Multiscale Modeling of Coupled Thermo-Hydro-Mechanical Problems in Granular Media

Jidong Zhao

Department of Civil and Environmental Engineering Hong Kong University of Science and Technology Clearwater Bay, Kowloon, Hong Kong e-mail: jzhao@ust.hk, web page: http://jzhao.people.ust.hk

ABSTRACT

The coupled thermo-hydro-mechanical (THM) behavior of granular media governs the performance of critical engineering systems, including permafrost-based infrastructure, carbon sequestration, methane hydrate extraction, and additive manufacturing. This work advances multiscale computational frameworks to model THM-coupled processes in granular media in contexts of these applications, addressing phase transitions, large deformations, and multiphysics interactions. For geotechnical systems, we present novel material point method (MPM)-based approaches: (1) a three-phase MPM simulating ice-water transitions and thawinduced failures in permafrost, validated against thaw consolidation and frost heave experiments; and (2) a multiscale MPM-DEM framework linking continuum-scale THM processes to grain-scale ice-bond mechanics for cyclic freeze-thaw analysis. These frameworks integrate ice saturation-dependent constitutive laws, fractional-step algorithms for numerical stability, and axisymmetric formulations. For granular systems undergoing thermalinduced phase changes in manufacturing, we extend the approach to CFD-DEM coupling for laser powder bed fusion (LPBF), resolving multiphase interactions (solid particles, melt pool, vapor) and thermal processes (melting, vaporization, solidification) via resolved immersed boundaries, evaporation models, and laser energy absorption schemes. Validations against synchrotron experiments demonstrate predictive capabilities in capturing melt pool dynamics, keyhole formation, and powder motion. The study underscores computational challenges in modeling THM-coupled phase transitions, multiphysics interactions, and failure mechanisms with explainable micro-macro linkages, emphasizing the need for versatile numerical methods to address granular media under extreme thermal-mechanical loading.

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