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Concurrent multiscale modeling of amorphous materials[1]

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An approach to multiscale modeling of amorphous materials is presented whereby atomistic scale domains coexist with continuum-like domains. The atomistic domains faithfully predict severe deformation while the continuum domains allow the computation to scale up the size of the model without incurring excessive computational costs associated with fully atomistic models and without the introduction of spurious forces across the boundary of atomistic and continuum-like domains. The material domain is firstly constructed as a tessellation of Amorphous Cells (AC). For regions of small deformation, the number of degrees of freedom is then reduced by computing the displacements of only the vertices of the ACs instead of the atoms within. This is achieved by determining, a priori, the atomistic displacements within such Pseudo Amorphous Cells associated with orthogonal deformation modes of the cell. Simulations of nanoscale polymer tribology using full molecular mechanics computation and our multiscale approach give almost identical prediction of indentation force and the strain contours of the polymer. We further demonstrate the capability of performing adaptive simulations during which domains that were discretized into cells revert to full atomistic domains when their strain attain a predetermined threshold.

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