Multiscale Material Point Method for Simulating the Interactions among Discrete Nano/Meso/Micro Structures under Impact Loading

Zhen Chen,^{1, 2}* Shan Jiang,^{2,3} Yong Gan,⁴ and Thomas D. Sewell³

¹State Key Laboratory of Structural Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Dalian 116024, China

²Department of Civil and Environmental Engineering, University of Missouri, Columbia, MO 65211, USA

³Department of Chemistry, University of Missouri, Columbia, MO 65211, USA

⁴School of Aeronautics and Astronautics, Zhejiang University, Zhejiang 310027, China

e-mail: chenzh@missouri.edu

ABSTRACT

Recent studies of energetic composites have underscored the need for an effective multiscale solution procedure for simulating the responses of discrete nano/meso/micro structures to impact loading [1, 2]. A particle-based computer test-bed is being developed with a concurrent link between the Dissipative Particle Dynamics (DPD) method and the Material Point Method (MPM), and a hierarchical bridge from Molecular Dynamics (MD) to DPD, in order to effectively discretize the multiphase interactions associated with multiscale failure evolution [3]. The proposed procedure has been illustrated using simulations of the dynamic and impact responses of discrete metallic nano/meso/micro structures. It appears that the DPD forces can be effectively coarse-grained using the MPM background grid, and that the concurrent link between the MPM and DPD enables near-seamless integration of constitutive modeling at the continuum level with force-based modeling at the mesoparticle level. By combining both MD and DPD within the MPM framework, an effort is being made to investigate the possibility of concurrently simulating the interactions among discrete nano/meso/micro structures under impact loading. Representative examples will be considered to demonstrate the recent research results.

REFERENCES

[1] Chen, Z., Jiang, S., Gan, Y., Oloriegbe, S.Y., Sewell, T.D., and Thompson, D.L., "Size Effects on the Impact Response of Copper Nanobeams," <u>Journal of Applied Physics</u>, Vol. 111, 113512, 2012 (This paper has been selected for publication in June 18, 2012 issue of <u>Virtual Journal of Nanoscale Science & Technology</u>).

[2] Chen, Z., Jiang, S., Sewell, T.D., Gan, Y., Oloriegbe, S.Y., and Thompson, D.L., "Effects of Copper Nanoparticle Inclusions on the Pressure-Induced Fluid-Polynanocrystalline Structural Transition in Krypton," Journal of Applied Physics, Vol. 116, 233506 (7pp), 2014.

[3] Chen, Z., Jiang, S., Gan, Y., Liu, H., and Sewell, T.D., "A Particle-Based Multiscale Simulation Procedure within the Material Point Method Framework," <u>Computational Particle Mechanics</u>, Vol. 1, pp. 147-158, 2014.