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# A High-Quality Preconditioning Technique for Multi-Length-Scale Symmetric Positive Definite Linear Systems

Ichitaro Yamazaki[1,*], Zhaojun Bai[1], Wenbin Chen[2] and Richard Scalettar[3]

[1] *Department of Computer Science, University of California, Davis, CA 95616, USA.*
[2] *School of Mathematical Sciences, Fudan University, Shanghai 200433, China.*
[3] *Department of Physics, University of California, Davis, CA 95616, USA.*

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**Abstract.** We study preconditioning techniques used in conjunction with the conjugate gradient method for solving multi-length-scale symmetric positive definite linear systems originating from the quantum Monte Carlo simulation of electron interaction of correlated materials. Existing preconditioning techniques are not designed to be adaptive to varying numerical properties of the multi-length-scale systems. In this paper, we propose a hybrid incomplete Cholesky (HIC) preconditioner and demonstrate its adaptivity to the multi-length-scale systems. In addition, we propose an extension of the compressed sparse column with row access (CSCR) sparse matrix storage format to efficiently accommodate the data access pattern to compute the HIC preconditioner. We show that for moderately correlated materials, the HIC preconditioner achieves the optimal linear scaling of the simulation. The development of a linear-scaling preconditioner for strongly correlated materials remains an open topic.

**AMS subject classifications**: 65F08, 65F10, 65F50, 81-08

**Key words**: Preconditioning, multi-length-scale, incomplete Cholesky factorization, quantum Monte Carlo simulation.

## 1. Introduction

We consider the solution of the linear system of equations

$$Ax = b, \tag{1.1}$$

where $A$ is an $n \times n$ *multi-length-scale* symmetric positive definite (SPD) matrix and $b$ is a given vector of length $n$, originating from the hybrid quantum Monte Carlo (HQMC)

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[*] Corresponding author. *Email addresses:* `ic.yamazaki@gmail.com` (I. Yamazaki), `bai@cs.ucdavis.edu` (Z. Bai), `wbchen@fudan.edu.cn` (W. Chen), `scalettar@physics.ucdavis.edu` (R. Scalettar)

simulation of a Hubbard model for studying electron interaction in correlated materials [2,15]. The properties of the coefficient matrix $A$, such as dimensionality and conditioning, depend on a set of multi-length-scale parameters from the underlying physical system to be simulated.

Preconditioning is recognized as one of the most critical components of a robust and efficient iterative linear solver. In this paper, we focus our attention on the development of a high-quality incomplete Cholesky (IC) factorization based preconditioner used in conjunction with the conjugate gradient method for solving the multi-length-scale system (1.1). An IC factorization is of the form

$$A = RR^T + E, \tag{1.2}$$

where $R$ is a sparse lower-triangular matrix with positive diagonals, and $E$ is an error matrix. A variety of IC factorization based preconditioners $R$ have been proposed [1,5–7,9–11,13,16,18]. The performance of many of these preconditioners for solving (1.1) has been reported in [3]. We observed that when a large number of elements are discarded into the error matrix $E$ to control the cost of computing $R$, the norm of the residual matrix $R^{-1}AR^{-T} - I$ increases significantly and the quality of the preconditioner is poor. To overcome these drawbacks, we propose combining the two most effective IC factorizations, namely the IC factorization with a global diagonal shift by Manteuffel [13] and the robust IC factorization by Kaporin [11]. The resulting factorization is referred to as a hybrid Incomplete Cholesky (HIC) factorization. The HIC can adaptively balance the cost and quality of preconditioner over a wide range of the multi-length-scale parameters of interest. We will present an algorithm to compute the HIC factorization. To efficiently accommodate the data access pattern of the proposed algorithm, we will introduce a sparse matrix storage format, which is an extension of the well-known compressed sparse column (CSC) sparse matrix storage format. We will present numerical results to demonstrate the adaptivity of the HIC preconditioner to varying multi-length-scale parameters. For moderately correlated materials, the HIC preconditioner based PCG solver achieves the optimal linear scaling of the simulation. This enables us to conduct the HQMC simulation for thousands of electrons.

The rest of this paper is organized as follows. In Section 2, we review the existing IC factorizations that are closely related to the HIC factorization proposed in this paper. In Section 3, we define the HIC factorization and present an algorithm to compute the factorization. In Section 4, we discuss an implementation of the HIC with a new sparse matrix storage scheme. After detailing the form of the multi-length-scale linear system (1.1) in Section 5, we present numerical results to demonstrate the effectiveness of the HIC preconditioner in Section 6. The concluding remarks are in Section 7.

## 2. Incomplete Cholesky factorizations

For a general SPD matrix $A$, the IC factorization of the form (1.2) could fail due to the occurrence of non-positive pivot, referred to as *pivot breakdown* [12]. The existence is proven only for some special classes of matrices [13,14,17]. Various IC factorizations