The Hong Kong Polytechnic University
Department of Applied Mathematics
Colloquium

Shrinking dimer dynamics for transition states/saddle points

by

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Exploring complex energy landscape is a challenging issue in many applications. Besides locating equilibrium states, it is often also important to identify the transition states given by saddle points. In this talk, we will discuss the mathematics and algorithms, in particular, the shrinking dimer dynamics, developed to compute transition states. Some applications will be considered, including the study of critical nuclei morphology in solid state transformations, optimal photonic crystal design and the generalized Thomson problem.

Date :   28 November, 2014 (Friday)
Time :   11:00a.m. – 12:00noon
Venue : TU717, The Hong Kong Polytechnic University

* * *   ALL ARE WELCOME   * * *