

# Spotlights in Computational Physics and Engineering (SCoPE)

Invited lectures on:

## Multi-scale modelling of advanced engineering materials: from understanding microphysics to enriched continuum description

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### Abstract

Advanced engineering materials with extraordinary properties have emerged to meet the continuously growing requirements in modern applications, e.g. aerospace, medical, automotive, tooling, and energy. As the governing microstructures are typically complex, computational modelling of advanced engineering materials with microstructures fully resolved over the entire macroscopic component domain is often prohibitive to perform. To address this, (hierarchical) multi-scale modelling approaches are being considered as suitable candidates, i.e. “divide-and-conquer” strategies whereby the entire range of material behaviour is divided into a hierarchy of scales. At each macroscopic material point, a microscopic unit cell is assigned. By upscaling, the microscopic phenomena are consistently and effectively bridged to the macroscopic behaviour.

Multi-scale modelling approaches adopting a classical continuum description at the macroscale are the mostly widely used to date. On one hand, they have exhibited remarkable success for many advanced engineering materials, e.g. closed-cell foams, fibre-matrix composites, and multi-phase metals. On the other hand, the classical continuum description fails for many others which may require enrichment of the macroscopic kinematics to resolve the microphysics as well as adaption of the scale transition. Despite a critical role in multi-scale modelling, what description shall be adopted at the macroscale is usually not known a-priori for a given material system.

In the lectures, a multi-scale modelling strategy from understanding microphysics to developing macroscopic enriched continuum description, will be introduced to address the challenges above. This strategy will be demonstrated through the recent advances for two advanced engineering materials: locally resonant acoustic metamaterials (LRAM) and dual-phase (DP) steels. Solid and shell problems will be covered for LRAM while interface problems will be focused on for DP steels.

The lectures are structured as follows:

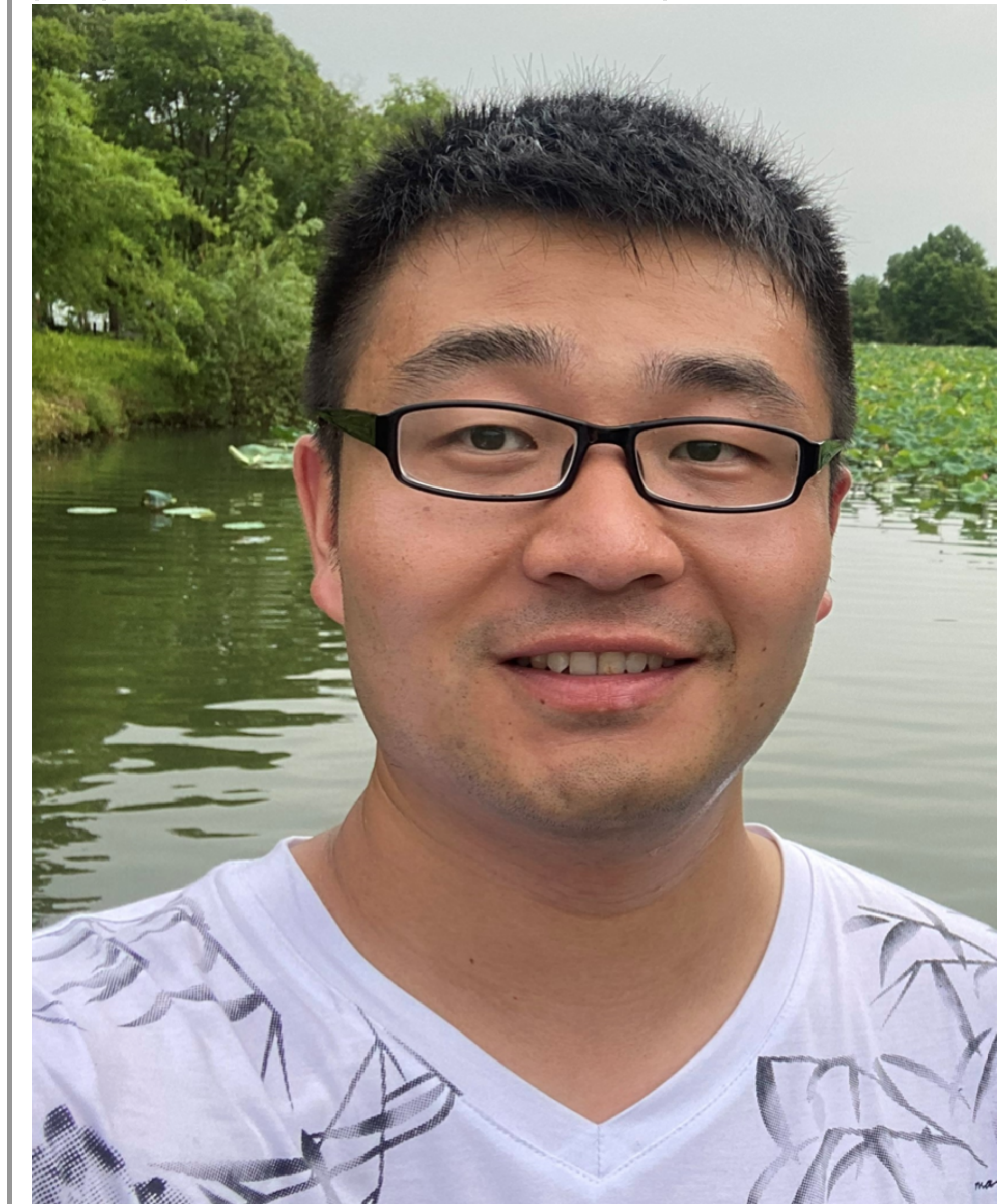
1. Basic concepts of multi-scale modelling approaches, with a focus on continuum-based two-scale modelling approaches (including solid, shell and interface problems). Challenges in multi-scale modelling of advanced engineering materials. An overview of the multi-scale modelling strategy from understanding microphysics to enriched continuum description.
2. Introduction to LRAM. 1D analytical modelling of LRAM to understand the microphysics (local resonance). Homogenization of LRAM towards enriched continuum. Application for double-negative LRAM (including dispersion and frequency domain analyses)
3. Introduction to LRAM panels. Homogenization of LRAM panels towards enriched continuum beam/shell structures. Application for negative-mass LRAM beams and plates (including dispersion, frequency domain and transient analyses). Application for LRAM plate sound transmission analyses.
4. Introduction to DP steels. Crystal plasticity modelling of martensite/ferrite interface microstructures to understand the microphysics (martensite substructure boundary sliding) governing the mesoscopic interface damage. Homogenization of martensite/ferrite interface microstructures towards enriched cohesive interfaces. Application for DP steel mesostructures.

### When and Where?

- ▶ 25.04.2024, 10:00-12:00, Maison du Savoir, MSA 2.230
- ▶ 26.04.2024, 10:00-12:00, Maison du Savoir, MSA 3.160

### Invitee: Lei Liu\*

**LEI LIU** is a Postdoctoral Researcher at Division of Material and Computational Mechanics, Chalmers University of Technology, Sweden since November 2023. Prior to joining Chalmers, he obtained his PhD degree at Mechanics of Materials Section, Eindhoven University of Technology, the Netherlands. His research interests focus on developing high-efficiency multi-scale modelling and homogenization approaches, and applying advanced computational tools to understand and predict the structure-property relations of complex materials.



### Selected Publications

- ▶ L. Liu, F. Maresca, T. Vermeij, J.P.M. Hoefnagels, M.G.D. Geers, and V.G. Kouznetsova. An integrated experimental-numerical study of martensite/ferrite interface damage initiation in dual-phase steels. *Scripta Materialia*, 239:115798, 2024.
- ▶ L. Liu, F. Maresca, J.P.M. Hoefnagels, M.G.D. Geers, and V.G. Kouznetsova. A multi-scale framework to predict damage initiation at martensite/ferrite interface. *Journal of the Mechanics and Physics of Solids*, 168:105018, 2022.
- ▶ L. Liu, A. Sridhar, M.G.D. Geers, and V.G. Kouznetsova. Computational homogenization of locally resonant acoustic metamaterial panels towards enriched continuum beam/shell structures. *Computer Methods in Applied Mechanics and Engineering*, 387:114161, 2021.
- ▶ L. Liu, F. Maresca, J.P.M. Hoefnagels, T. Vermeij, M.G.D. Geers, and V.G. Kouznetsova. Revisiting the martensite/ferrite interface damage initiation mechanism: The key role of substructure boundary sliding. *Acta Materialia*, 205:116533, 2021.
- ▶ A. Sridhar, L. Liu, V.G. Kouznetsova, and M.G.D. Geers. Homogenized enriched continuum analysis of acoustic metamaterials with negative stiffness and double negative effects. *Journal of the Mechanics and Physics of Solids*, 119:104-117, 2018.