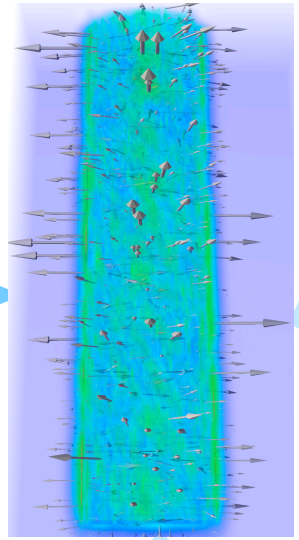
data

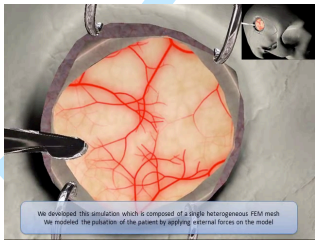
Build synthetic microstructures with similar statistical properties to microscopic images (GAN) to generate data ‘in silico’ and support the design, optimisation and fabrication of artificial menisci.



Generate synthetic microstructures (GAN)

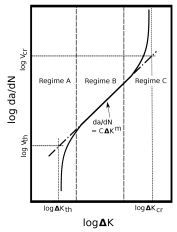
CFD





Surgical simulation

Olga Barrera, Oxford



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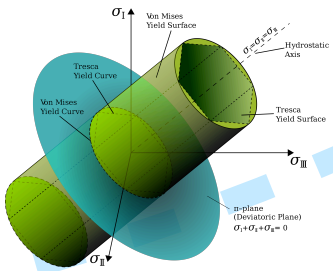
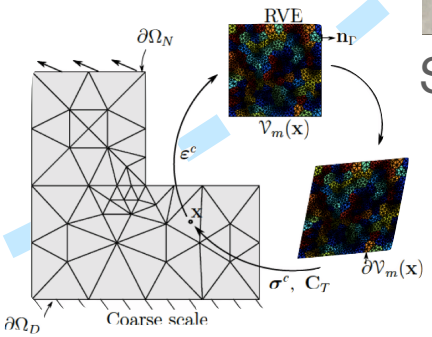


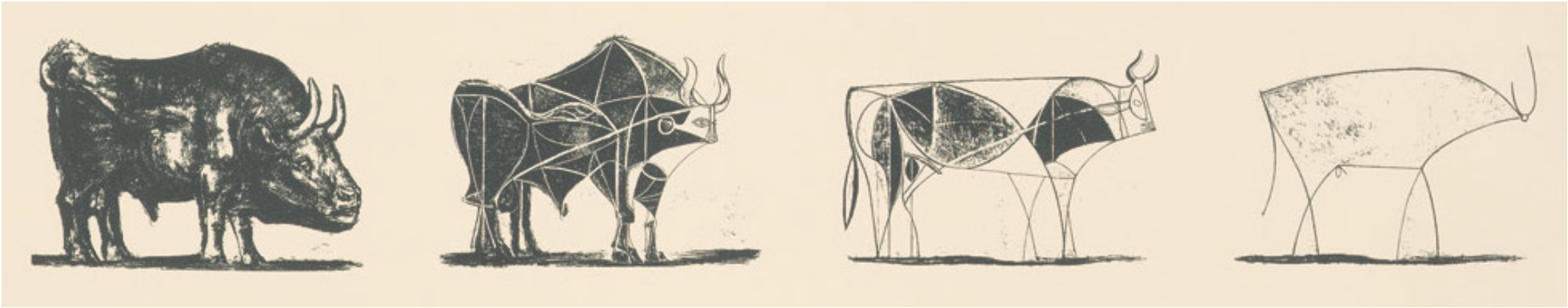
Non-linear fracture



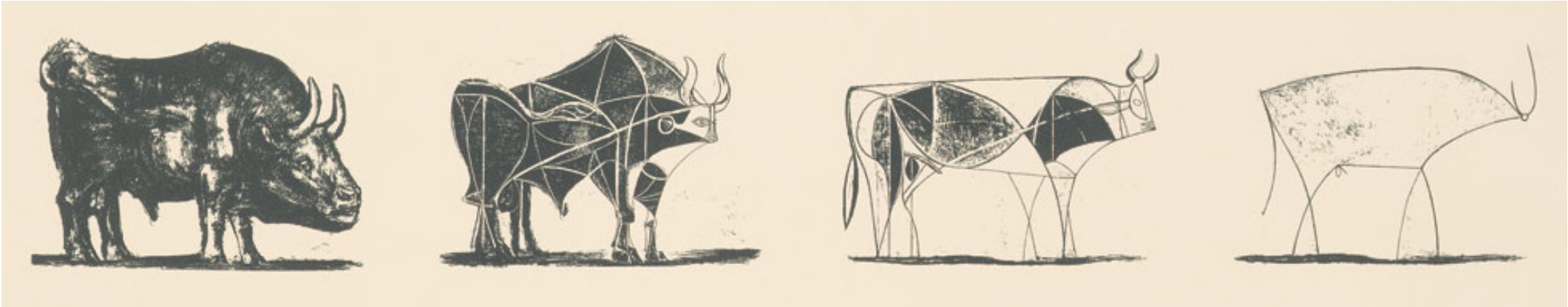
Multi-scale fracture

2003 2006 2009 2013 Today

ENGINEERING CANCER CARE



Surgical assistance for breast cancer treatment



Arnaud Mazier

Anatoscope

François Faure, Benjamin Gilles, Sophie Ribes, Frederick Van Meer, Christopher Masri, Clément Darche.

CHU Montpellier

Dr Gauthier Rathat (surgeon), Pr Guillaume Captier (surgeon)
Pr Patrice Taourel (radiology)

AnatoScope

MARIE CURIE ACTIONS

RAINBOW Rapid Biomechanics Simulation for Personalized Clinical Design
A Marie Skłodowska-Curie European Training Network

SOFA Simulation Open Framework Architecture

Breast Cancer Surgical Assistance

Worldwide numbers on cancer in 2018

- Each year 18.1 million new cancer case
- 2nd most spread with 11.6% for breast (1 in 4 cancers among women)
- 6.6% of mortality (5th most deadly)
- 1 woman on 8

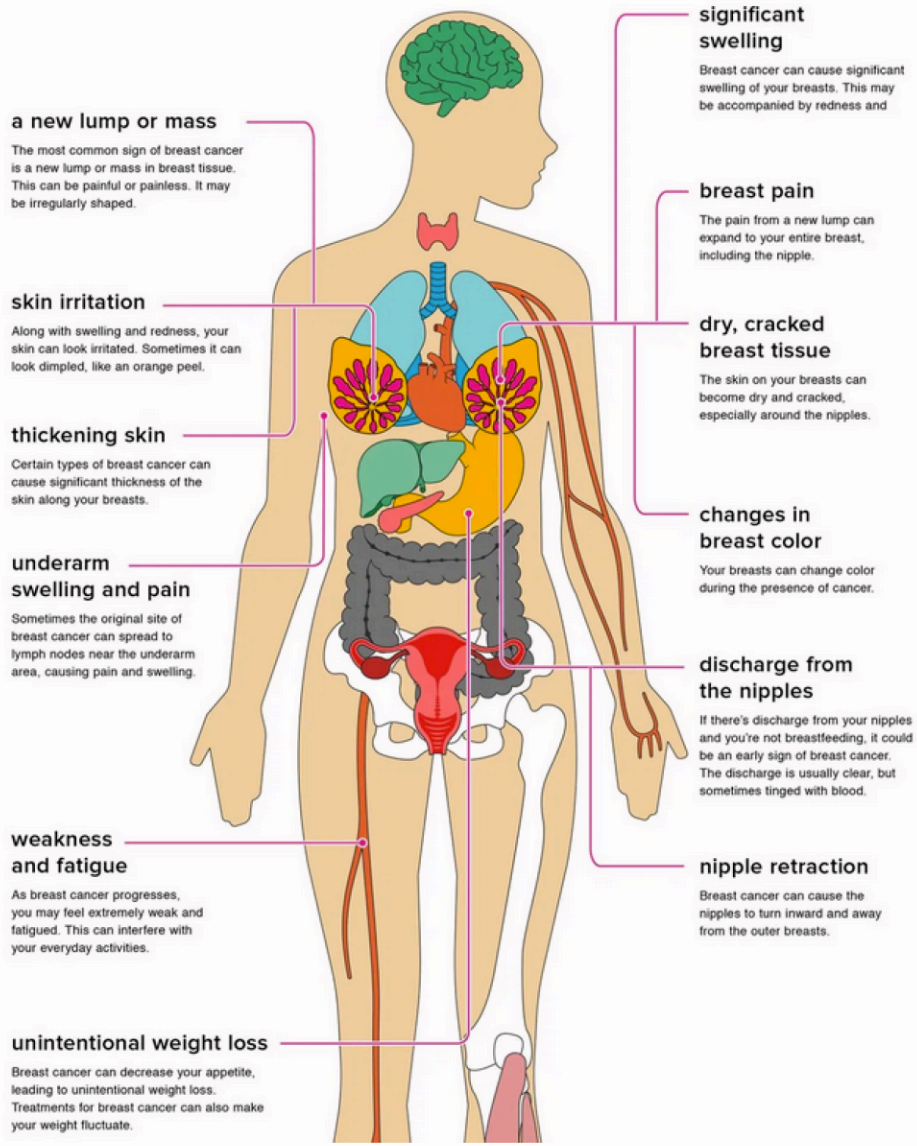


Figure: Breast cancer symptoms

Source: www.healthline.com & www.gco.iarc.fr

Breast Cancer Surgical Assistance

Different types of cancer

- LCIS (Lobular Carcinoma In Situ)
- DCIS (Ductal Carcinoma In Situ)
- IBC (Inflammatory Breast Cancer)
- Stages from 1 to 4 (Metastasis : spread to other organs)

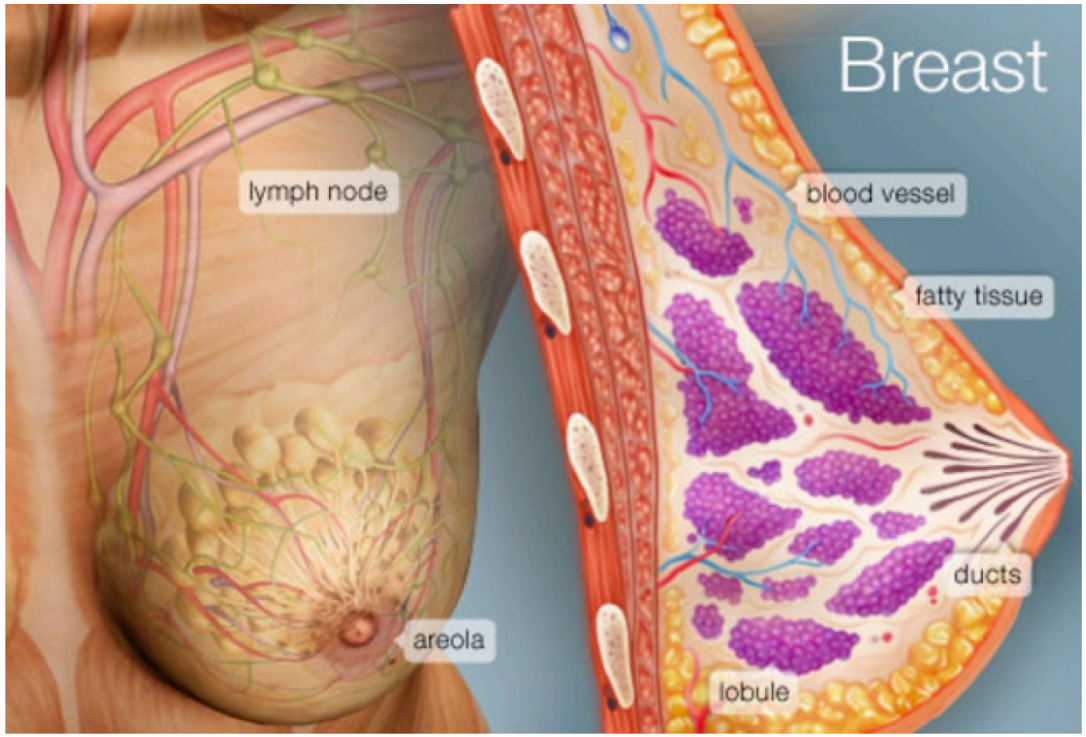
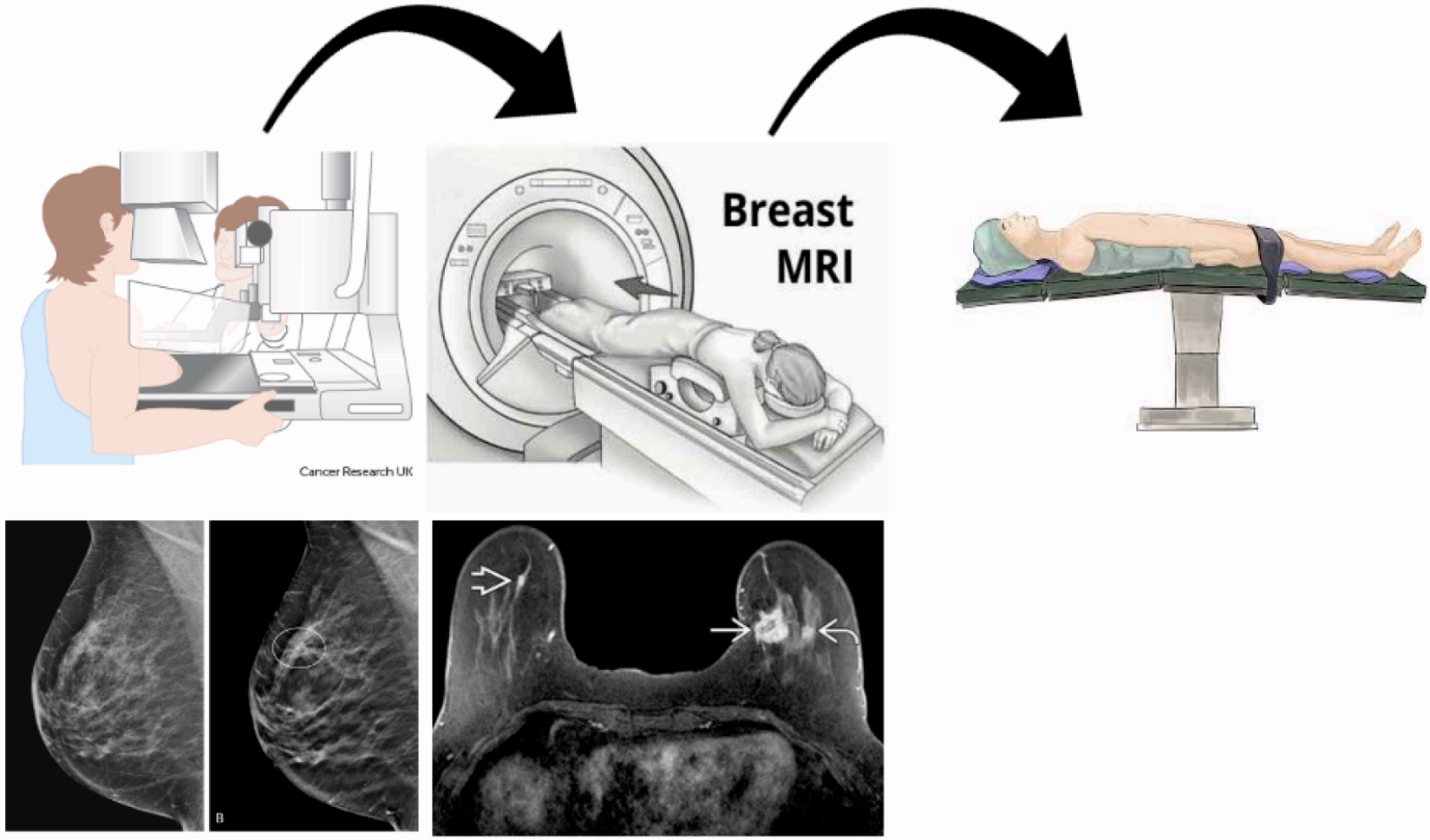


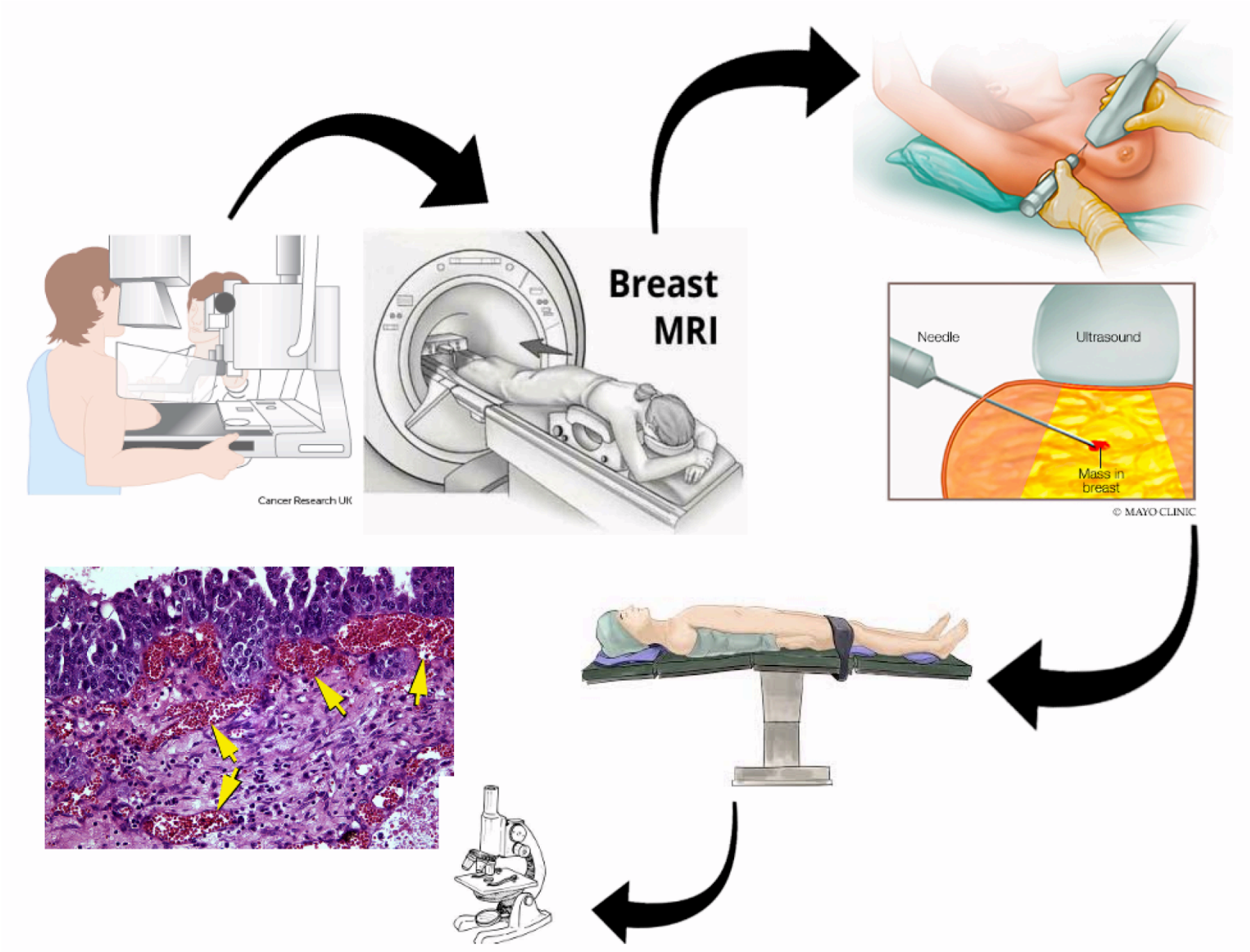
Figure: Breast anatomy

Source: www.webmd.com & www.nationalbreastcancer.org

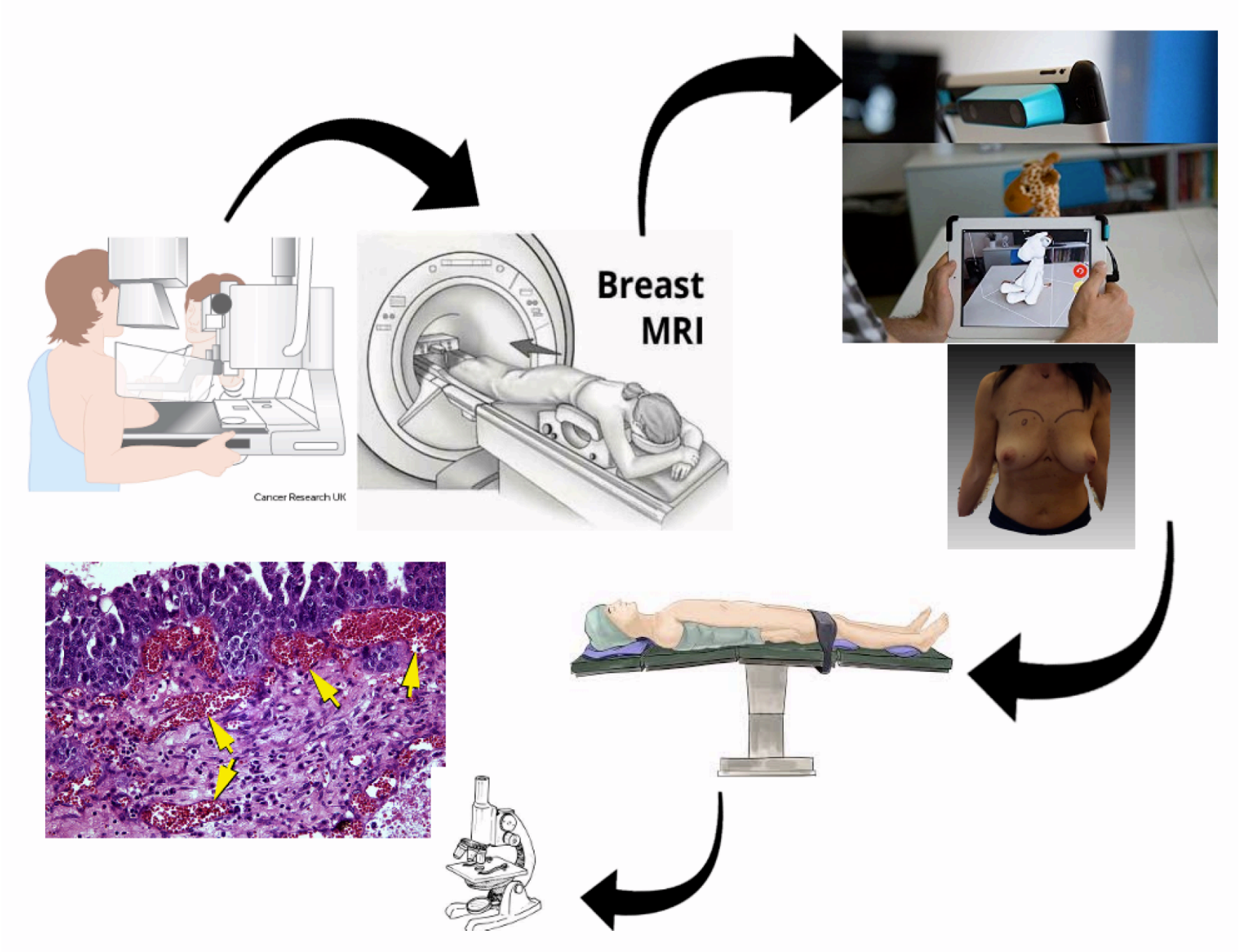
Breast Cancer Surgical Assistance



Detection to surgery: current practice



Our solution



Generating a patient database in silico

What is image registration ?

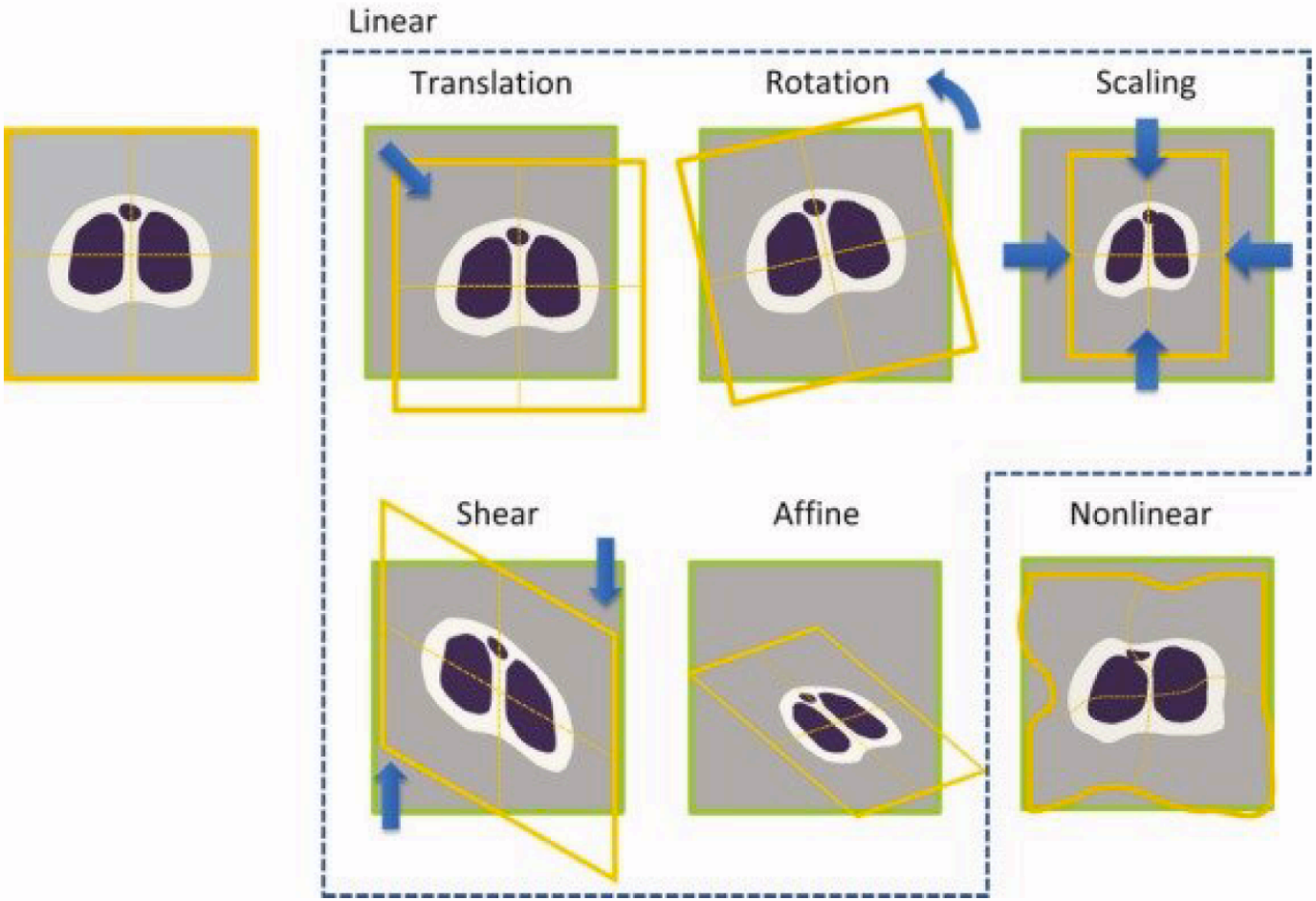
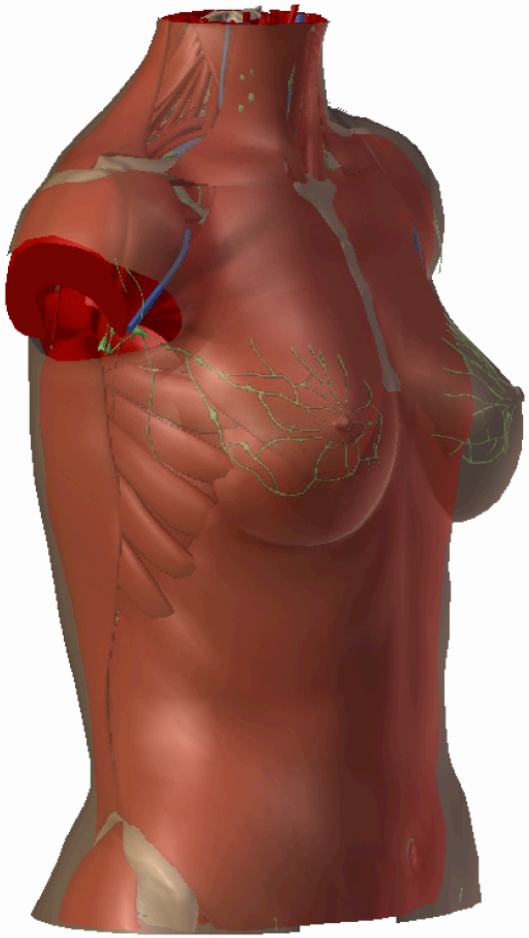


Figure: Geometric transformations

Generating a patient database

What is mesh registration ?



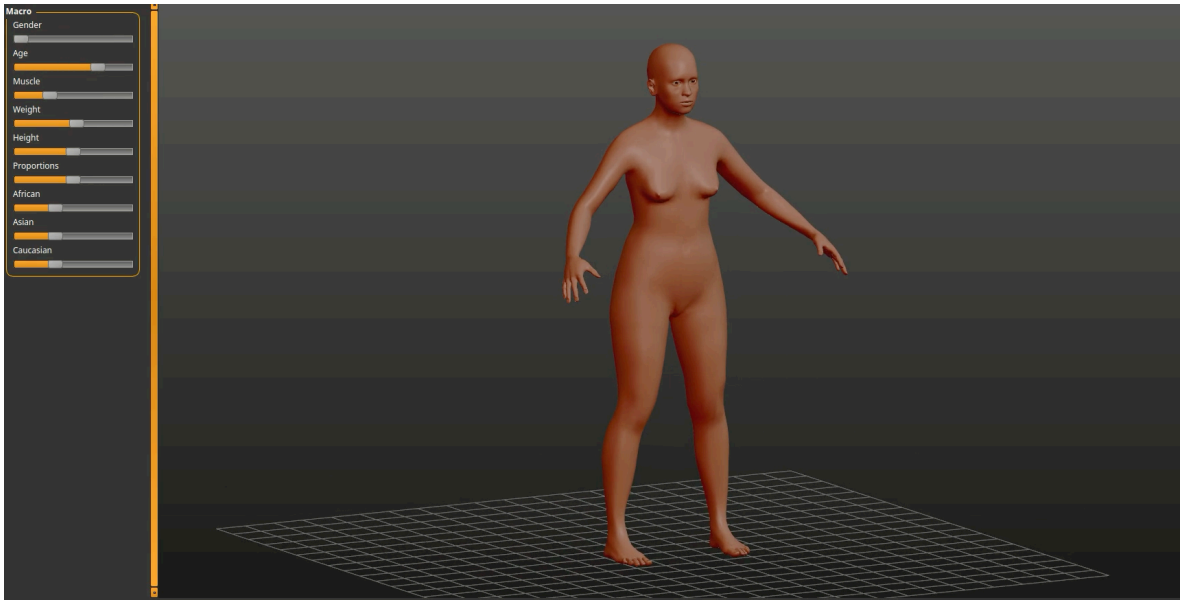


Figure: Anatoscope model

Generating a patient database

What is mesh registration ?

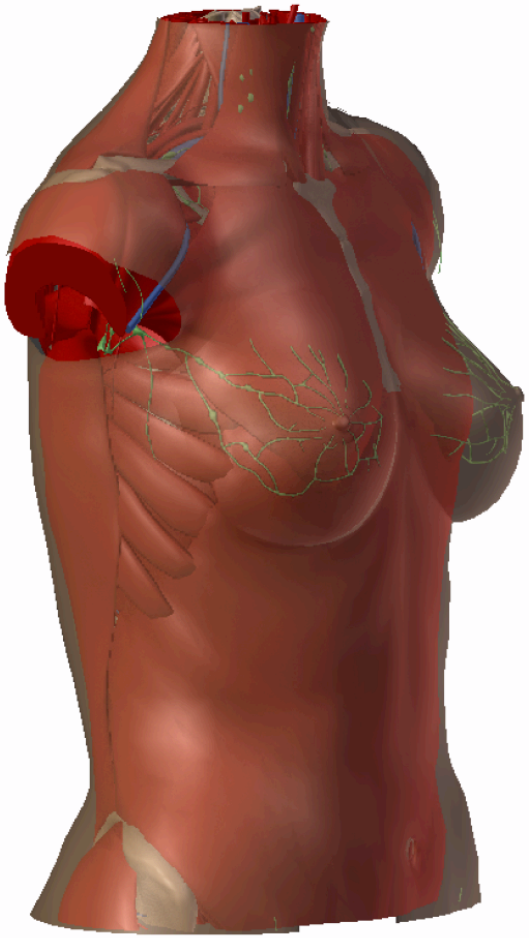


Figure: Anatoscope model

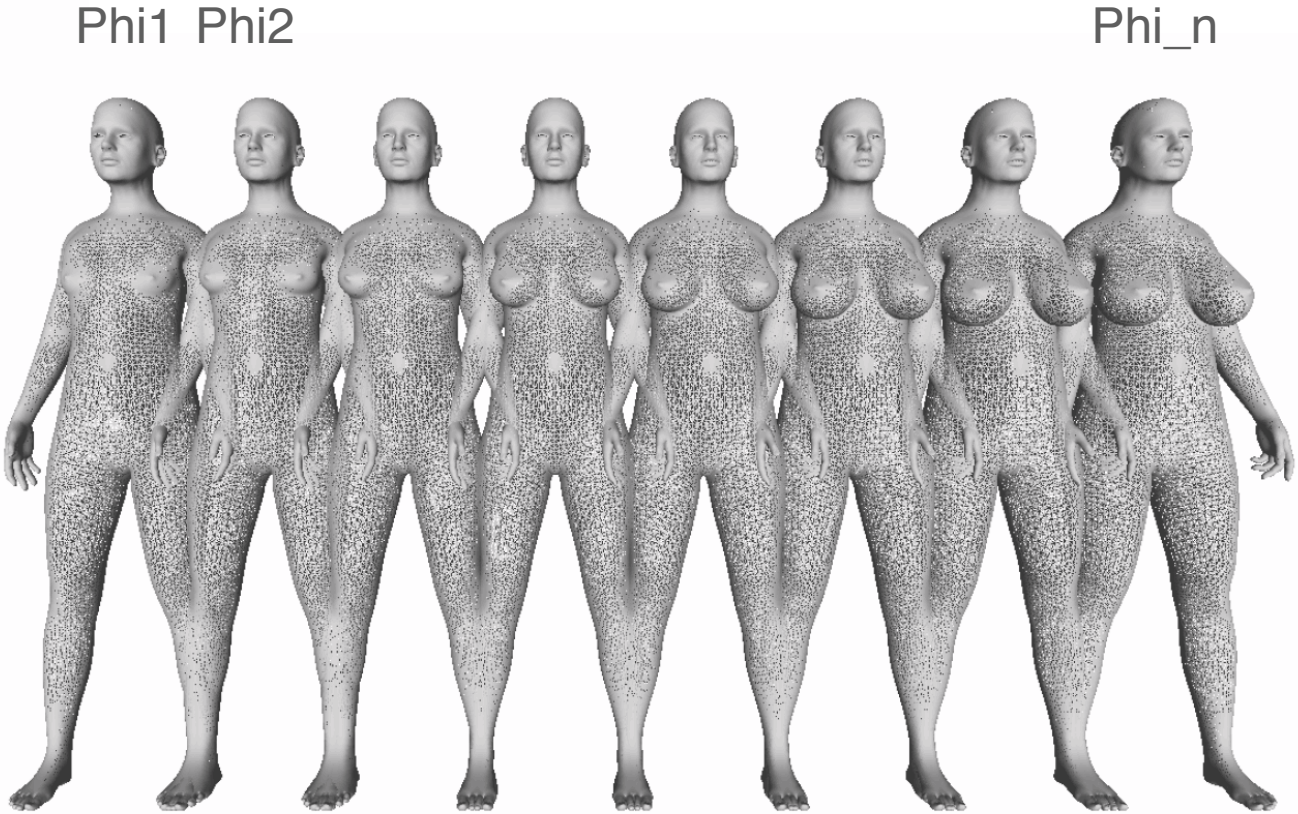
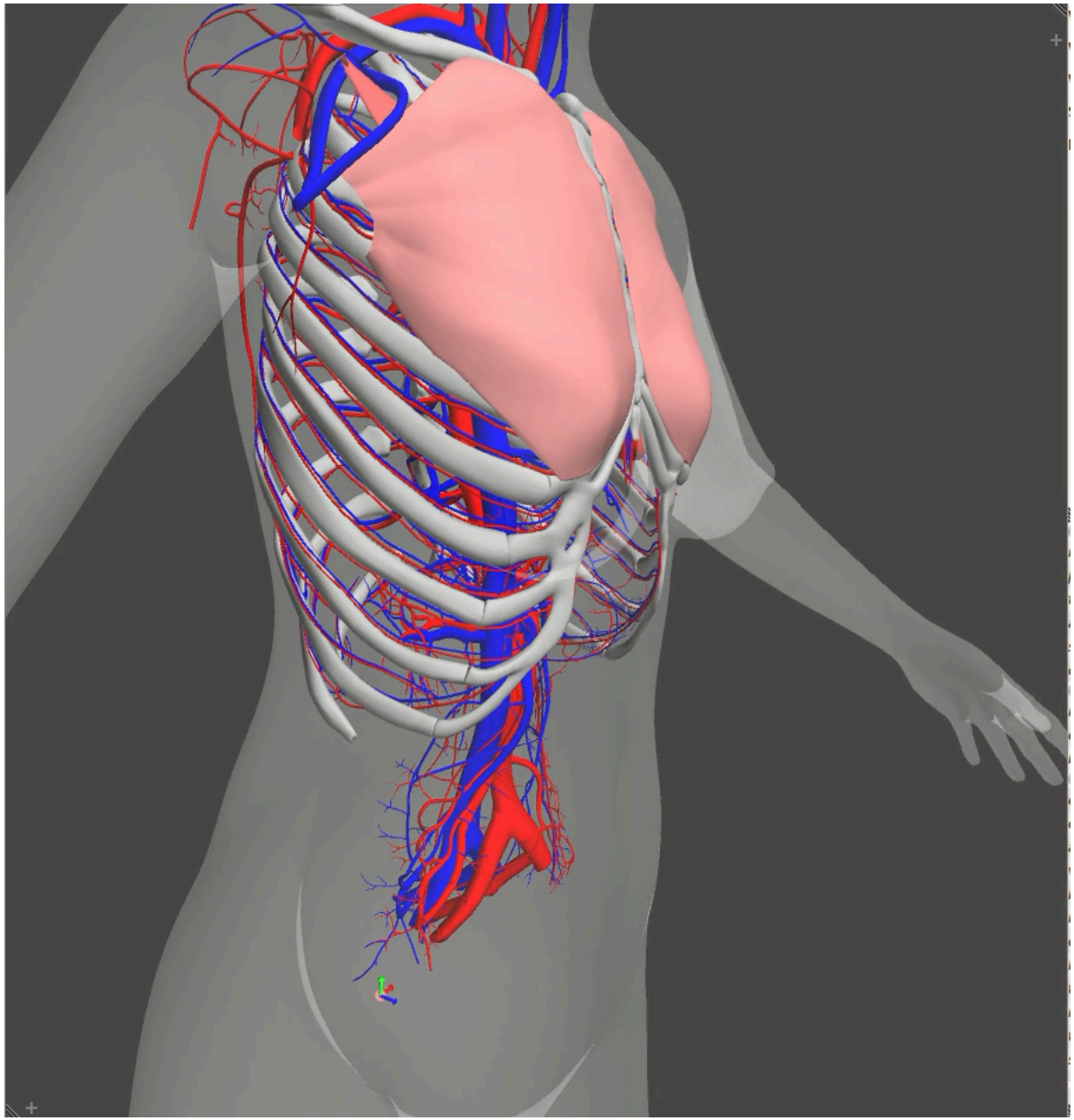


Figure: MakeHuman generation

Avoids re-segmentation…

- Collect simulation examples $\{\mathbf{u}_i\}$
- Subtract the average $\{\mathbf{X}_i\} = \{\mathbf{u}_i - \mu\}$
- Construct data matrix $\mathbf{X} = (\cdots \mathbf{X}_i \cdots)$
- Eigen of covariance matrix $\mathbf{X}\mathbf{X}^\mathsf{T} = \mathbf{U}\,\mathrm{diag}(\boldsymbol{\lambda})\mathbf{U}^\mathsf{T}$
- Truncate basis. Discard columns of U corresponding to the smallest eigenvalues

PCA application



Generating a patient database

Skin to skin ICP (Iterative Closest Point) registration

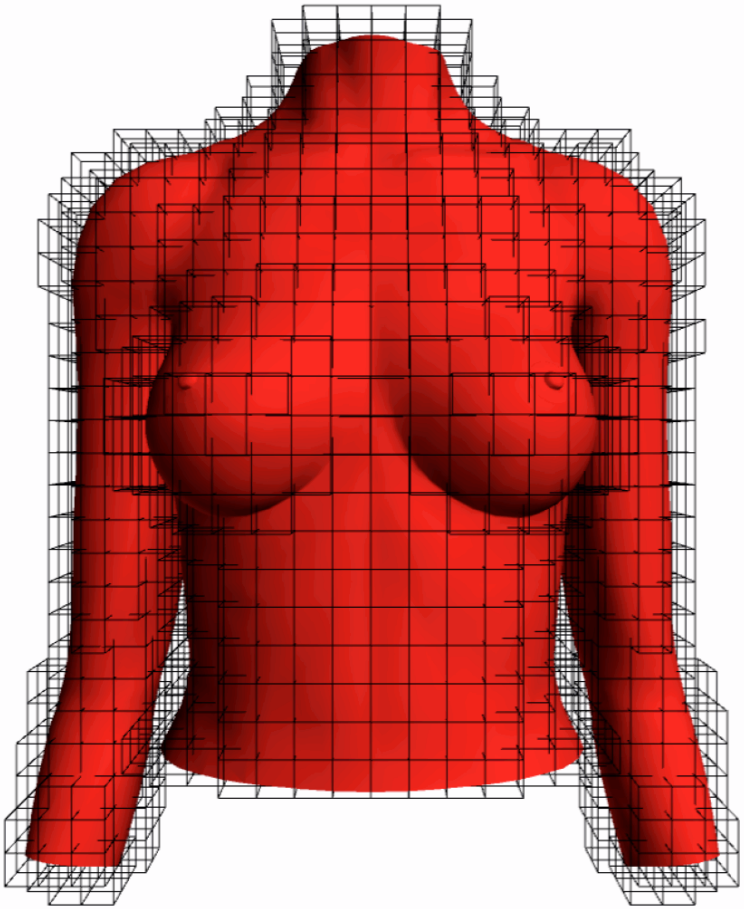


Figure: Anatoscope model embedded in a FE grid

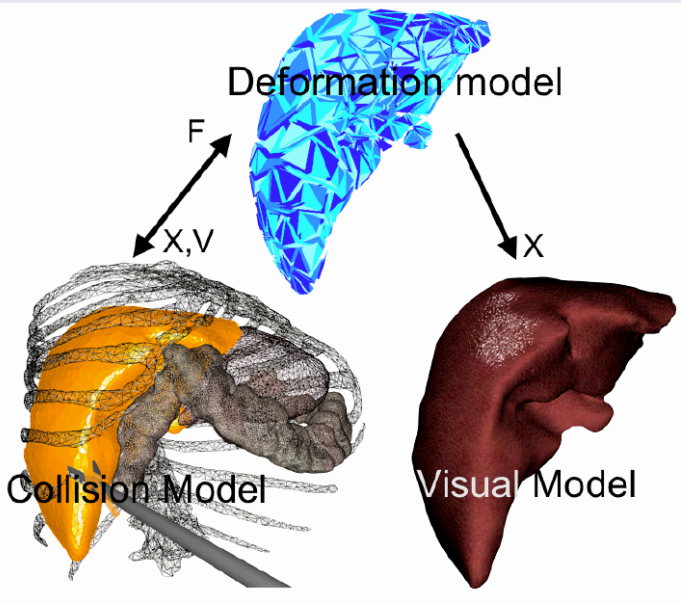
Real-time simulation framework SOFA

SOFA : Mappings

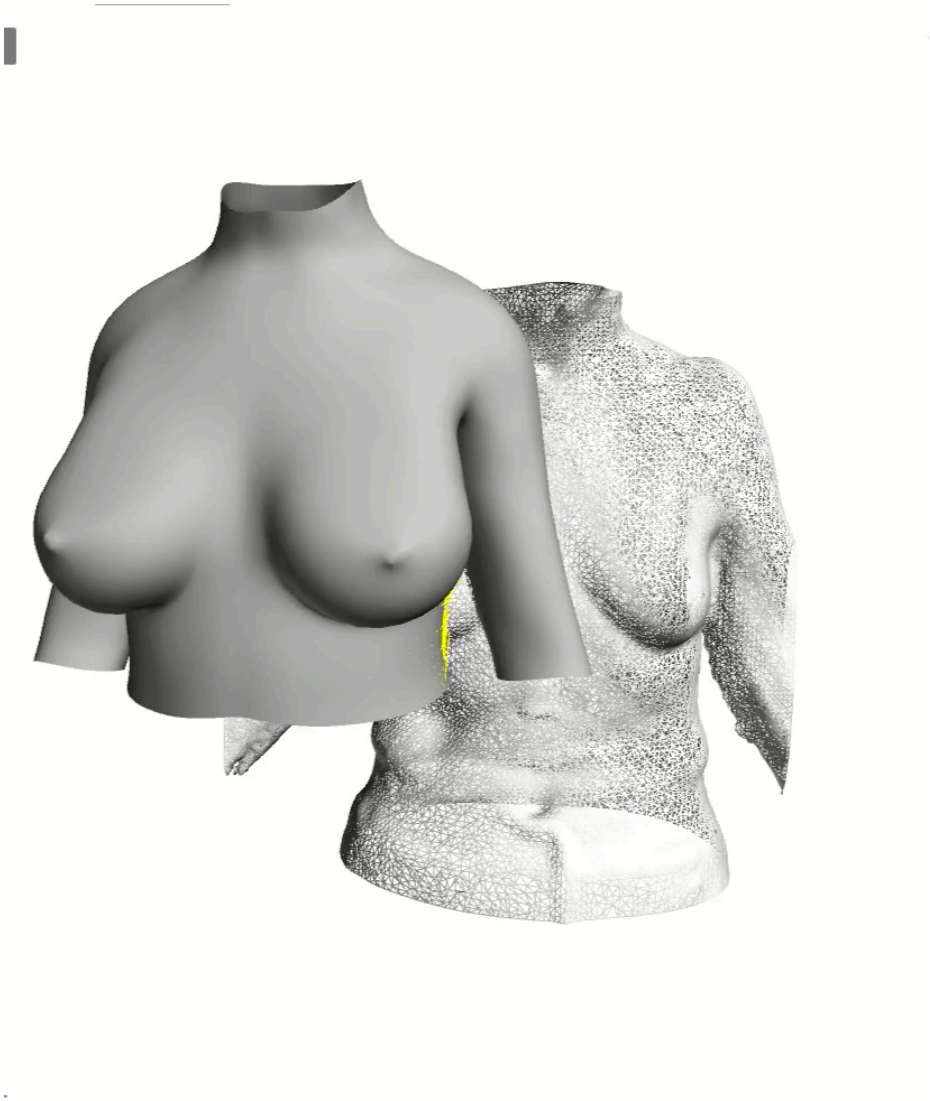
In linear :

$$\mathbf{f}_m = \mathbf{J}^T \mathbf{f}_s \tag{1}$$

$$\mathbf{a}_s = \mathbf{J}\mathbf{a}_m + \frac{\partial \mathbf{J}}{\partial \mathbf{x}_m}\mathbf{v}_m \tag{2}$$

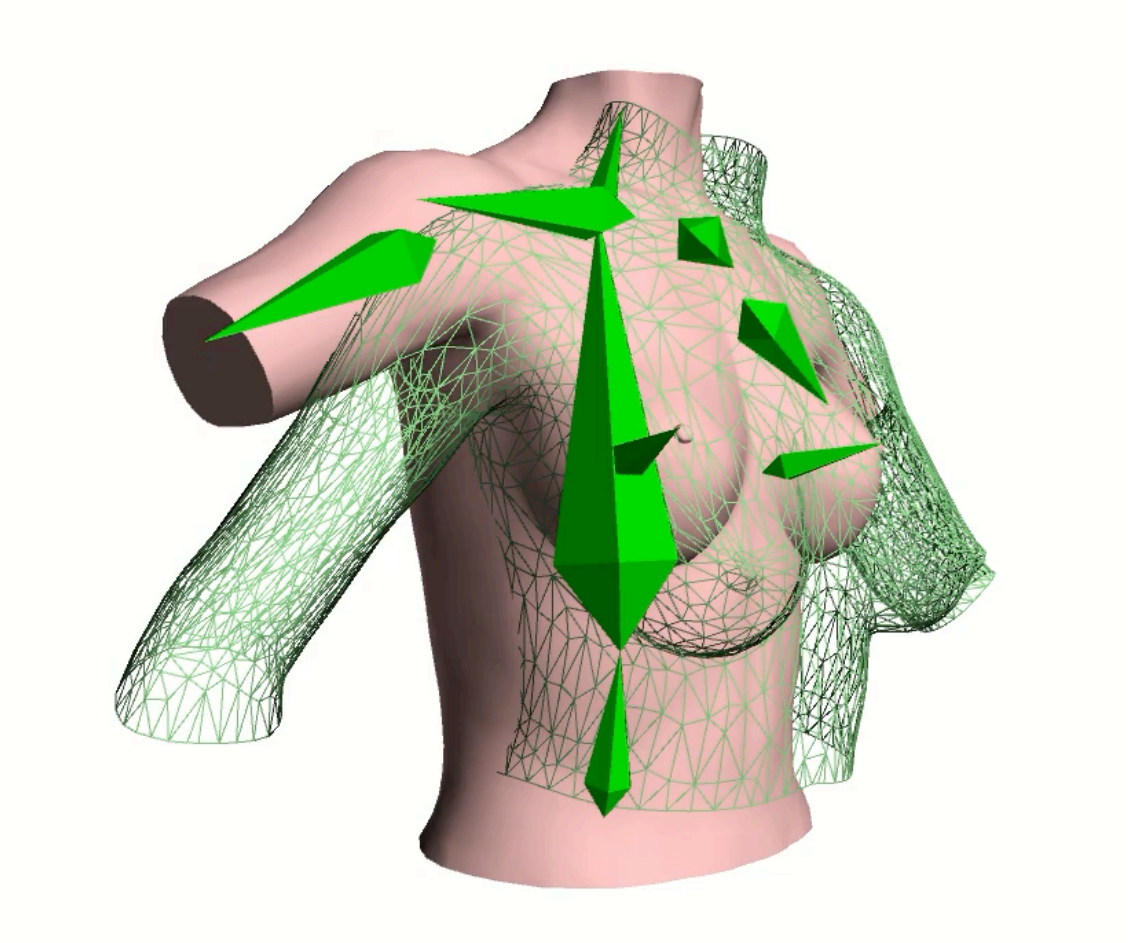


PCA to surface scan

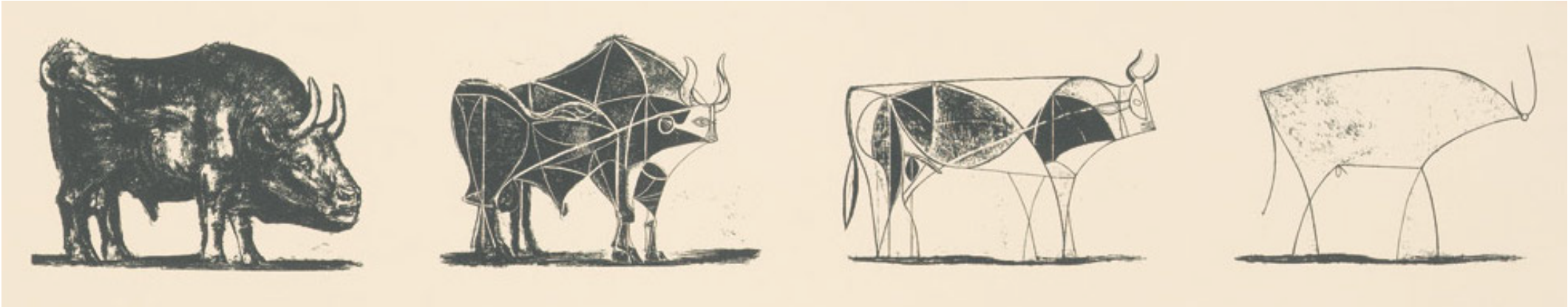


Future work and improvements

- Use Gaussian distribution on parameters
- For MakeHuman generation use quasi-random low-discrepancy sequences (i.e. Sobol) for parameters
- PCA limit main drawback : does not take into account movements of the arms



Data-driven neuro-oncology



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T. Duval, PhD, Toulouse Neuroimaging Center, FR

G. Sciumè, PhD, Associate Prof. Univ. Bordeaux, FR

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Glioblastoma - experimental-theoretical computational approach

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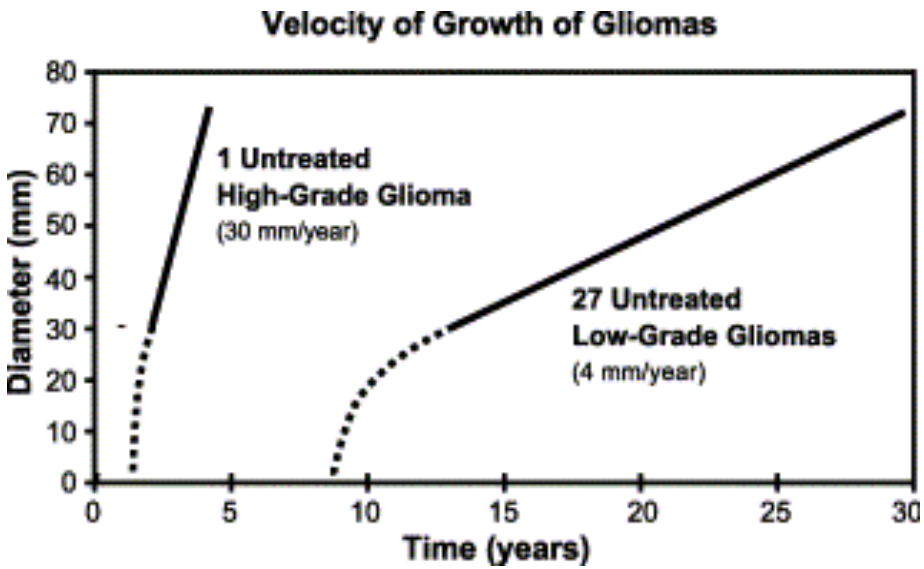
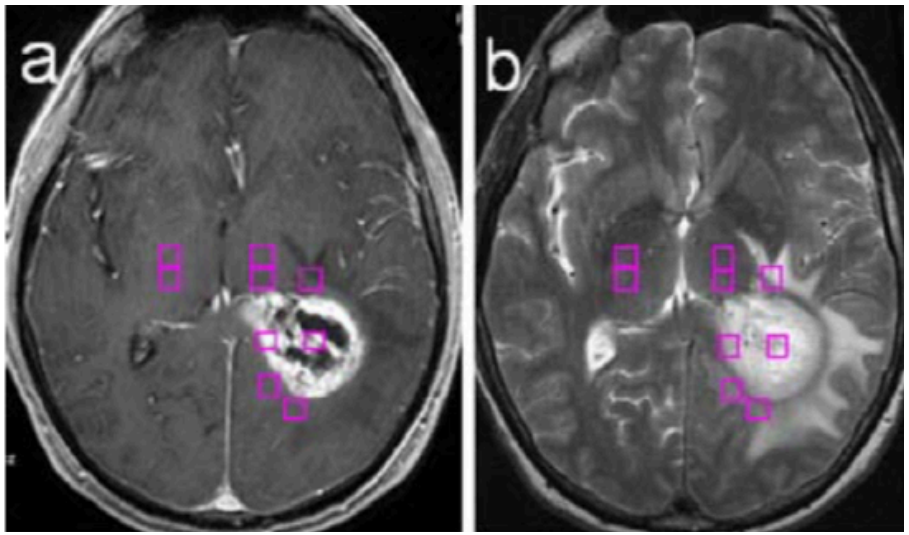
erc RealTCut

Glioblastomas



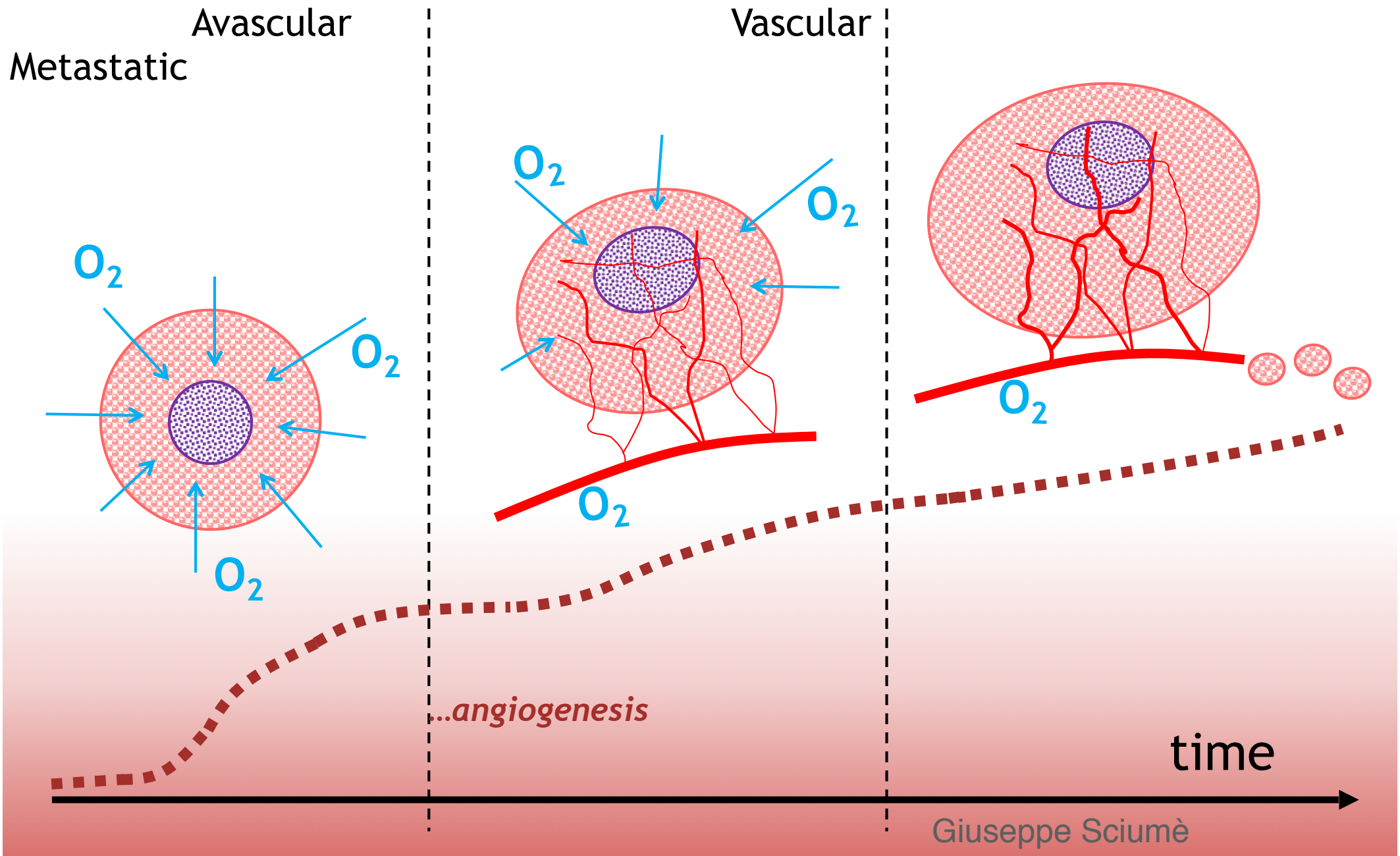


Doi 10.1007/s00234-006-0102-3

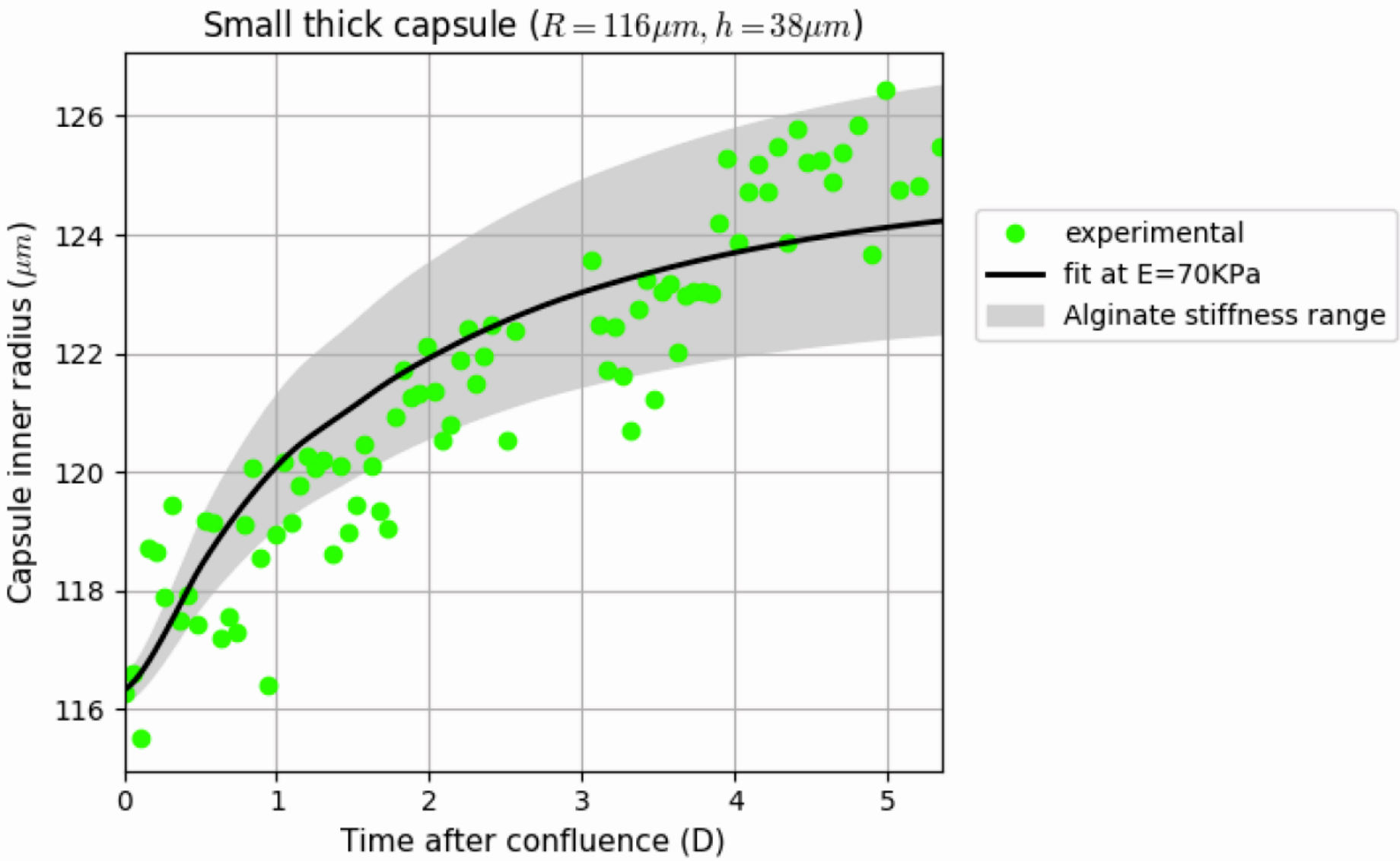
Glioblastomas (WHO grade 4)

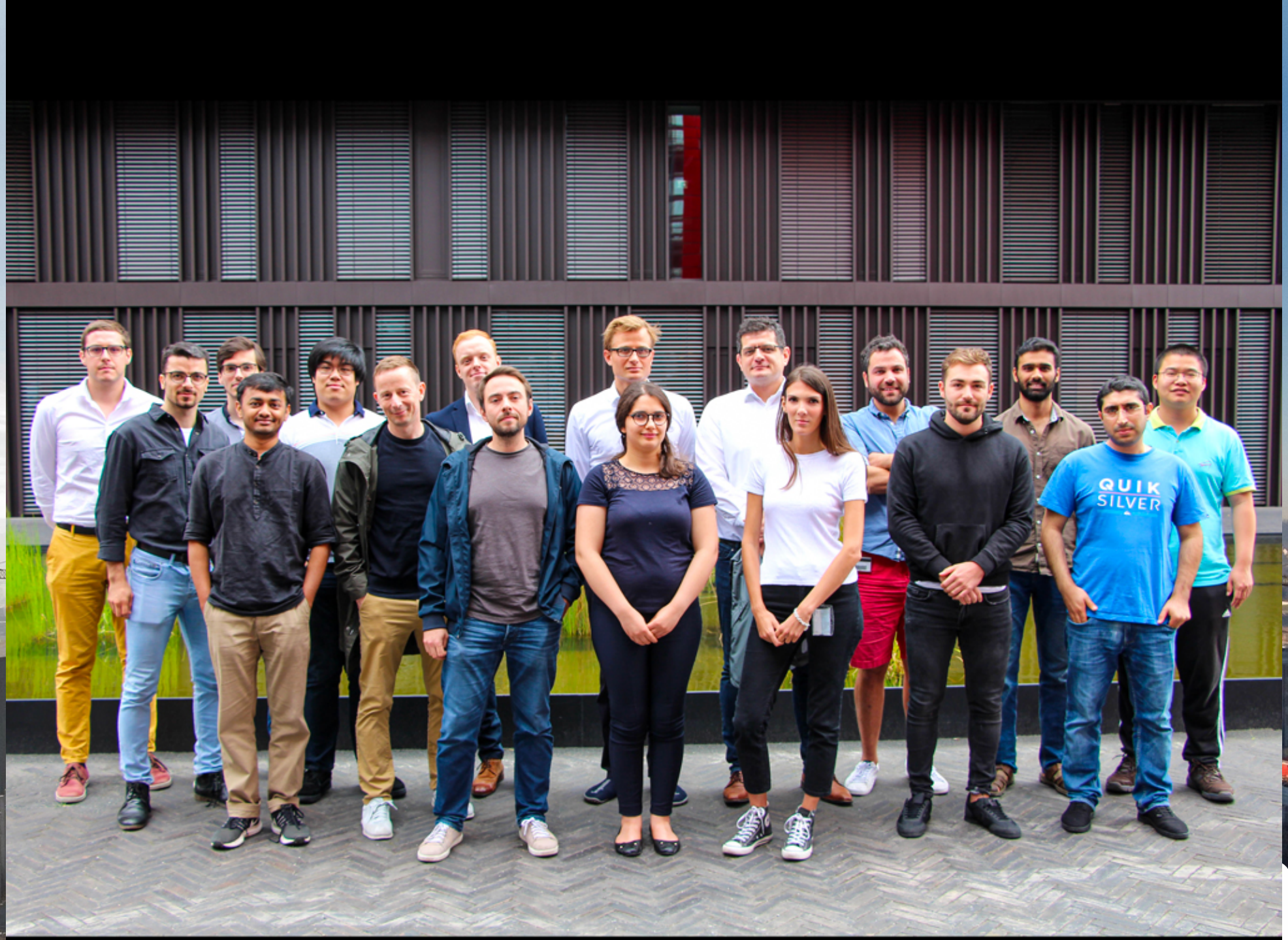
- Third non-operable
- Maximal surgical resection, plus radiotherapy, plus concomitant and adjuvant TMZ
- 90% of the tumors recur at the original site

Stages of tumor growth

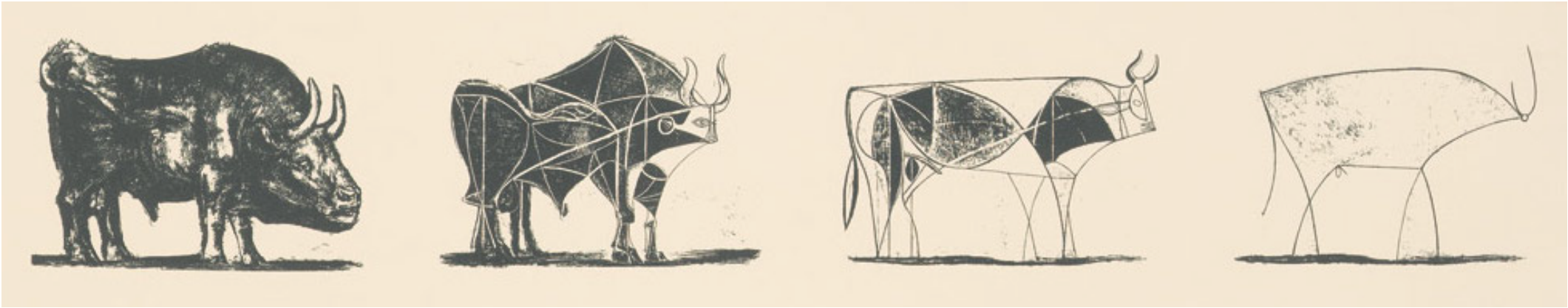


Giuseppe Sciumè


Small thick capsule ($R = 116\mu m$, $h = 38\mu m$)
Capsule inner radius (μm)
126
124
122
120
118
116
0
1
2
3
4
5
Time after confluence (D)
experimental
fit at E=70KPa
Alginate stiffness range


QUIK
SILVER

ACTIVITY REPORTS



Presentations and activity reports

- DTU DRIVEN report = https://drive.google.com/file/d/1mSzNb7hrc0mBWU7r3GXCYw769Q1ICuT4
- DTU DRIVEN overview = https://drive.google.com/file/d/1VQx0VE8BTee1LAsrqJkOA4vgwbdAvJOy
- CES Paul Würth = https://drive.google.com/file/d/1I0BHt9Qf_IuCwiuDcf04VcM2RtyV5prx

What makes Data Science different?
http://hdl.handle.net/10993/30235

Error control in deep brain stimulation simulations
http://hdl.handle.net/10993/30937

Energy-minimal crack growth
http://hdl.handle.net/10993/29414

Uncertainty Quantification in biomechanics
http://hdl.handle.net/10993/28618

Real-time error estimation for needle insertion
http://hdl.handle.net/10993/28624

Bayesian parameter identification in mechanics
http://orbilu.uni.lu/bitstream/10993/29561/3/template.pdf
http://orbilu.uni.lu/bitstream/10993/28631/1/1606.02422v4.pdf

Real-time Error Control for Surgical Simulation
http://dx.doi.org/10.1109/TBME.2017.2695587

Shape optimization directly from CAD: An isogeometric boundary element a…
http://dx.doi.org/10.1016/j.cma.2016.11.012

Linear smoothed polygonal and polyhedral finite elements
http://dx.doi.org/10.1002/nme.5324

2018 Lab Report
http://hdl.handle.net/10993/33806
http://orbilu.uni.lu/bitstream/10993/33806/1/2018labReport.pdf

2016 Lab Report
http://hdl.handle.net/10993/19425

Selected publications

		2020
Quantifying discretization errors for soft tissue simulation in computer assisted surgery: A preliminary		2020
Fracture mechanism simulation of inhomogeneous anisotropic rocks by extended finite element		2019
Structural shape optimization of three dimensional acoustic problems with isogeometric boundary	3	2019
Parameter identification problem in bimaterial human skin and sensitivity analysis: Uncertainties in		2019
Mechanical parameters identification of keloid and surrounding healthy skin using Digital Image		2019
An implicit boundary approach for viscous compressible high Reynolds flows using a hybrid	1	2019
A new locking-free polygonal plate element for thin and thick plates based on Reissner-Mindlin plate	1	2019
A stochastic Galerkin cell-based smoothed finite element method (SGCS-FEM)		2019
A gradient weighted extended finite element method (GW-XFEM) for fracture mechanics	3	2019
A unified polygonal locking-free thin/thick smoothed plate element	1	2019
Coupled molecular-dynamics and finite-element-method simulations for the kinetics of particles		2019
Weak and strong from meshless methods for linear elastic problem under fretting contact conditions		2019
Multiscale modeling of material failure: Theory and computational methods	1	2019
Advances in Crystals and Elastic Metamaterials		2019
A unified enrichment approach addressing blending and conditioning issues in enriched finite	3	2019
A simple and robust computational homogenization approach for heterogeneous particulate	5	2019
Model order reduction accelerated Monte Carlo stochastic isogeometric method for the analysis of	1	2019
Multiscale fracture: a natural connection between reduced order models and homogenisation		2019
Displacement based polytopal elements a strain smoothing and scaled boundary approach		2019

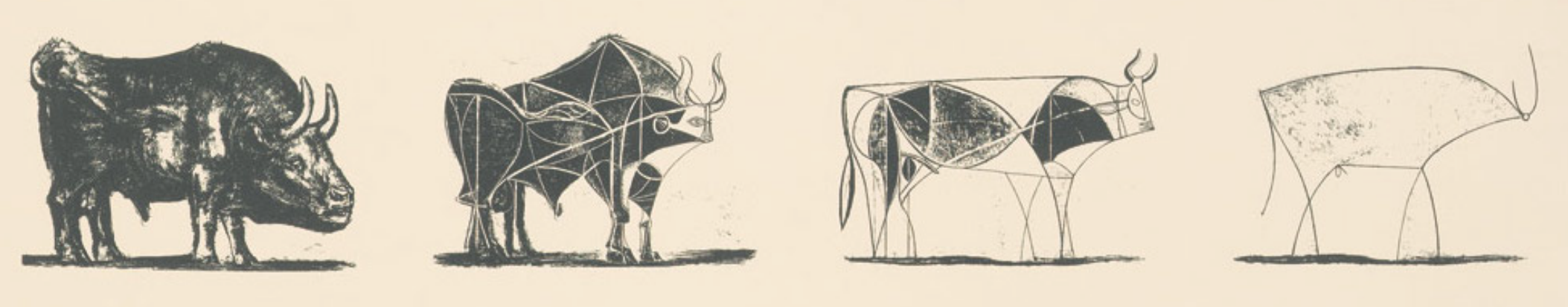
Selected publications

	10	2019
A one point integration rule over star convex polytopes	2	2019
A parallel and efficient multi-split XFEM for 3-D analysis of heterogeneous materials	7	2019
ADVANCES IN GEOMETRY INDEPENDENT APPROXIMATIONS		2019
Deep neural network with high–order neuron for the prediction of foamed concrete strength	10	2019
Improving the conditioning of XFEM/GFEM for fracture mechanics problems through enrichment quasi-	11	2019
Model I cohesive zone models of different rank coals	2	2019
Corotational cut finite element method for real-time surgical simulation: Application to needle insertion	3	2019
Introduction to Isogeometric Analysis		2019
Classification of states and model order reduction of large scale Chemical Vapor Deposition processes	5	2019
Linear smoothed extended finite element method for fatigue crack growth simulations	5	2019
Modelling Complex Systems: a primer-agent-based models, equation-based models, statistical models		2019
B-spline FEM for time-harmonic acoustic scattering and propagation	7	2019
The elastic properties of composites reinforced by a transversely isotropic random fibre-network		2019
Meshing or not meshing-Iso/sub/super-geometric analysis (adaptive unfitted methods for real-time		2019
Taylor-series expansion based numerical methods: A primer, performance benchmarking and new	1	2019
Geometrical and material uncertainties for the mechanics of composites		2019
A tutorial on Bayesian inference to identify material parameters in solid mechanics	10	2019
Advances in carbon based nanomaterials for bio-medical applications	1	2019
The influence of fracture geometry variation on non-Darcy flow in fractures under confining stresses	6	2019
A hyper-reduction method using adaptivity to cut the assembly costs of reduced order models	1	2019
Identifying elastoplastic parameters with Bayes' theorem considering output error, input error and model	10	2019

Thank you!!

Programmable matter

with Jakub Lengiewicz
Marie-Skłodowska Curie Fellow

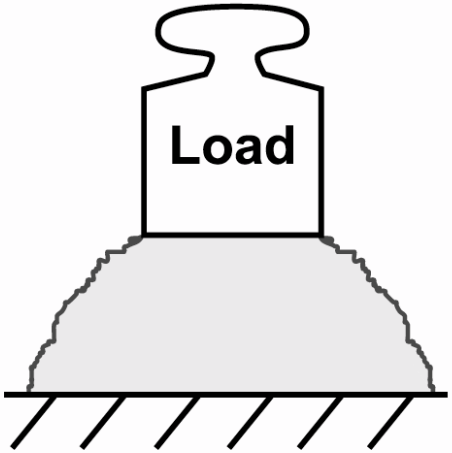


Institute of Fundamental Technological Research (IPPT)
Polish Academy of Sciences
Warsaw, Poland
Paweł Hołobut

Partially supported by Polish National Science Centre (NCN)
"Micromechanics of Programmable Matter", 2012-2017
Grant No. 2011/03/D/ST8/04089

Programmable Matter – definition

A class of future meta-materials which have the ability to freely and actively change their shape or other physical properties in a programmable and controllable manner.

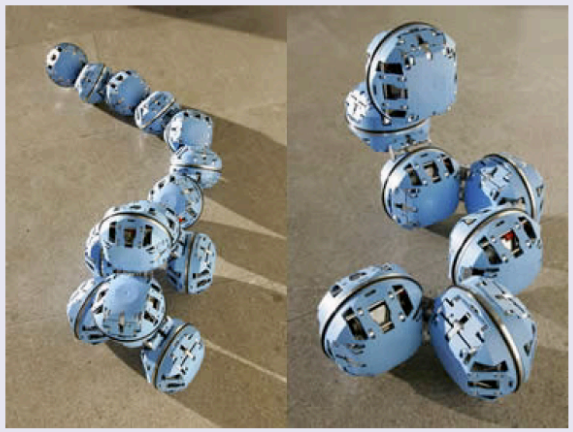


Hardware – provides the ability to *perform physical actions* and *process information* at a very *fine length-scale*.
Software – defines the *actual behavior* of the system, and *can be modified* if needed.

Modular robotic approach

Miche (MIT)

PolyBot (Xerox PARC)



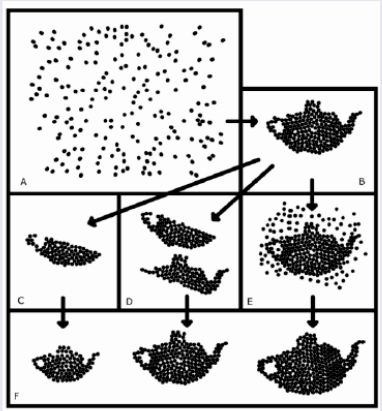
ATRON (Univ. South. Denmark)

and many more

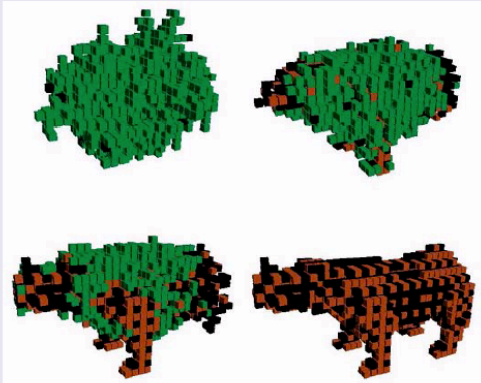
see [Yim et al., 2007]

With large amounts of modules

Pure shape-change problems $\Longrightarrow$ transforming sculptures

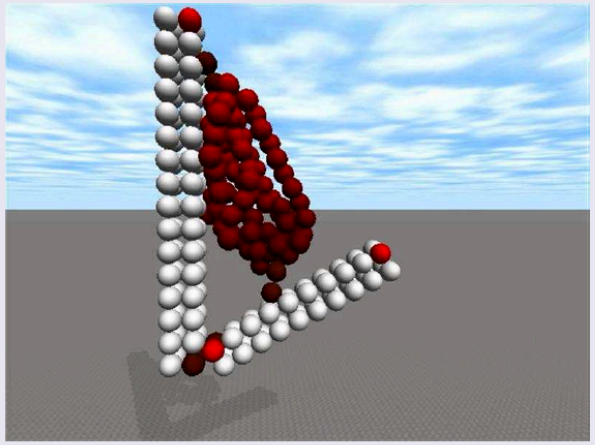


[Rubenstein et al., IROS, 2009],

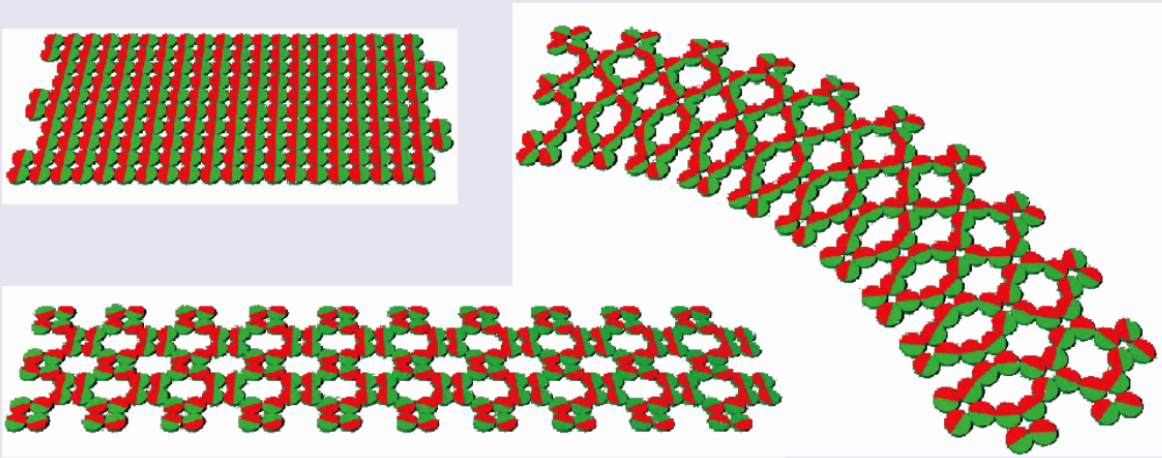


[Stoy, Springer, 2006]

Collective actuation



[Christensen et al., Neur.Comp.Appl., 2010]

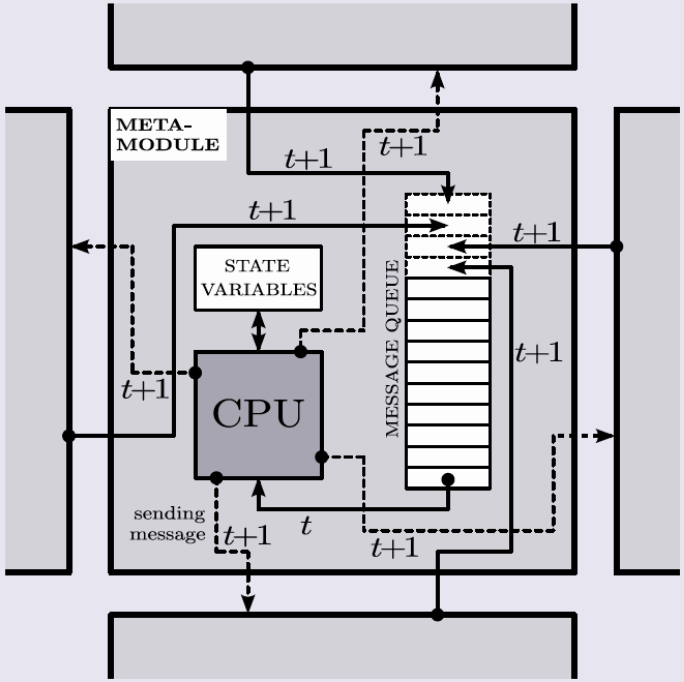


[J. Campbell and P. Pillai, IJRR, 2008]

Data flow and module design

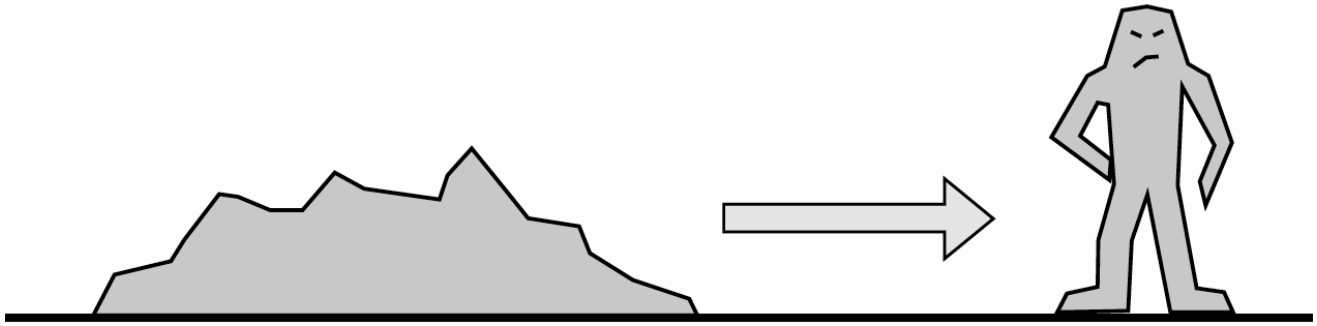
Organization of information exchange and processing

- modular robot is an asynchronous distributed computing architecture – MIMD (multiple instruction, multiple data)
- independent CPU and memory is located in every module
- communication with direct neighbors
- possibility to reconfigure



→ special distributed algorithms need to be developed

Pure shape change and locomotion



assumptions:

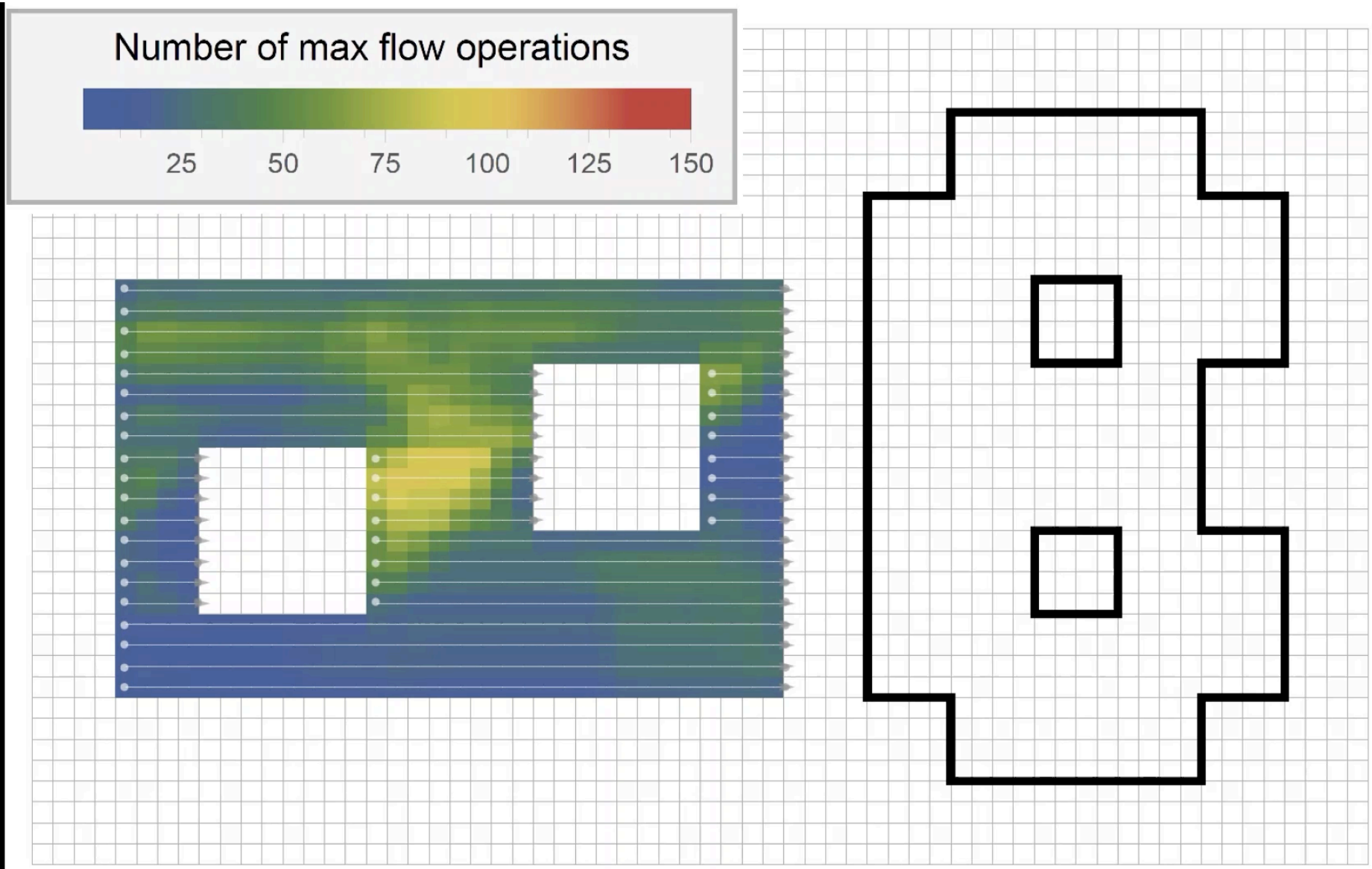
- system under external load (e.g. gravity)
- mobile (active) connections are weak (may be locked beneath the surface)
- CPU time $\ll$ communication time $\ll$ module physical motion time

our approach:

- maintain a porous frame structure and engage a **volume** of modules to move
- expected improved overall reconfiguration time

[J. Lengiewicz and P. Hołobut, Efficient Collective Shape Shifting and Locomotion of Massively-Modular Robotic Structures, *in review*, ***2017***]

Maximal flow between the source and the target boundaries

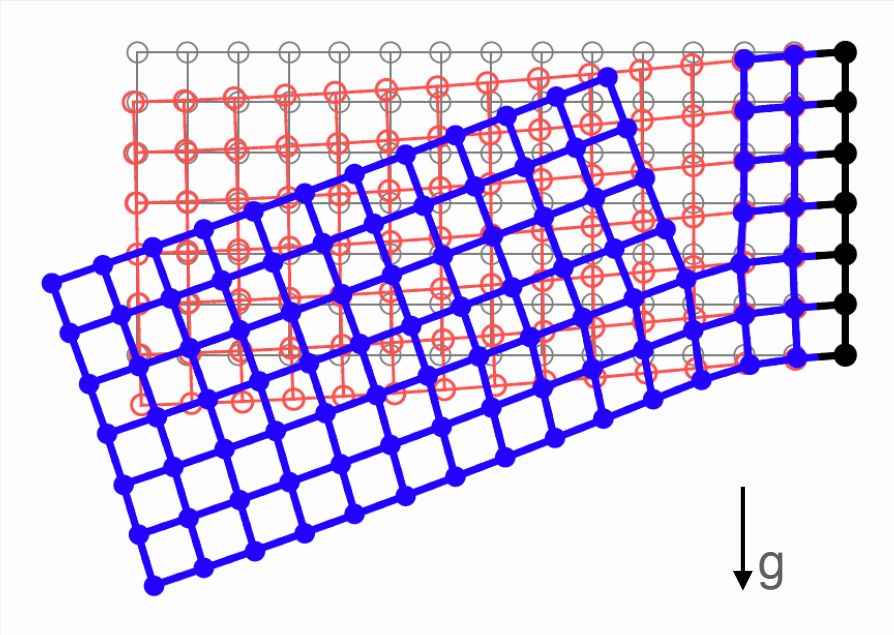


Distributed and asynchronous Edmonds-Karp algorithm to search for a maximal flow in a graph

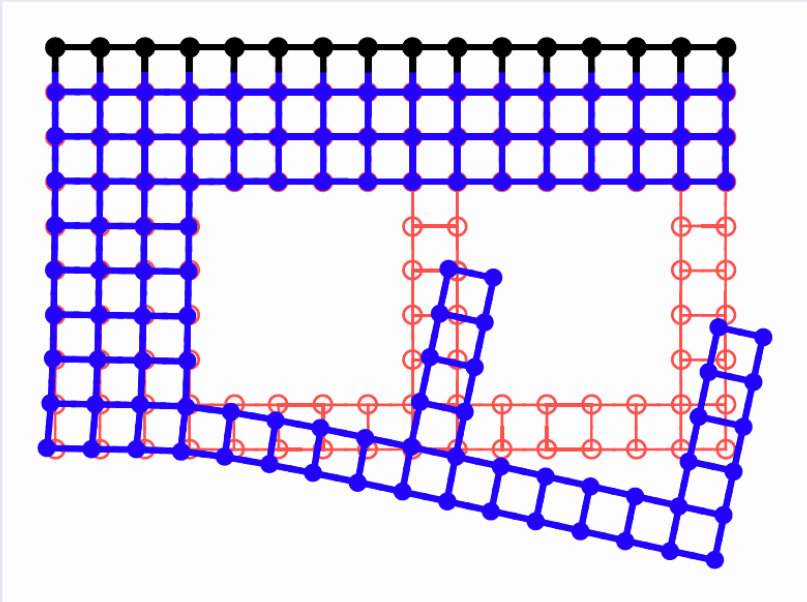
Predict consequences of breaking connections

Examples

- four connections are planned to be released
- three configurations: undeformed, deformed and predicted

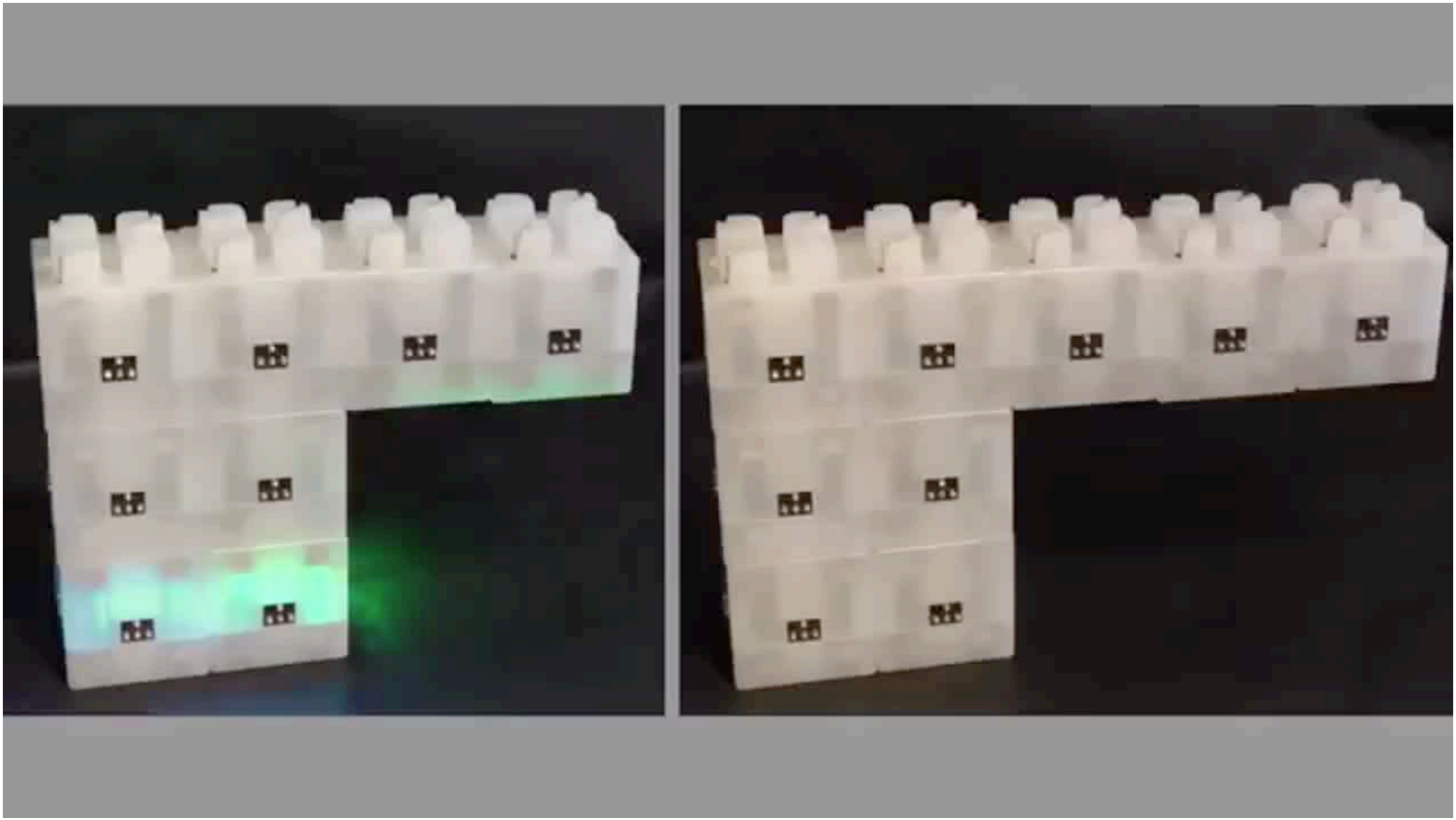


Example 1

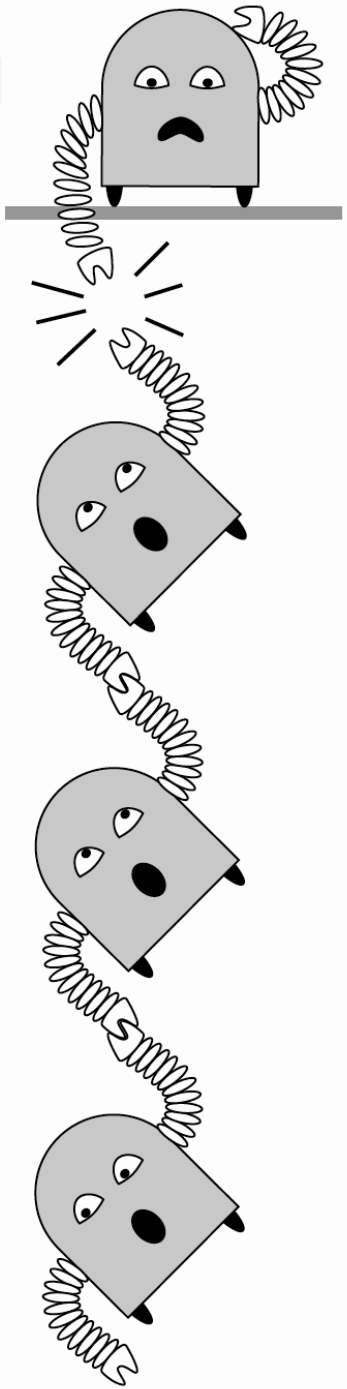


Example 2

Blinkyblocks - colour the blocks depending on stresses



Thank you!



Our approach to Programmable Matter:

[1] P. Hołobut, M. Kursa, and J. Lengiewicz, A class of microstructures for scalable collective actuation of Programmable Matter, *Proceedings of the IEEE/RSJ International Conference on Intelligent Robots and Systems* ***2014***.

[2] P. Hołobut, M. Kursa, and J. Lengiewicz, Efficient modular-robotic structures to increase force-to-weight ratio of scalable collective actuators, *Proceedings of the IEEE/RSJ International Conference on Intelligent Robots and Systems* ***2015***.

[3] P. Hołobut, P. Chodkiewicz, A. Macios, and J. Lengiewicz, Internal localization algorithm based on relative positions for cubic-lattice modular-robotic ensembles, *Proceedings of the IEEE/RSJ International Conference on Intelligent Robots and Systems* ***2016***.

[4] P. Hołobut and J. Lengiewicz, Distributed computation of forces in modular-robotic ensembles as part of reconfiguration planning, *Proceedings of the IEEE International Conference on Robotics and Automation* ***2017***

[5] J. Lengiewicz, M. Kursa, and P. Hołobut, Modular-Robotic Structures for Scalable Collective Actuation, *Robotica*, **2017**.

[6] J. Lengiewicz and P. Hołobut, Efficient Collective Shape Shifting and Locomotion of Massively-Modular Robotic Structures, *in review*, ***2017***.

DTU
DRIVEN

20 PhD students in
Data-Driven Science

Luxembourg National
Research Fund

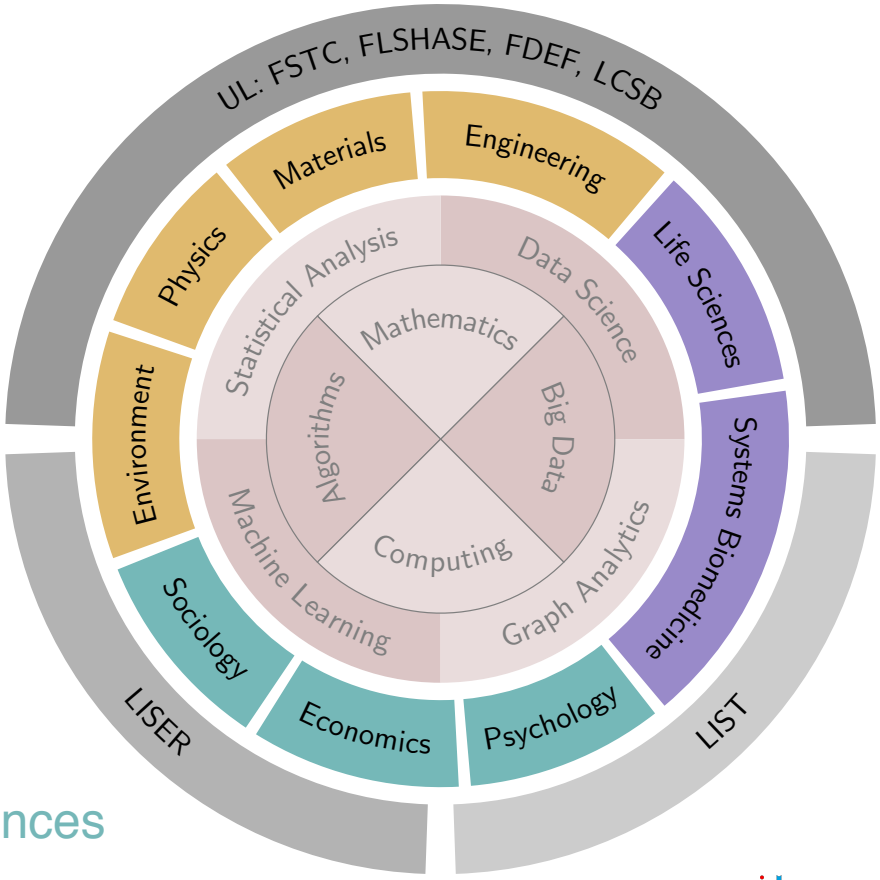
Challenges, Objectives & Research

Challenges

- scientific advances through data exploration
- machine learning techniques seen as black boxes in non-technical fields
- current lack of disciplinary ability to employ data-driven predictive modelling

Objectives and Novelty

- empower domain experts to identify, utilise and evaluate the potential of data-driven predictive modelling
- explore, adapt and employ established machine learning methods to a selection of research directions
- enhance existing expertise and research the disciplinary utility of emerging methods



Research Fields and Consortium

- Computational Physics and Engineering
- Computational Biology and Life Sciences
- Computational Behavioural and Social Sciences

Interdisciplinary Data-driven Research

Outcomes & Impact

Environment for doctoral candidates

- 20-30 PIs and co-PIs, 100+ research staff
- wide spectrum of subject-specific data
- HPC facilities at UL

Scientific outcomes & impact

- scientific advancement through innovative disciplinary results
- design of novel (transferable) multi-disciplinary methodologies

- DCs trained to leverage mathematical commonalities
- DCs trained to work at the interface between fields ("translators")
- DCs trained to drive innovation, education and cutting edge research

Economic outcomes & impact

- contribute to key strengths unique to Luxembourg: international Data hub & IT infrastructure
- contribute to develop a diversified, knowledge-based economy in Luxembourg

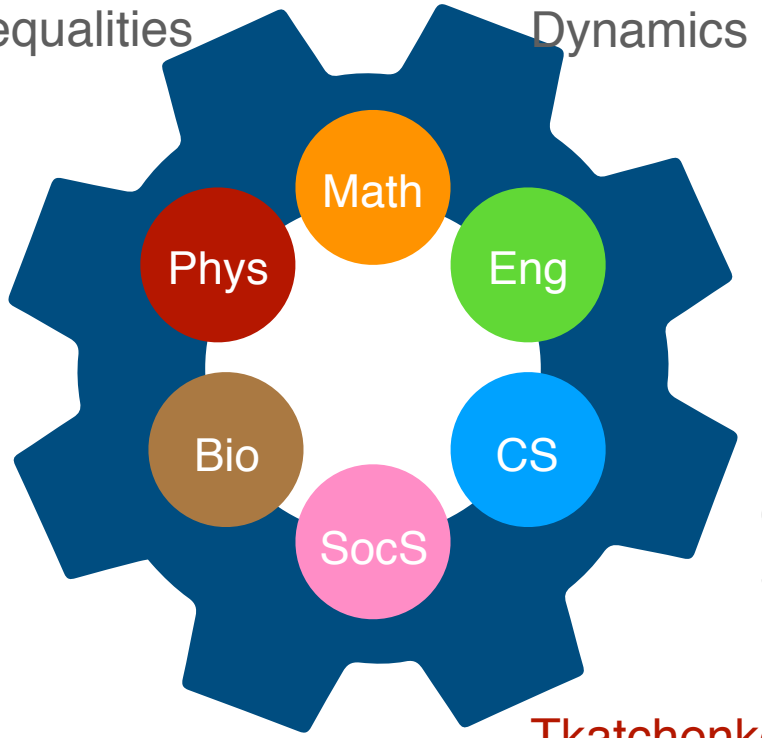
Data and Computational Sciences Doctoral Programme

Example Projects

D'Ambrosio & Tkatchenko
Social Inequalities

Peters & Bouvry
Computational Fluid Dynamics

Skupin, Bordas, & Sauter
Tumour Growth



Hale & Nourdin
Risk Quantification

Schommer, Gilles & Theobald
Computational Linguistics

Fickers & Theobald
Gender Aspects in Science

Fleming & Zilian
Microfluidic Devices

Tkatchenko, Beex & Bordas
Quantum-Continuum-Coupling

Luxembourg Institutes	University of Luxembourg	Private Sector

Methodological Core

Statistical Inversion

Bayesian Inference

Bayesian statistics

Constrained Regression

Classification SVM, Decision Trees

Feature Selection

Manifold learning

Feature Extraction

Deep learning

Clustering

Network Analytics

Random

Probability

Sampling

Least Squares

Linear Algebra

Optimisation

Gradient-based

Penalty Methods

Greedy Methods

Lagrange

Interpolation

Radial Basis Fcts

PCA

SVD

POD

Partitioning

Graph Analysis

Uncertainty Quantification

Metropolis-Hastings, Malliavin Derivatives

Weighted Residual Methods

Large Sparse/Dense Linear Systems of Equations

Discretisation and Solution of Nonlinear Coupled PDE

Problems with Constraints

Meshfree Approximation

Reduced Order Modelling

Parallel Computing

Flow Control

New priorities for the Luxembourg funding council

https://www.fnr.lu/national-research-priorities-for-luxembourg-approved/?utm_source=SLIDER&utm_medium=SLIDER%20HOM

Fundamental tools and data-driven modelling and simulation

Mastering control and understanding of the data revolution requires multidisciplinary research at the interface between computer science and mathematics (as a tool to gain insight into highly complex systems) and application areas such as engineering, life sciences, physics, as well as the social sciences.

A key novel topical area is the assimilation of hypothesis-driven mathematical models in complex systems vs. purely data-driven machine learning (ML) algorithms (differentiation of causality vs. correlation). In other words, the transition from Small Data (hypothesis-driven) to Big Data (ML paradigm). Other relevant topical areas are the quantification of uncertainties and risks in complex systems and multi-scale/reduced-order modelling (reducing complexity while maintaining information content).

RESEARCH & INNOVATION
in Luxembourg