# RESEARCH GROUP

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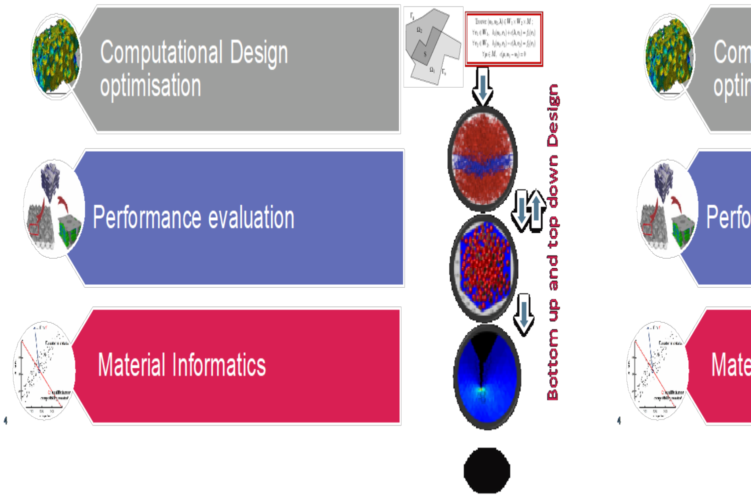
# Composite Modelling

This group combines computational mathematics, computer science, and composite materials science and engineering to i) develop physically-meaningful multiscale design frameworks augmented by data-driven approaches, ii) accelerate development, adoption and use of new composite materials; and iii) increase the fraction of critical design and decisions informed by modelling and simulation.




Combining Computational Mathematics, Computer Science, and Composite Materials Science and Engineering, our research group acts “horizontally” in a world of vertically oriented disciplines providing the knowledge and the machinery needed to:

- Develop a physically meaningful composite material design thanks to the integration of advanced materials modelling coupled with uncertainty management and reliability analysis.
- Accelerate development, adoption and use of new composite materials.
- Increase the fraction of critical design and decisions informed by modelling and simulation.

## Main expertise fields

1. Computational Design optimisation
   - Microstructure reconstruction, generation, analysis and optimisation.
   - Functional Design: right-the-first time thanks to end-to-end modelling and simulation workflows with increased accuracy and interoperability.

- Performance evaluation and interoperability
  - Predictive multiscale material relations that bridge microstructures with the continuum concurrently via statistical averaging and monitoring the microstructure/defect evolutions (i.e., manufacturing processes).
  - Materials-Process Relationships to truly close the loop between as-designed and as-manufactured composites material, products and structures.

- Material Informatics (MI)
  - MI for material microstructure analysis: Use data-centric approaches and leveraging machine learning technology for composite materials design and manufacturing.
  - MI for material selection/design: Inductive methodologies and tools for microstructure-property correlations.
  - MI to accelerate composite material design: Innovative approaches to accelerate the "forward" direction of innovation (properties are realised for an input material) and to enable the "inverse" direction (materials are designed given desired properties).

## Research challenges

The core of our research philosophy/methodology is to develop collaborations and research that effectively mesh computation with experiment (data-driven computational modelling) to tailor functional composites. In view of their sheer computational complexity, such topics cannot be successfully tackled without a simultaneous application of specialized robust solution techniques, high performance algorithms, and software tools for highly advanced computer facilities, including those based on parallel and distributed processing.

### Challenge 1: Composite material microstructure description and evolution

- Development of consistent theory and tools for microstructure-properties relationships. This microstructure level methodology needs to be supported by experimental characterization techniques to understand the anchoring physics and to design the optimized composite material microstructure.
- Material Twin: The challenge is to organize the information of reliable digital twin microstructure and Representative Volume Element and reveal the interconnection between the microstructure and the composite performances.
- Integrating manufacturing process modelling within a material design process.

### Challenge 2: Model coupling and linking

- Multiscale methods that bridge the different length scales and time scales and physics.
- Top-down and bottom-up design through a multi-component software suite (interoperability) based on community standards.

### Challenge 3: Data-driven model augmented physics-based model capabilities.

- Data-driven computational mechanics.
- Alleviate the computational burden of multiscale methods by employment of model order reduction techniques to derive the effective material response on the component level.

### Challenge 4: Multidisciplinary Design Optimisation (MDO) and decision making

- Optimize concurrently composite material microstructure with the effective use of materials models at different scales.
- Multi-criteria optimisation over all stages of product development, taking uncertainties, risks and opportunities into account.

## Application areas

- Microstructure Multiscale Modelling and Functional Design
- Manufacturing Process Modelling and Design
- Microstructure Modelling, Generation, Reconstruction and Analysis
- Material and process modelling empowered decision making
- Performance Evaluation
- Virtual Characterisation
- Functional Composite Structures Modelling and Design

## Main assets

- Internationally leading and talented researchers with proven track record offering the knowledge in mathematical modelling, optimization techniques, numerical methods, high-performance and parallel algorithms, and large-scale scientific computation.
- Long-term collaborations with world-leading companies and research groups.
- Wide range of In-house software capabilities.
- Proficient use of scientific software tools and programming languages:  Abaqus, ANSYS, COMSOL, Matlab, Simulink, Scilab, Fortran, C/C++ and Python.

## Selected publications


- Efficient uncertainty quantification and management in the early stage design of composite applications.
- Data-driven multiscale finite element method: From concurrence to separation.
- Transverse compaction of 2D glass woven fabrics based on material twins: Part 1 and Part 2.
- A data-driven analysis on bridging techniques for heterogeneous materials and structures.
- Identification of the material parameters of a viscous hyperelastic constitutive law from spherical indentation tests of rubber and validation by tensile tests.
- Global sensitivity analysis of solid oxide fuel cells with Bayesian sparse polynomial chaos expansions.
- A two-phase self-consistent model for the deformation and phase transformation behaviour of polymers above the glass transition temperature: application to PET.
- Effective conductivity in isotropic heterogeneous media using a strong-contrast statistical continuum theory.
- A micro-meso-model of intra-laminar fracture in fiber-reinforced composites based on a discontinuous Galerkin/cohesive zone method.
- An XFEM crack-tip enrichment for a crack terminating at a bi-material interface.
- An ABAQUS toolbox for multiscale finite element computation.
- X-FEM implementation of VAMUCH: Application to active structural fiber multi-functional composite materials.
- Static, free vibration and stability analysis of three-dimensional nano-beams by atomistic refined models accounting for surface free energy effect.
- Integration of material and process modelling in a business decision support system: Case of COMPOSELECTOR H2020 project.
- Optimal design of multi-step stamping tools based on response surface method.


## Partners

Goodyear Technical Centre, e-Xstream Engineering, ArcelorMittal, Siemens-Samtech, Saint Gobain Research, Dow Europe, Airbus, ESI-Group, ESTECO, Alcuilux , Weber , ESA (European Space Agency) , Open Engineering, SIMEDA-Antogyr, IEE, Luxembourg, Euro-Composites, Tarkett, Saint-Gobain, Abrasives, Luxembourg, Rioatrex Puretec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