Multiresolution molecular mechanics: surface effects and iso-parametric analysis

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ABSTRACT

Within the generalized framework of the newly presented energy-based concurrent atomistic/continuum method Multiresolution Molecular Mechanics (MMM) [1], two proposed summation rules, the bulk summation and the edge summation rule to efficiently determine the bulk and surface energy distribution respectively, consists the optimal MMM summation rule. In Ref. [1], the bulk summation rule has been verified and proved to outperform the widely used Gauss quadrature. In this study, the edge summation rule will be employed to specifically capture surface effects. This is achieved in three steps: (i) use the edge summation rule to determine the surface energy distribution for any given finite element method (FEM) shape function analytically; (ii) select the optimal number of surface primary sampling atoms on the surfaces, and (iii) determine the weight for each surface primary sampling atoms using the edge summation rule and then use their energies to sampling the surface energy. In particular, the effect of the selection of surface primary sampling atoms on the accuracy of capturing surface effect will be studied. In addition, the sampling errors introduced by employing the edge summation rule will be determined through error structure analysis. Then iso-parametric analysis within the generalized framework of MMM will be performed to standardize the implementation procedure of MMM, as is widely employed in conventional FEM. The iso-parametric analysis is achieved by performing the surface summation rule and the bulk summation rule within some specifically designed surface parent elements and bulk parent elements. In particular, the iso-parametric analysis will be performed with respect to linear, bilinear, and quadratic elements undergoing tensile, shear, and bending deformations and will be compared against full atomistic to show the effectiveness of MMM.

REFERENCES

[1]   Yang, Q., To, A.C. Multiresolution molecular mechanics: a unified and consistent framework for general finite element shape functions. *Comp. Meth. Appl. Mech. Eng*. (under review).

[2]   Yang, Q., Biyikli, E., To, A.C. Multiresolution molecular mechanics: statics. *Comp. Meth. Appl. Mechanics Eng.* 2013, 258, 26-38.

[3]   Yang, Q., Biyikli, E., To, A.C. Multiresolution molecular mechanics: convergence and error structure analysis. *Comp. Meth. Appl. Mech. Eng.* 2014, 269, 20-45 .

[4]   Biyikli, E., Yang, Q., To, A.C. Multiresolution molecular mechanics: dynamics. *Comp. Meth. Appl. Mech. Eng.* 2014, 274, 42-55.