SIMULATIONS OF MULTIFUNCTIONAL MATERIALS BRIDGING METHODS, SCALES, AND DISCIPLINES

1600 - MULTISCALE AND MULTIPHYSICS SYSTEMS

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ABSTRACT

The macroscopic, observable behavior of advanced materials is governed by the structure at different scales. Non-exhaustively, these scales include atomistic and mesoscopic levels. Of utmost interest, understanding failure and evaluating strength and fracture toughness requires multiscale approaches. Advanced materials include nanocomposites, polymer blends, inorganic amorphous materials, smart materials, and hierarchical materials. Advanced materials can also be extended to biological materials, which display complex multiscale features.

A possible classification categorizes the required multiscale approaches into sequential and concurrent methods. Sequential methods obtain findings on the fine scale, which are then applied to the coarse scale in a separate simulation. In contrast, concurrent methods simultaneously consider the coarse and fine-scale in hierarchical or partitioned-domain approaches. In hierarchical methods, both scales are evaluated in the entire simulation domain, while the partitioned-domain strategies only resolve the regions of interest, e.g., the vicinity of fillers in nanocomposites at the fine scale.

Commonly, multiscale strategies do not only bridge scales but also methods and disciplines, which is the scope of this mini-symposium.

Possible topics include (non-exclusive list):

- **Materials**: Bulk polymers (e.g., thermosets, thermoplastics, elastomers, gels), composites, bio-based materials, biological materials, graphene, inorganic glasses, piezoelectric materials, meta-materials, dielectrics, phase-change materials, architected materials, liquid-crystal;
- **Methods**:
    - **Continuum approaches**: Finite element method, peridynamics, numerical homogenization, phase-field methods, topology optimization,
    - **Particle-based methods**: Ab initio, molecular mechanics/dynamics, dissipative particle dynamics,
    - **Multiscale methods**: Atomistic-continuum coupling (sequential, concurrent, hierarchical, partitioned-domain methods), heterogeneous multiscale method, quasicontinuum method, QM-MM, FE^2, FE-FFT,
    - **Multi-physics coupling**: Piezoelectricity, flexoelectricity, thermoelasticity, photomechanics, magnetorheology, mechanochemistry, phase transition;
- **Scales**: Atomistic, molecular, coarse-grained, mesoscale, macroscale;
- **Applications**: Prediction of mechanical properties, characterization of processing conditions and production methods, understanding of fracture mechanisms, development of new nanocomposites, identification of structure-property relationships, sensors, smart materials, solar cells, batteries.