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COMPARISON OF SEVERAL STAGGERED ATOMISTIC-TO-CONTINUUM CONCURRENT COUPLING STRATEGIES

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The atomistic and continuum descriptions of matter are concurrently coupled in a staggered manner. The continuum-to-atomistic link is implemented using an affine assumption for the outer region of the atomistic description, where the ions are fully enslaved to the continuum solution. The atomistic-to-continuum link is based on fields that are calculated from the atomistic solution [4, 5]. It utilizes the atomistic-to-continuum correspondence, obtained by spatial averaging in the spirit of Irving and Kirkwood, and Noll [1, 2, 3].

In this work, different mechanisms to pass the information from the atomistic domain to continuum are studied [6]. The schemes considered here are decomposed into the surface-type (displacement or traction boundary conditions) and the volume-type. The latter restrict the continuum displacement field (and possibly its gradient) in some sense to the atomistic (discrete) displacements using Lagrange multipliers.

The described coupling methods are numerically examined using two examples: uniaxial deformation and a plate with a hole relaxed under surface tension. Accuracy and convergence rates of each method are reported. It was found that the displacement (surface) coupling scheme and the Lagrangian (volume) scheme based on either discrete displacements or the H1 norm derived from continuous displacement fields provide the best performance.

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REFERENCES

[1] D. Davydov and P. Steinmann. Reviewing the roots of continuum formulations in molecular systems. Part I: Particle dynamics, statistical physics, mass and linear momentum balance equations. *Mathematics and Mechanics of Solids*, 1–23, 2013.

[2] D. Davydov and P. Steinmann. Reviewing the roots of continuum formulations in molecular systems. Part II: Energy and Angular Momentum Balance Equation. *Mathematics and Mechanics of Solids*, 1–16, 2013.

[3] D. Davydov and P. Steinmann. Reviewing the roots of continuum formulations in molecular systems. Part III: Stresses, Couple Stresses, Heat Fluxes. *accepted*.

[4] D. Davydov, A. Javili and P. Steinmann. On molecular statics and surface-enhanced continuum modeling of nano-structures. *Computational Materials Science*, Vol. **69**, 510–519, 2013.

[5] D. Davydov, A. Javili, P. Steinmann, A. McBride. A comparison of atomistic and surface enhanced continuum approaches at finite temperature. In H. Altenbach and N. F. Morozov (eds.), *Surface Effects in Solid Mechanics*, Advanced Structured Materials, Vol **30**, 43–57, 2013.

[6] D. Davydov, J-P. Pelteret, P. Steinmann. Comparison of several staggered atomistic-to-continuum concurrent coupling strategies. *submitted*.