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A Cohesive Finite Element Method for Quasi-continua

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ABSTRACT

In this work, a cohesive finite element method (FEM) is proposed for quasi-continua (QC), i.e. continuum media whose constitutive behaviors are modeled by underlying atomistic microstructures.

Most cohesive laws used in conventional cohesive FEMs are based on either empirical or idealized constitutive models that do not accurately reflect the actual atomistic lattice structures. The proposed cohesive-QC finite element method, cohesive-QC FEM in short, is a step forward in the sense that: (1) the cohesive relation between interface traction and displacement opening is now obtained based on atomistic potentials along the interface, rather than empirical assumptions; (2) it allows the local quasi-continuum method to simulate certain inhomogeneous deformation patterns.

We introduce a surface Cauchy-Born rule such that the interfacial cohesive relation is consistent with the atomistically enriched hyperelasticity inside the solid, and with this one can simulate inhomogeneous or discontinuous displacement fields by using a simple local quasi-continuum model.

In this presentation, we shall present numerical examples of dynamic fracture and dislocation propagation to demonstrate the validity, efficiency, and versatility of the method.

REFERENCES

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