

# COUPLING METHODS FOR CONTINUUM MODEL WITH MOLECULAR MODEL

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## ABSTRACT

Coupling methods for continuum models with molecular models are developed. Two methods are studied here: a bridging domain coupling method, which has an overlapping subdomain, and an edge-to-edge coupling method, which has an interface between two models. We enforce the compatibility on the overlapping subdomain or interface nodes/atoms by the Lagrange multiplier method or the augmented Lagrangian method. Static solution and dynamic solution are given respectively. For dynamic problems, we develop an explicit algorithm and the results show that the bridging domain coupling method can avoid spurious reflections without any additional filtering procedures. A multiple-time-step algorithm is also implemented and it saves considerable computation time. These methods are used to study the nanotube fracture.

## References:

- [1] T. Belytschko and S. P. Xiao, "Coupling methods for continuum model with molecular model", *International Journal for Multiscale Computational Engineering*, v 1(1), p. 115-126, 2003.
- [2] T. Belytschko, S. P. Xiao, G. C. Schatz and R. Ruoff, "Atomistic simulations for nanotube fracture", *Physical Review B*, v 65, p. 235430, 2002.
- [3] M. Arroyo and T. Belytschko, "An atomistic-based finite deformation membrane for single layer crystalline films", *Journal of the Mechanics and Physics of Solids*, v 50, p. 1941-1977, 2002.
- [4] F. F. Abraham, J. Q. Broughton, N. Bernstein and E. Kaxiras, "Spanning the length scales in dynamic simulation", *Computational Physics*, v 12(6), p. 538-546, 1998.