数学与系统科学研究院 计算数学所系列学术报告

### <u>报告人:</u> Prof. Arieh Iserles

( University of Cambridge )

## 报告题目:

# Computing the Schrödinger equation with no fear of commutators

<u>邀请人:</u> 洪佳林 研究员

# <u>报告时间</u>: 2013 年 4 月 8 日 (周一) 上午 9:30~10:30

<u>报告地点</u>: 科技综合楼三层 **311** 计算数学所报告厅

#### Abstract:

In this talk I report recent work on the solution of the linear Schrödinger equation (LSE) by exponential splitting in a manner that separates different frequency scales. The main problem in discretizing LSE originates in the presence of a very small parameter, which generates exceedingly rapid oscillation in the solution. However, it is possible to exploit the features of the graded free Lie algebra spanned by the Laplacian and by multiplication with the interaction potential to split the evolution operator in a symmetric Zassenhaus splitting so that the arguments of consecutive exponentials constitute an asymptotic expansion in the small parameter. Once we replace the Laplacian by an appropriate differentiation matrix, this results in a high-order algorithm whose computational cost scales like O(N log N), where N is the number of degrees of freedom and whose error is uniform in the small parameter.

欢迎大家参加!