Fast Solvers for Force-based Multi-physics Coupling Models

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Force-based multi-physics coupling models have become popular since they provide a simple and efficient coupling mechanism, avoiding the difficulties in formulating and implementing a consistent coupling energy. They are the only known consistent methods for coupling a general atomistic model to a continuum model, for coupling a quantum mechanics model to a molecular mechanics model, for coupling atomistic polymer models to coarse-grained polymer models, etc. However, the development of efficient and reliable iterative solution methods for force-based coupling methods presents a challenge due to the non-symmetric and indefinite structure of the linearized force-based models as well as to their unusual stability properties. We present rigorous numerical analysis and computational experiments to systematically study the stability and convergence rate for a variety of fast solvers for the force-based quasicontinuum approximation as an example of more general phenomena.