数学与系统科学研究院

计算数学所学术报告

(定期学术报告)

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报告题目： **Mathematical Modeling and Computation at Micro– and Nano–Scale**

报告时间： 2007 年 12 月 20 日(周四)

下午 4:00—5:00

报告地点： 科技综合楼三层 311

计算数学所报告厅

Abstract：

As the size of devices and structures has become smaller and smaller and entered the nano–scale, the physical principles governing their operation are changing dramatically. The

macroscopic descriptions of physical problems are based on phenomenological laws, such as the Fourier law for heat conduction, and the Maxwell equations for electromagnetic problems. While this engineering approach was adequate for most engineering applications in the past, it becomes increasingly insufficient for other evolving and emerging technologies, particularly nanotechnology, direct energy conversion technologies, biotechnology, microelectronics and photonics.

In this talk, I would like to introduce the recent advances of our group in multiscale

Analysis. First, I will talk about some new concepts such as size effects, scale invariance and scale gap. These concepts are, of course, of great mathematical and physical interest. I will give our new theoretical results. For instance, we have proven that the elastic constants and the dielectric constants are approximate scale invariants for a nanocrystal in the framework of the local density approximation of density

functional theory(DFT–LDA). From this, I will give some typical applications in CMOS transistor, photonic crystals and the protein structures in solution. We have proven that the size of the quantum region in the weak conjecture is of the order of a few Fermi wave–lengths , i.e. typically the inter–atomic distance, on the basis of DFT–LDA. It is a rigorous mathematical justification on the principle of "nearsightedness" and order N methods in quantum mechanics, which forms the basis of the multiscale methods such as QM/MM and QM/MD/FEM.

Finally, I will discuss the mathematical modeling and multiscale computations for electromagnetics and heat transfer at micro– and nano–scale. Numerous numerical results will be presented, which support strongly our methods.

欢迎大家参加！