



The Hong Kong University of Science and Technology

Department of Mathematics

Mathematics Colloquium

**On the Cauchy-Born approximation at finite
temperature: modeling, simulation and analysis**
by

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Abstract

The recent development of molecular dynamics models has dramatically improved and enriched traditional continuum mechanics models. It provides an atomistic-based constitutive model, taking into account detailed atomic interactions. At zero temperature, the Cauchy–Born (CB) rule offers an efficient constitutive model. In this talk, we will extend the CB approximation to finite temperature for systems at thermodynamic equilibrium. I will address several issues regarding the derivation and implementation of the CB approximation of the stress at finite temperature. In particular, an asymptotic expansion is employed to derive a closed form expression for the first Piola–Kirchhoff stress. For systems under periodic boundary conditions, a derivation is presented, which takes into account the translational invariance and clarifies the removal of the zero phonon modes. Also revealed by the asymptotic approach is the role of the smooth-ness of the interatomic potential. Several numerical examples are provided to validate this approach, both for simple and for complex lattices. The issue of the validity and accuracy of the CB rule will also be discussed.

Date: Friday, 22 February 2019

Time: 3:00p.m. - 4:00p.m.

**Venue: Lecture Theater F,
Academic Building, 1/F
(near Lifts 25 - 26), HKUST**

All are welcome!