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Quasicontinuum Method: Novel Theories and Implementation

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ABSTRACT

The theoretical and computational limitations of continuous description and atomistic modeling on capturing phenomena at the micro- or nano-scale have called for the need to fuse atoms with finite elements. Atomistic modeling has been used to address a wide variety of deformation processes in solids in the past decades. Nevertheless, the length scale restriction of atomistic modeling has long been a substantial obstacle in making useful prediction. In the past few years, a very promising method called the quasicontinuum (QC) method has been developed to circumvent this length scale problem [1-5]. By using kinematic constraints through finite element interpolation, the method allows for developing fully atomistic scale resolution near defects while exploiting coarser description further away to reduce redundant degrees of freedom. The QC method has received broad attention since its debut, partly due to its theoretical elegance in thinning redundant degrees of freedom and partly due to its computational generality in treating a wide range of problems relating to defect nucleation and evolution in solids. However, the formulation of QC conceived and developed in [1, 2] suffers from its inherent deficiency of calculating forces at the transition region between the atomistic and continuum. This inconsistency produces non-physical forces (a.k.a., ghost forces) even when the crystal is undeformed, let alone for more demanding inhomogeneous phenomena.

In this study, we present recent theoretical and computational advances on the QC method. On the theoretical side, we resolve the local and non-local mismatch through analyzing the error induced by the Cauchy-Born based QC method between atoms and finite elements. The origin of ghost forces is analyzed and it has found that the non-local effect between atoms and finite elements needs to be taken into account. Consequently, the energy and force in this transition region need to be resolved atomistically. To this end, a physical-based scheme with the concept of transition atoms is established. The undesirable ghost forces caused by local and non-local match have been successfully remedied by the transition atoms (Figure 1).

On the computational side, we present recent progress to ease implementation of the QC mesh generation in 3D. As atoms and finite elements are adaptively evolving in the QC

analysis, it requires automatic mesh generation in 3D. Nevertheless, the additional constraints imposed by the QC method in which the local representative atoms need to be coincided with the nodes of finite elements pose a challenge for a Delaunay-based mesh generation. To this end, the theories proposed herein have been extended to eliminate such constraints. It thus allows for using a general purpose mesh generator for the QC method. The robustness of our implementation is demonstrated by studying indentation size effects for various samples at nanoscale.

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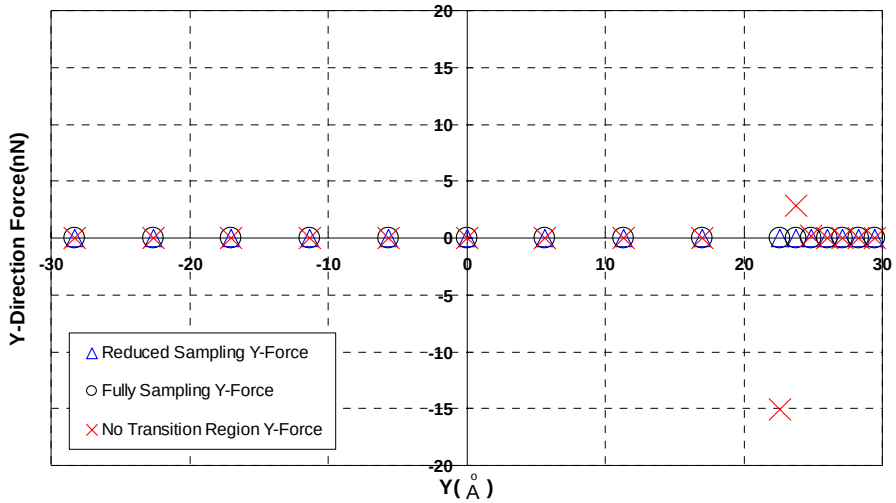

Figure 1: QC force calculations for a perfect crystal: mismatch induced ghost forces are observed between atoms and finite elements if no transition region is adopted. The undesirable ghost forces have been successfully remedied by the transition atoms.