III.2. Multi-length scale matrix computation problems: synopsis

Forefront problems of scientific and engineering computing often require solutions involving large scale matrix computations. Great progress has been made both in general procedures and also in more focused situations which exploit specific matrix structure and sparsity patterns. A generation of excellent algorithms has been developed and presented in textbooks and research monographs. Vast amounts of public and proprietary software libraries, packages and templates have been made widely accessible, such as LAPACK and ScaLAPACK among many others. The impact of progress in large scale matrix computations to the advancement of computational science and engineering cannot be overstated. However, challenges of the advancement of multi-scale mathematical modeling and simulation to numerical linear algebra theory and algorithms have not been widely addressed. Most solvers are not designed in ways that are robust and efficient for underlying multi-length scale simulations. This is an emerging research area. A broad range of scientific and engineering modeling and simulation problems involve multiple scales for which traditional monoscale approaches have proven to be inadequate, even with the largest supercomputers.

In recent years, there is a wide range of synergistic activities on development of robust and efficient linear algebra solvers which are specially designed for multi-length scale numerical linear algebra problems arising from quantum mechanical simulations of materials. This includes new algorithm design and analysis, hybrid use of existing algorithms and development of high-performance software.

We have focused on the following computational kernels arising from Quantum Monte Carlo simulations:

- Study of the dynamics of the eigenvalue distributions, condition numbers and other critical properties of multi-length scale matrices.
- Development of robust and efficient self-adapting linear algebra solvers, direct and iterative.
- Development of high performance software solving real multi-length scale phenomena.

The following is a conference paper to summarize some of our efforts:

- Z. Bai, W. Chen, R. Scalettar and I. Yamazaki, Robust and efficient numerical linear algebra solvers and applications in quantum mechanical simulations. Proceedings of the 4th International Congress of Chinese Mathematician (ICCM), Edited by Lizhan Ji, Kefeng Liu, Lo Yang, Shing-Tung Yau, Vol.III, pp.253–268, Higher Education Press, China. 2007.

A lecture-note style presentation on the derivation details of physical model and numerical computational problems and algorithms is described in the following 114-page long chapter

- Z. Bai, W. Chen, R. Scalettar and I. Yamazaki, *Numerical Methods for Quantum Monte Carlo Simulations of the Hubbard Model*, in "Multi-Scale Phenomena in Complex Fluids" edited by Thomas Y. Hou, Chun Liu and Jian-Guo Liu, Higher Education Press, Feb. 2009

Issues and challenges on the development of stable linear solvers and robust preconditioning techniques are discussed in the following papers

- Z. Bai, R. Lee, R.-C. Li and S. Xu, *Stable solution of linear systems invovling long chain of matrix multiplications*, submitted, 2009

- I. Yamazaki, Z. Bai, W. Chen and R. Scalettar, *A high-quality preconditioning technique for multi-length-scale symmetric positive definite linear systems.* Numer. Math. Theor. Meth. Appl. 2:469-484, 2009

QUEST (Quantum Electron Simulation Toolbox) is a Fortran 90/95 package that implements the Determinant Quantum Monte Carlo method, it is available at

- http://www.cs.ucdavis.edu/∼bai/PETAMAT

For the discussion on parallelization, see

- C.-R. Lee, I-H. Chung and Z. Bai, *Hybrid granularity parallelization scheme for determinant quantum Monte Carlo simulations for strongly correlated electron systems*, submitted to the 24th IEEE Inter. Parallel and Distributed Processing Symposium, April, 2010