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Multiscale Modeling Schemes Spanning a Large Range of Scales

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This paper presents effective multiscale modeling schemes to carry out analyses spanning a large range of scales. The proposed concepts in the continuum realms is to use the medium of the intermediate scale as a means to connect variables at the lower scale with those at the upper scale through developing equivalent constitutive equations. These equations are developed based on microstructures of the lower scale through making the variables satisfy corresponding mechanics principles. In the realm of joint atomistic and continuum scales, a mixed particle and molecular dynamics (MD) method will be coupled with quantum methods. The particle method is used to lump many atoms together as a molecular particle to reduce degrees of freedom in the low-stress gradient region. This lumped molecular particle can further connect to structure particles that are used in mesh-free finite element analysis to make the transition from the atomic scale to the continuum possible.

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