数学与系统科学研究院

计算数学所系列学术报告

系列专题报告题目：**An Introduction to the Quasi-continuum Approximation and Its Analysis**

特邀报告人：**Prof. Ping Lin**

(Division of Mathematics, University of Dundee, UK)

邀请人：陈志明研究员

内容简介：

Many scientific systems such as materials may be modeled by a large number of particles (or atoms) where any particle interacting with any other through, for example, a pair potential energy. The equillibrium configuration is a minimizer of the total energy of the system. The computational cost is extremely high since the number of particles (or atoms) is usually huge. An approximate sparse representation of the system is necessary to reduce the computational cost. Recently in material research much attention has been paid to a so-called quasicontinuum (QC) approximation which may be seen as an approximate representation of the accurate atomistic model. The QC approximation solves a fully atomistic problem in regions where

the material contains defects, but uses finite elements (continuum) to integrate out the majority of the atomistic degrees of freedom in regions where there is no defect. It is a typical atomistic-to-continuum multiscale model. Mathematical/numerical analysis is still at its infancy. Many issues are open for further studies. This lecture series will include four lectures with the following subtitles. The goal of these lectures is to introduce the QC and its variants as well as some basic analysis methods. Some possible research problems may be mentioned during lectures for graduate students who might be interested in working a bit in this topic.

Programme

Thursday 10th June

Course: 1. Quasicontinuum methods for materials with simple lattice structure
Abstract: Introduce the idea and basic concepts of the QC approximation for 1D and 2D models and under the finite element framework estimate the error between the QC solution and the atomistic solution.
Time: 9:00 am-11:15 am
Venue: Lecture Hall 311 of ICMSEC

Thursday 17th June

Course: 2. The unphysical force and its removing strategies for the quasicontinuum method
Abstract: Explain the unphysical force (called ghost force) at the local (continuum) and nonlocal (atomistics) interface through a 1D periodic atomistic system. Discuss and compare three ghost force removing methods: quasinonlocal method, geometrically consistent reconstruction, QC projection method.
Time: 9:00 am-12:00 am
Venue: Lecture Hall 311 of ICMSEC

Thursday 24th June

Course: 3. A one-dimensional dynamical QC model and nonlinear wave equation of mixed type

Abstract: It is difficult to make the method work for dynamics (zero temperature). We will consider the simplest case, 1D nearest neighbor interaction and formulate the dynamic QC. To study the error between the dynamic QC solution and the atomistic dynamic solution, analysis of a nonlinear wave equation of mixed type is involved.

Time: 9:00 am-11:15 am

Venue: Lecture Hall 311 of ICMSEC

Monday 28 June

Course: 4. Quasicontinuum methods for materials with complex lattice structure

Abstract: Introduce the QC for materials with more complicated periodic structure, allowing different species of atoms (interacting with different pair potential energies).

Time: 9:00 am-12:00 am

Venue: Lecture Hall 311 of ICMSEC

欢迎大家参加！