Comparative study of molecular dynamics and material point method for simulating failure evolution

†Zhen Chen[1,2]*, Yu-Chen Su[2], and Jun Tao[1]

[1]Department of Engineering Mechanics, Dalian University of Technology, China
[2]Department of Civil and Environmental Engineering, University of Missouri, USA

*Presenting author: chenzh@missouri.edu
†Corresponding author: chenzh@missouri.edu

Abstract

There exist two types of model-based simulation procedures available for evaluating failure evolution, namely, continuous and discontinuous ones. Molecular dynamics (MD) is a representative example of discontinuous methods, in which a cut-off radius associated with the discrete forcing function for a given molecule is specified to describe the interactions among this molecule and other molecules within a domain of influence. On the other hand, the material point method (MPM) is a continuum-based particle method, in which a constitutive model is required for a given material point such that the interaction among this material point and other points are described via the first or higher order gradients of deformations. It has been shown that the evolution of interfacial failure between different material phases has the nonlocal feature [1]. As continuous approaches, nonlocal elastoplasticity and elastodamage models, in terms of strain gradients or integrals, have been proposed to predict the interactions among material points (particles) during the evolution of failure, for which the size effect is the key to calibrate these constitutive models based on experimental data. The size effect in continuous approaches is similar to the cut-off radius in discontinuous approaches, but the quantitative analysis of their relationship has not been performed in a systematic manner. Based on the recent research efforts on the MPM [2-6], a case study is conducted to compare the numerical results with both MD and MPM in simulating an impact test to evaluate cartilage failure, and an effective way to integrate nonlocal modeling and spatial discretization is explored within the MPM framework to better evaluate multi-phase (solid-fluid-gas) interactions involving failure evolution.

References

[1] Chen, Z., and Schreyer, H.L., "On Nonlocal Damage Models for Interface Problems," International Journal of Solids and Structures, Vol. 31(9), pp. 1241-1261, 1994.
[2] Gan, Y., Sun, Z., Chen, Z., Zhang, X., and Liu, Y., "Enhancement of the Material Point Method Using B-spline Basis Functions," International Journal for Numerical Methods in Engineering, Vol. 113, pp. 411-431, 2018.
[3] He, L., Gan, Y., and Chen, Z., "Preliminary Effort in Developing the Smoothed Material Point Method for Impact," Computational Particle Mechanics, Vol. 6, pp. 45-53, 2019.
[4] Lu, M., Zhang, J., Zhang, H., Zheng, Y., and Chen, Z., "Time-discontinuous Material Point Method for Transient Problems," Computer Methods in Applied Mechanics and Engineering, Vol. 328, pp. 663-685, 2018.
[5] Tao, J., Zhang, H., Zheng, Y., Chen, Z., "Development of Generalized Interpolation Material Point Method for Simulating Fully Coupled Thermomechanical Failure Evolution," Computer Methods in Applied Mechanics and Engineering, Vol. 332, pp. 325-342, 2018.
[6] Zhang, X., Chen, Z., and Liu, Y., The Material Point Method – A Continuum-Based Particle Method for Extreme Loading Cases, Academic Press, Elsevier, 2016.