

## MODELLING AND DESIGN OF ADVANCED MATERIALS

MARTIN DOŠKÁŘ\* AND MARTIN HORÁK\*

\* Department of Mechanics, Faculty of Civil Engineering  
Czech Technical University in Prague  
Thakurova 7, Prague  
Czech Republic  
{Martin.Doskar, Martin.Horak}@cvut.cz

**Key words:** Multiscale Modelling, Homogenisation, Computational Material Design, Metamaterials, Advanced Numerical Techniques

### ABSTRACT

Modelling and design of advanced, active, and architected materials remain at the forefront of challenges in computational mechanics. These materials, with their unique architectures and tailored behaviours, require methods that effectively connect their microstructure to their overall performance. Achieving this goal demands computational approaches that strike a balance between accuracy and efficiency while addressing the complex physical processes at play.

Homogenization techniques are essential for simplifying detailed material behaviours into effective properties, retaining the most critical microstructural influences. Similarly, multiscale simulations offer insights into how small-scale features shape larger-scale responses. Together, these methods provide the tools needed to understand and predict how materials behave in diverse real-world applications.

Recent advances in computational methods are pushing the limits of active materials and metamaterial design. Numerical simulations now enable the exploration of new geometries and functionalities, driving innovation in areas like structural mechanics, energy absorption, and wave control. Furthermore, interfacial phenomena—such as surface energies and contact mechanics—play a pivotal role in multiscale and multiphysics interactions, especially in systems where boundaries critically influence performance.

This minisymposium aims to bring together researchers tackling these challenges in modelling, simulation, and design. Topics of interest include:

- Multiscale simulation techniques for understanding material behaviour,
- Homogenization methods for complex material systems,
- Computational strategies for designing advanced and architected materials,
- Modelling of interfacial phenomena like surface energies and contact mechanics,
- Applications of these methods in structural, functional, and smart materials.

By encouraging collaboration and knowledge exchange, this minisymposium seeks to advance the computational techniques needed to model and design advanced materials effectively. It offers a forum to discuss the latest developments and practical applications, supporting innovation in computational mechanics and material science.