

MS 1-7: Multiscale Materials Modelling from Atoms to Macroscale

Organizers:

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This mini-symposium will focus on new ideas in multiscale materials modelling including coupled approaches between discrete (molecular dynamics, dislocation dynamics, for instance) and continuum modelling strategies. It aims to bring together experts across the disciplines to discuss new models and new trends for a wide range of materials classes (polymers, metals and alloys, ceramics, glasses, geomaterials, etc.)

The relevant topics are (non-comprehensive list)

Discrete, continuous, and coupling models and methods:

- Ab-initio approaches, molecular mechanics & dynamics, dissipative particle dynamics, peridynamics;
- Continuum mechanics, finite elements, fast-Fourier transform, phase-field methods, homogenization approaches;
- Sequential, hierarchical, and domain-decomposition coupling techniques;
- Multiphysical coupling

Scales: Atomistic & molecular, coarse-grained, mesoscale, macroscale, scale-bridging

Materials and applications:

- Amorphous and crystalline materials
- Scale-bridging aspects of elasticity, viscosity, and plasticity including micromechanics and microstructures;
- Studies of fracture across the scales, including crack nucleation and propagation
- Coupled material modelling (discrete and continuous, multiphysics)
- Prediction of mechanical properties
- Structure-property relationships