8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

A QUASI-STATIC MOLECULAR DYNAMICS-CONTINUUM MULTISCALE MODEL FOR NANO-SCALE CONTACT PROBLEMS

Liu Tianxiang[1, 2], Wriggers Peter[1] and Liu Geng[2]

[1] Institute of Mechanics and Computational Mechanics, Leibniz University of Hannover, Hannover, Appelstr. 9A, 30167, Germany
nwpuliutx@hotmail.com,
wriggers@ibnm.uni-hannover.de

[2] Northwestern Polytechnical University
PO Box 324, No. 127, Youyi Xi Road, Xi'an 710072, P.R. China
npuliug@nwpu.edu.cn

Key Words: *Multiscale, Nano-scale, Contact.*

ABSTRACT

Analyzing the contact performances between two surfaces plays a key role in studying friction, wear, and lubrication in tribological systems. Advancements of micro/nano-electro-mechanical system (MEMS/NEMS) and nanotechnology in recent years demand the developments of multiscale contact mechanics.

By using multiscale methods, the calculation domain which needs to consider the local mechanical behaviors with nano-scale characteristic would be simulated by atomistic methods and the other domains still can use the traditional methods for larger length and time scale in order to save computational cost or achieve calculations for larger scale systems. A multiscale method presented by Liu et al. [1] called bridging scale method (BSM), which can implement the energy equilibrium and force equilibrium both, is studied. However, the BSM must use the finite element method in the whole calculation domain, which is not advantaged for contact problems because it will produce two scales of contact boundaries, especially when some atoms on the contacting surfaces are adhered out of the substrate, the continuum contact boundary conditions can no longer follow such phenomenon very easily. Therefore, An adjusted boundary conditions for the continuum domain which can eliminate the finite elements in the atomistic domain is presented.

A 2-D wave propagation problem is implemented by using the adjusted BSM. A model is constructed by atoms in the middle of the calculation domain whose unit cell of crystal structure is hexagonal and the nearest-neighbor interactions of 6-12 Lennard-Jones potential are considered. In the regions out of the atomic domain, the finite element method is employed. The results show that the wave can be diffused from the MD region to the coarse scale successfully. By comparing the transfer of the total energy in the MD region, the results from the adjusted BSM agree well with the pure MD simulation.

A quasi static molecular dynamics-continuum multiscale model which can deal with the nano-scale contact problems is presented. Comparing to the existing multiscale

models for contact problems, such as in Ref. [2], the present model not only can implement the equilibrium of the energy field and force field in different scale domains, but also can implement the thermal transfer from the MD region to the coarse scale region. In the MD simulation, the speed of the approaching probe is very small in comparing with the longitudinal sound speed which is usually in the order of 10^3 m/s, the results of the contact process could be recognized approximately as the quasi static case in nature. After every step of loading, the system is then relaxed for thousands of time steps to its minimum energy configuration. For the continuum simulaton, the Cauchy-Born rule [3] is employed to evaluate the non-linear constitutive relationship of the coarse scale. The mulscale boundary conditions based on the adjusted BSM is used. By using the present mutiscale model, the simulation of the nano-scale adhesive contact between a cylinder and a substrate is implemented. The results show that the boundary conditions are effective for the contact problems. Furthermore, the 2-D adhesive contacts of rough surfaces with and without friction are investigated. Some behaviors of the nano-scale contact processes are discussed and the differences between the multiscale model and the pure MD simulation are revealed.

REFERENCES

[1] W. K. Liu, H. S. Park, 2006, “Bridging Scale Methods for Computational Nanotechnology,” *Handbook of Theoretical and Computational Nanotechnology*, Editors M. Rieth and W. Schommers, American Scientific Publishers, 1st edition.

[2] B. Q. Luan, S. Hyun, J. F. Molinari, et al., 2006, “Multiscale Modeling of Two-Dimensional Contacts,” *Physical Reviews E*, **74**(4), pp. 046710.

[3] Sauer, R. A., Li, S., 2007, “An Atomic Interaction-Based Continuum Model for Adhesive Contact Mechanics,” *Finite Elements in Analysis and Design*, **43**, pp. 384-396.