

A Left-Looking Selected Inversion Algorithm and Task Parallelism on Shared Memory Systems

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Abstract—Given a sparse matrix A , the selected inversion algorithm is an efficient method for computing certain selected elements of A^{-1} . These selected elements correspond to all or some nonzero elements of the LU factors of A . In many ways, the type of matrix updates performed in the selected inversion algorithm is similar to that performed in the LU factorization, although the sequence of operation is different. In the context of LU factorization, it is known that the left-looking and right-looking algorithms exhibit different memory access and data communication patterns, and hence different behavior on shared memory and distributed memory parallel machines. Corresponding to right-looking and left-looking LU factorization, selected inversion algorithm can be organized as a left-looking and a right-looking algorithm. The parallel right-looking version of the algorithm has been developed in [1]. The sequence of operations performed in this version of the selected inversion algorithm is similar to those performed in a left-looking LU factorization algorithm. In this paper, we describe the left-looking variant of the selected inversion algorithm, and based on task parallel method, present an efficient implementation of the algorithm for shared memory machines. We demonstrate that with the task scheduling features provided by OpenMP 4.0, the left-looking selected inversion algorithm can scale well both on the Intel Haswell multicore architecture and on the Intel Knights Corner (KNC) manycore architecture. Compared to the right-looking selected inversion algorithm, the left-looking formulation facilitates pipelining of work along different branches of the elimination tree, and can be a promising candidate for future development of massively parallel selected inversion algorithms on heterogeneous architecture.

Index Terms—selected inversion; shared memory; parallel algorithm; openmp; multicore; manycore; task; scheduling; high performance computation;

I. INTRODUCTION

Given a non-singular, sparse matrix $A \in \mathbb{C}^{N \times N}$, the selected inversion algorithm is an efficient method for computing selected elements of A^{-1} . These selected elements correspond to all or a subset of the nonzero entries of the LU factors of A . The computation of such selected elements has recently received an increasing level of attention, notably in the context of density functional theory [2], [3], [4], [5], quantum transport [6], [7], dynamical mean field theory [8], [9], and uncertainty quantification [10], to name a few.

The sequence of operations performed in the selected inversion of A can be described in terms of a traversal of the elimination tree associated with A . Elimination tree traversal can also be used to describe the sequence of operations performed in an LU factorization of A . However, in selected inversion, the elimination tree is traversed from the root down to the leaves, whereas a bottom-up traversal from the leaves to the root is performed in the LU factorization. Hence, the sequence of operations performed in the selected inversion of A can be viewed as “mirrored” operations performed in the LU factorization of A .

There are several ways to implement the LU or Cholesky factorization of A . Two of the most widely used implementations are the left-looking and right-looking factorization algorithms. They differ in the way data is fetched from the factored part of matrix and applied to the part of the matrix that remains to be factored.

It is well known that the left-looking and right-looking algorithms exhibit different memory access and data communication patterns. As a result, their performance can be quite different on shared memory and distributed memory parallel machines. The right-looking LU factorization can sometimes achieve higher parallel scalability on distributed memory parallel machines with a relatively large number of processors [11], [12].

There are at least two ways to implement the selected inversion algorithm. The right-looking variant has been developed in [13]. Its parallelization for a distributed memory machine has been described in [1]. Although the parallel right-looking algorithm can scale to as many as 4,096 processors [14], further performance improvement appears to be challenging due to the complex data communication patterns employed in this variant of the selected inversion algorithm.

In this paper, we present a left-looking selected inversion algorithm. We will show that it is much easier to schedule multiple tasks that can be executed concurrently in the left-looking algorithm. As a result, the left-looking implementation may reach higher parallel scalability than what is possible at present.

As a first step, we develop an efficient implementation of the

left-looking selected inversion algorithm for shared memory parallel machines. The parallelization makes use of the task scheduling features provided by OpenMP 4.0. We demonstrate the performance of our implementation on a number of test problems. The performance study is carried out on both the Intel Haswell multicore architecture and the Intel Knights Corner (KNC) manycore architecture.

The rest of the paper is organized as follows. In the next section, we review the basic algorithmic ingredients of a selected inversion algorithm, and point out the main differences in different variants of the algorithm. We also describe the left-looking selected inversion in detail. In section III, we discuss how various updates performed in a left-looking selected inversion can be divided as individual tasks, how these tasks depend on each other, and how we can use dependency analysis to avoid write conflict. We also show how the execution of different tasks can be scheduled dynamically based on dependency analysis, and how task scheduling can be implemented with the new OpenMP primitives. The numerical results that demonstrate the efficiency of the left-looking algorithm are presented in section IV.

II. THEORY

A. Selected inversion algorithm

The selected inversion algorithm has been discussed in [13], [1], and here we only briefly recall its formulation. To simplify the discussion as well as its implementation, in this paper, we assume the matrix A is at least *structurally symmetric*, i.e. $A_{ij} \neq 0$ implies $A_{ji} \neq 0$ for any i, j . If A is not structurally symmetric we can fill zeros to the matrix A and treat these added zeros as nonzero entries, so that the resulting modified matrix becomes structurally symmetric. Given a 2-by-2 block partitioning of the matrix A with $A_{1,1}$ being a scalar,

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix}, \quad (1)$$

its LU decomposition is

$$A = \begin{pmatrix} L_{1,1} & 0 \\ L_{2,1} & I \end{pmatrix} \begin{pmatrix} U_{1,1} & U_{1,2} \\ 0 & S_{2,2} \end{pmatrix}. \quad (2)$$

Here $S_{2,2}$ is called the Schur complement, and is obtained from the trailing submatrix of column 1, denoted by $A_{2,2}$, modified by a rank one matrix from the L, U factors. We can express A^{-1} as

$$A^{-1} = \begin{pmatrix} (\hat{U}_{1,1})^{-1}(\hat{L}_{1,1})^{-1} + \hat{U}_{1,2}S_{2,2}^{-1}\hat{L}_{2,1} & -\hat{U}_{1,2}S_{2,2}^{-1} \\ -S_{2,2}^{-1}\hat{L}_{2,1} & S_{2,2}^{-1} \end{pmatrix}, \quad (3)$$

where

$$\begin{aligned} \hat{L}_{1,1} &= L_{1,1}, & \hat{U}_{1,1} &= U_{1,1}, \\ \hat{L}_{2,1} &= L_{2,1}(L_{1,1})^{-1}, & \hat{U}_{1,2} &= (U_{1,1})^{-1}U_{1,2}. \end{aligned} \quad (4)$$

Assume the inverse of the Schur complement $S_{2,2}^{-1}$ has already been computed, and denote by \mathcal{C} the set of indices

$$\{i \mid (L_{2,1})_i \neq 0\}. \quad (5)$$

Due to the structural symmetry property of A , the set $\{j \mid (U_{1,2})_j \neq 0\}$ is identical to \mathcal{C} . The basic idea of the selected inversion algorithm is that in order to update $A_{1,1}^{-1}$, we only need the entries

$$\{(S_{2,2}^{-1})_{i,j} \mid i \in \mathcal{C}, j \in \mathcal{C}\}. \quad (6)$$

Applying this principle recursively, we obtain a pseudo-code for demonstrating this column-based selected inversion algorithm for symmetric matrix, which is given in [13].

In practice, a column-based sparse factorization and selected inversion algorithm may not be efficient due to the lack of level 3 BLAS operations. For a sparse matrix A , the columns of A and the L factor can be partitioned into supernodes. A supernode is a maximal set of contiguous columns $\mathcal{J} = \{j, j+1, \dots, j+s\}$ of the L factor that have the same nonzero structure below the $(j+s)$ -th row, and the lower triangular part of $L_{\mathcal{J},\mathcal{J}}$ is dense. This definition can be relaxed to limit the maximal number of columns in a supernode (i.e. sets are not necessarily maximal). With slight abuse of notation, both a supernode index and the set of column indices associated with a supernode are denoted by uppercase script letters such as $\mathcal{I}, \mathcal{J}, \mathcal{K}$ etc.. $A_{\mathcal{I},*}$ and $A_{*,\mathcal{J}}$ are used to denote the \mathcal{I} -th block row and the \mathcal{J} -th block column of A , respectively. $A_{\mathcal{I},\mathcal{J}}^{-1}$ denotes the $(\mathcal{I}, \mathcal{J})$ -th block of the matrix A^{-1} , i.e. $A_{\mathcal{I},\mathcal{J}}^{-1} \equiv (A^{-1})_{\mathcal{I},\mathcal{J}}$. When the block $A_{\mathcal{I},\mathcal{J}}$ itself is invertible, its inverse is denoted by $(A_{\mathcal{I},\mathcal{J}})^{-1}$ to distinguish from $A_{\mathcal{I},\mathcal{J}}^{-1}$. Using the supernode notation, a pseudo-code for the selected inversion algorithm is given in Algorithm 1. Here $L_{\mathcal{I},\mathcal{K}} \neq 0$ means that it is not an empty matrix block.

Algorithm 1: Selected inversion algorithm based on LU factorization.

(1) The supernode partition of columns of A : $\{1, 2, \dots, \mathcal{N}\}$

Input: (2) A supernodal LU factorization of A with LU factors L and U .

Output: Selected elements of A^{-1} , i.e. $A_{\mathcal{I},\mathcal{J}}^{-1}$ such that $L_{\mathcal{I},\mathcal{J}}$ is not an empty block.

for $\mathcal{K} = \mathcal{N}, \mathcal{N} - 1, \dots, 1$ **do**

1 | Find the collection of indices
 $\mathcal{C} = \{\mathcal{I} \mid \mathcal{I} > \mathcal{K}, L_{\mathcal{I},\mathcal{K}} \neq 0\}$

2 | $\hat{L}_{\mathcal{C},\mathcal{K}} \leftarrow L_{\mathcal{C},\mathcal{K}}(L_{\mathcal{K},\mathcal{K}})^{-1}, \hat{U}_{\mathcal{K},\mathcal{C}} \leftarrow (U_{\mathcal{K},\mathcal{K}})^{-1}U_{\mathcal{K},\mathcal{C}}$

end

for $\mathcal{K} = \mathcal{N}, \mathcal{N} - 1, \dots, 1$ **do**

Find the collection of indices
 $\mathcal{C} = \{\mathcal{I} \mid \mathcal{I} > \mathcal{K}, L_{\mathcal{I},\mathcal{K}} \neq 0\}$

3 | Calculate $A_{\mathcal{C},\mathcal{K}}^{-1} \leftarrow -A_{\mathcal{C},\mathcal{K}}^{-1}\hat{L}_{\mathcal{C},\mathcal{K}}$

4 | Calculate $A_{\mathcal{K},\mathcal{K}}^{-1} \leftarrow U_{\mathcal{K},\mathcal{K}}^{-1}L_{\mathcal{K},\mathcal{K}}^{-1} - \hat{U}_{\mathcal{K},\mathcal{C}}A_{\mathcal{C},\mathcal{K}}^{-1}$

5 | Calculate $A_{\mathcal{K},\mathcal{C}}^{-1} \leftarrow -\hat{U}_{\mathcal{K},\mathcal{C}}A_{\mathcal{C},\mathcal{K}}^{-1}$

end

B. Left-looking, right-looking, and multifrontal algorithms

There are three main variations of an LU or LDL^T factorization algorithms. They are the left-looking, right-looking and multifrontal algorithms [15], [16], [17], [11], [18]. The difference among these approaches lies mainly in the way the

Schur complement is updated. In the left-looking algorithm, the update of the \mathcal{J} -th supernode within the Schur complement is delayed until the supernodes \mathcal{K} of L (and U) have been computed for all $\mathcal{K} < \mathcal{J}$. When the \mathcal{J} -th supernode is updated, the updating procedure looks to the left of the \mathcal{J} -th supernode, and collects contributing matrix blocks from supernodes \mathcal{K} with $\mathcal{K} < \mathcal{J}$. The collected contributing matrix blocks are accumulated by means of matrix inner products.

In the right-looking algorithm, the entire Schur complement to the right of \mathcal{J} -th supernode is updated when the \mathcal{J} -th supernode of L becomes available. The update is performed as a matrix outer product of the L and U factors from the \mathcal{J} -th supernode.

The multifrontal algorithm can be considered as an variant of the right-looking algorithm. In a multifrontal algorithm, the update of the Schur complement is organized in a hierarchical fashion, and guided by the elimination tree [19] that describes the dependency among all supernodes in the LU factorization. The hierarchical update requires the contributions of a supernode to its ancestors to be kept on a stack.

The left-looking, right-looking and multifrontal algorithms all have advantages and disadvantages over each other. Their relative performance depends on the sparsity structure of the matrix and the architecture of the machine on which they are performed. We refer readers to references [20] on comparisons of these algorithms in the context of LU or LDL^T factorizations.

From the perspective of the elimination tree, an LU factorization traverses from the bottom (leaf nodes) of the tree upwards until reaching the top (root node). The selected inversion algorithm shown in Alg. 1, on the other hand, can be described in terms of a top-down traversal of the elimination tree. In Alg. 1, the main computational bottlenecks are steps 3 and 5. In order to compute $A_{\mathcal{C},\mathcal{K}}^{-1}$, contributing blocks need to be fetched from the trailing submatrix $A_{\mathcal{C},\mathcal{C}}^{-1}$, which is to the right the supernode \mathcal{K} . In this sense, the most straightforward implementation of the selected inversion algorithm is a right-looking algorithm. The contributions to the update of $A_{\mathcal{C},\mathcal{J}}^{-1}$, are accumulated as an inner product between row blocks of $A_{\mathcal{C},\mathcal{C}}^{-1}$ and $\hat{L}_{\mathcal{C},\mathcal{J}}$ (or $\hat{U}_{\mathcal{J},\mathcal{C}}$).

The implementation details of a sequential right-looking selected inversion algorithm for general sparse symmetric matrices have been described in [13]. In [1], [14], we presented a parallel implementation of this right-looking algorithm. Our numerical experiments indicate that such an algorithm can scale to 4096 or more processors.

The selected inversion algorithm can also be implemented in a way that is analogous to the multifrontal method used for a LU factorization of A . This variant of the selected inversion algorithm is described in [4], which was referred to as a hierarchical Schur complement method. The parallel implementation of such method for a Laplacian type of matrices was presented in [21]. However, a load-balanced implementation of this approach on massively parallel computers for general sparse matrices can become challenging.

C. Left-looking selected inversion algorithm

We now describe the left-looking variant of the selected inversion algorithm. This variant offers some advantages in terms of load-balancing, memory access patterns and scheduling compared to the other variants on massively parallel computer architectures.

In the left-looking selected inversion algorithm, when the computation for the supernode \mathcal{K} is finished and $A_{\mathcal{C},\mathcal{K}}^{-1}$ becomes available, we update all matrix blocks of A^{-1} corresponding to the descendants of \mathcal{K} within the nonzero sparsity pattern of the LU factors. This type of update is motivated by the right-looking factorization algorithm in which all ancestors of \mathcal{K} corresponding to the nonzero sparsity pattern of the LU factor are updated, when $L_{\mathcal{C},\mathcal{K}}$ and $U_{\mathcal{K},\mathcal{C}}$ become available.

To be specific, let us consider the update of the lower triangular part of A^{-1} first. Define the sets

$$\mathcal{C} = \{\mathcal{I} \mid \mathcal{I} > \mathcal{K}, L_{\mathcal{I},\mathcal{K}} \neq 0\}, \quad \mathcal{C}' = \{\mathcal{I} \mid \mathcal{I} < \mathcal{K}, L_{\mathcal{K},\mathcal{I}} \neq 0\}, \quad (7)$$

and the computation for the supernode \mathcal{K} is finished when $A_{\mathcal{C},\mathcal{K}}, A_{\mathcal{K},\mathcal{C}}$ and $A_{\mathcal{K},\mathcal{K}}$ are computed. When the matrix blocks $A_{\mathcal{C},\mathcal{K}}^{-1}$ become available, according to step 3 of Alg. 1, we can apply updates to matrix blocks indexed by \mathcal{C} and \mathcal{C}' as follows

$$A_{\mathcal{C},\mathcal{C}'}^{-1} \leftarrow A_{\mathcal{C},\mathcal{C}'}^{-1} - A_{\mathcal{C},\mathcal{K}}^{-1} \hat{L}_{\mathcal{K},\mathcal{C}'}. \quad (8)$$

The update described by Eq. (8) is clearly a block outer product. This is similar to the outer product used to update the Schur complement in a right-looking factorization algorithm. However, we should note that not all matrix blocks of $A_{\mathcal{C},\mathcal{C}'}$ need to be updated in the selected inversion algorithm. Only the matrix blocks of $A_{\mathcal{I},\mathcal{I}'}$ such that $\mathcal{I} \in \mathcal{C}, \mathcal{I}' \in \mathcal{C}'$ and $L_{\mathcal{I},\mathcal{I}'} \neq 0$ need to be updated. Therefore, to be precise, Eq. (8) should be replaced by

$$A_{\mathcal{I},\mathcal{I}'}^{-1} \leftarrow A_{\mathcal{I},\mathcal{I}'}^{-1} - A_{\mathcal{I},\mathcal{K}}^{-1} \hat{L}_{\mathcal{K},\mathcal{I}'}, \quad \mathcal{I} \in \mathcal{C}, \mathcal{I}' \in \mathcal{C}', L_{\mathcal{I},\mathcal{I}'} \neq 0. \quad (9)$$

We should note that all the blocks below and to the right of $A_{\mathcal{K},\mathcal{K}}^{-1}$ should have been computed when the $(\mathcal{K} + 1)$ -th supernode has been traversed. Hence, to complete the computation for the \mathcal{K} -th supernode, only the diagonal block $A_{\mathcal{K},\mathcal{K}}^{-1}$ needs to be updated. This is the first update performed in the second loop of Alg. 1.

Once $A_{\mathcal{K},\mathcal{K}}^{-1}$ becomes available, we can also update the \mathcal{K} -th block row of A^{-1} by

$$A_{\mathcal{K},\mathcal{I}'}^{-1} \leftarrow A_{\mathcal{K},\mathcal{I}'}^{-1} - \sum_{\substack{\mathcal{I} \in \mathcal{C}, \\ L_{\mathcal{I},\mathcal{I}'} \neq 0}} A_{\mathcal{K},\mathcal{I}}^{-1} \hat{L}_{\mathcal{I},\mathcal{I}'}, \quad \mathcal{I}' \in \mathcal{C}'. \quad (10)$$

The update performed in Eq. (10) is a block inner product calculation.

The update to the upper triangular blocks of A^{-1} can be performed in a similar fashion. The pseudo-code that outlines the main steps of the sequential left-looking selected inversion algorithm is given in Alg. 2.

For symmetric matrices, the LU factorization can be simplified into the LDL^T factorization. The update of upper triangular part in step 6 and 7 in Alg. 2 can simply be obtained by the transpose of the lower triangular part without further

Algorithm 2: Left-looking selected inversion algorithm based on LU factorization.

(1) The supernode partition of columns of A : $\{1, 2, \dots, \mathcal{N}\}$
Input: (2) A supernodal LU factorization of A with LU factors L and U .
Output: Selected elements of A^{-1} , i.e. $A_{\mathcal{I},\mathcal{J}}^{-1}$ such that $L_{\mathcal{I},\mathcal{J}}$ is not an empty block.

for $\mathcal{K} = \mathcal{N}, \mathcal{N} - 1, \dots, 1$ **do**

1 Find the collection of indices
 $\mathcal{C} = \{\mathcal{I} \mid \mathcal{I} > \mathcal{K}, L_{\mathcal{I},\mathcal{K}} \neq 0\}$

2 $\hat{L}_{\mathcal{C},\mathcal{K}} \leftarrow L_{\mathcal{C},\mathcal{K}}(L_{\mathcal{K},\mathcal{K}})^{-1}, \hat{U}_{\mathcal{K},\mathcal{C}} \leftarrow (U_{\mathcal{K},\mathcal{K}})^{-1}U_{\mathcal{K},\mathcal{C}}$

end

Set A^{-1} to be a zero sparse matrix, with sparsity pattern given by $L + U$

for $\mathcal{K} = \mathcal{N}, \mathcal{N} - 1, \dots, 1$ **do**

Find the collection of indices
 $\mathcal{C} = \{\mathcal{I} \mid \mathcal{I} > \mathcal{K}, L_{\mathcal{I},\mathcal{K}} \neq 0\}$

3 Update the matrix diagonal block
 $A_{\mathcal{K},\mathcal{K}}^{-1} \leftarrow U_{\mathcal{K},\mathcal{K}}^{-1}L_{\mathcal{K},\mathcal{K}}^{-1} - \hat{U}_{\mathcal{K},\mathcal{C}}A_{\mathcal{C},\mathcal{K}}^{-1}$
Find the collection of indices
 $\mathcal{C}' = \{\mathcal{I} \mid \mathcal{I} < \mathcal{K}, L_{\mathcal{K},\mathcal{I}} \neq 0\}$

4 Outer product phase for the lower triangular part:

$$A_{\mathcal{I},\mathcal{I}'}^{-1} \leftarrow A_{\mathcal{I},\mathcal{I}'}^{-1} - A_{\mathcal{I},\mathcal{K}}^{-1}\hat{L}_{\mathcal{K},\mathcal{I}'}, \quad \text{for } \mathcal{I} \in \mathcal{C}, \mathcal{I}' \in \mathcal{C}', L_{\mathcal{I},\mathcal{I}'} \neq 0. \quad (11)$$

5 Inner product phase for the lower triangular part:

$$A_{\mathcal{K},\mathcal{I}'}^{-1} \leftarrow A_{\mathcal{K},\mathcal{I}'}^{-1} - \sum_{\substack{\mathcal{I} \in \mathcal{K} \cup \mathcal{C}, \\ L_{\mathcal{I},\mathcal{I}'} \neq 0}} A_{\mathcal{K},\mathcal{I}}^{-1}\hat{L}_{\mathcal{I},\mathcal{I}'}, \quad \text{for } \mathcal{I}' \in \mathcal{C}'$$

6 Outer product phase for the upper triangular part:

$$A_{\mathcal{I}',\mathcal{I}}^{-1} \leftarrow A_{\mathcal{I}',\mathcal{I}}^{-1} - \hat{U}_{\mathcal{I}',\mathcal{K}}A_{\mathcal{K},\mathcal{I}}^{-1}, \quad \text{for } \mathcal{I} \in \mathcal{C}, \mathcal{I}' \in \mathcal{C}', U_{\mathcal{I}',\mathcal{I}} \neq 0. \quad (12)$$

7 Inner product phase for the upper triangular part:

$$A_{\mathcal{I}',\mathcal{K}}^{-1} \leftarrow A_{\mathcal{I}',\mathcal{K}}^{-1} - \sum_{\substack{\mathcal{I} \in \mathcal{K} \cup \mathcal{C}, \\ U_{\mathcal{I}',\mathcal{I}} \neq 0}} \hat{U}_{\mathcal{I}',\mathcal{I}}A_{\mathcal{I},\mathcal{K}}^{-1}, \quad \text{for } \mathcal{I}' \in \mathcal{C}'$$

end

computation. As discussed in [1], for symmetric matrices, it is important to symmetrize the diagonal block once $A_{\mathcal{K},\mathcal{K}}^{-1}$ is computed in step 3 of Alg. 2 as

$$A_{\mathcal{K},\mathcal{K}}^{-1} \leftarrow \frac{1}{2}(A_{\mathcal{K},\mathcal{K}}^{-1} + A_{\mathcal{K},\mathcal{K}}^{-T}),$$

in order to reduce the propagation of the symmetrization error. This is particularly important for large matrices. The modification for Hermitian matrices is similar, simply by replacing the transpose operation into the Hermitian transpose operation whenever suitable.

At first sight, the left-looking selected inversion algorithm has some disadvantages compared to the right-looking variant. The order of operations of the two algorithms are very

different, and the implementation of the left-looking algorithm is more complicated. Furthermore, the left-looking selected inversion algorithm could result in higher memory consumption. In the right-looking selected inversion algorithm, one can gradually overwrite the LU factors by A^{-1} , and hence the LU factor and the A^{-1} can share the same memory space. On the other hand, each update of A^{-1} in the left-looking algorithm requires both the LU and the A^{-1} matrix blocks. Hence the storage cost of the left-looking algorithm can be close to twice as large as that in the right-looking algorithm.

On the other hand, the left-looking algorithm can become advantageous in the massively parallel computational environment by exploiting concurrency more naturally. In order to facilitate parallelism in the right-looking selected inversion algorithm, a task scheduling procedure guided by the traversal of the elimination tree is used to pipeline multiple tasks [1]. However, it is difficult to optimize this task scheduling procedure in the right-looking algorithm. This is because when the computation of a given supernode \mathcal{K} is finished, the matrix blocks $A_{\mathcal{C},\mathcal{K}}$ can be requested repeatedly by supernodes to the left of \mathcal{K} in later computational stages (see step 3 in Alg. 1). This creates complex task dependencies, and hinders parallelism on distributed parallel computer architecture. The left-looking algorithm, on the other hand, has the advantage that once the contributions from $A_{\mathcal{C},\mathcal{K}}^{-1}$ and $A_{\mathcal{K},\mathcal{C}}^{-1}$ have been included in the matrix blocks associated with the descendants of \mathcal{K} , $A_{\mathcal{C},\mathcal{K}}^{-1}$ and $A_{\mathcal{K},\mathcal{C}}^{-1}$ will no longer be needed in any subsequent calculations. This can greatly simplify the task dependency, and allows the selected inversion algorithm to become more load balanced and scalable on massively parallel computers.

III. TASK BASED PARALLELISM AND OPENMP IMPLEMENTATION

As supercomputer nodes grow “fatter” with multicore and manycore processors, the performance of an application relies increasingly on using high level programming models such as OpenMP to achieve intra-node parallelism. Due to the relatively complex data dependency in the selected inversion algorithm, simple parallelization strategies such as those based on multi-threaded BLAS or parallel for loops cannot achieve satisfactory scalability on manycore shared memory nodes. Scalable implementation of the selected inversion algorithm requires a careful organization of the computation into relatively independent computational tasks with properly described task dependency and granularity. In the following, we demonstrate how the left-looking algorithm can be parallelized on a shared memory node by using OpenMP to manage concurrent threads for symmetric matrices. The computational tasks and dependencies can be described relatively easily thanks to the task and task dependency feature in OpenMP 4.0. A distributed memory parallel implementation and a hybrid MPI+OpenMP version will be described in a separate report.

A. Task based scheduling procedure

The left-looking selected inversion in Alg. 2 can be organized into a “pre-selected inversion” phase (step 1-2) and the “selected inversion” phase (step 3-7). The pre-selected inversion phase computes the normalized LU factors \hat{L} and \hat{U} , respectively. This can be performed independently for each supernode \mathcal{K} and its parallelization can be simply performed by means of a parallel for loop.

The main difficulty is in the selected inversion phase. For each supernode \mathcal{K} , the computation can be divided into three stages: (1) Diagonal block update (2) Outer-product update, and (3) Inner-product update. In the following, and as depicted in Figures 1 and 2, we assume that \mathcal{K} is the current supernode being processed. Supernodes \mathcal{L}, \mathcal{M} and $\mathcal{N} \in \mathcal{C}$ are three supernodes that have already been computed, and they are ancestors of \mathcal{K} in the elimination tree. Supernodes \mathcal{J} and $\mathcal{I} \in \mathcal{C}'$ are descendants of \mathcal{K} in the elimination tree. They need to be updated by contribution from supernode \mathcal{K} .

The diagonal block $A_{\mathcal{K},\mathcal{K}}^{-1}$ is computed in an independent task denoted by $D_{\mathcal{K},\mathcal{K}}$.

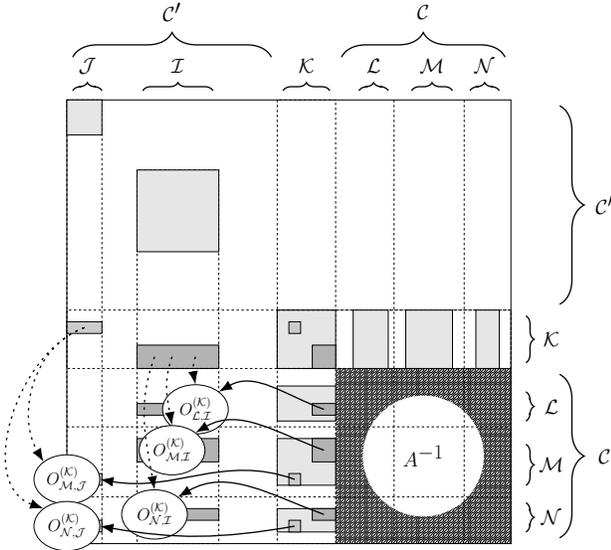


Fig. 1: Outer-product task parallelism. $O_{*,\mathcal{I}}^{(\mathcal{K})}$ and $O_{*,\mathcal{J}}^{(\mathcal{K})}$ correspond respectively to the outer-product updates from supernode \mathcal{K} to two supernodes \mathcal{I} and \mathcal{J} in \mathcal{C}' . Data dependencies from previously computed values of A^{-1} are denoted with solid arrows. Data dependencies from values in LU factors are indicated using dashed arrows.

In the outer product stage, the update to the lower triangular part of $A_{\mathcal{C},\mathcal{C}'}$ may be divided into several updating tasks, and each task corresponds to a submatrix update defined by (9). The update to each block $A_{\mathcal{I},\mathcal{I}'}^{-1}$, denoted by $O_{\mathcal{I},\mathcal{I}'}^{(\mathcal{K})}$, can be computed as an individual task, and all tasks may be executed concurrently if there are enough threads (Figure 1).

In the inner product stage, every matrix block $A_{\mathcal{K},\mathcal{I}'}^{-1}, \mathcal{I}' \in \mathcal{C}'$ is updated according to (10). This corresponds to a block-sparse inner product between $A_{\mathcal{K},*}^{-1}$ and $L_{*,\mathcal{I}'}$. There are two

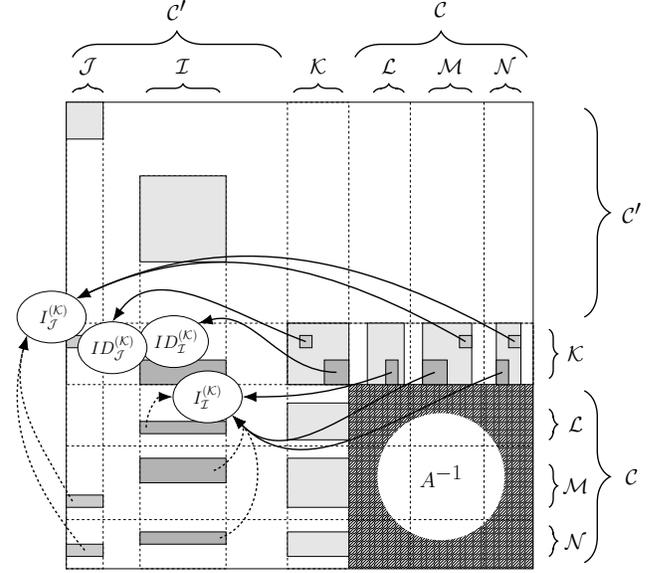


Fig. 2: Inner-product and update from diagonal task parallelism. $I_{\mathcal{I}}^{(\mathcal{K})}$ and $I_{\mathcal{J}}^{(\mathcal{K})}$ correspond to two inner-product updates from supernode \mathcal{K} to two supernodes \mathcal{I} and \mathcal{J} in \mathcal{C}' . $ID_{\mathcal{I}}^{(\mathcal{K})}$ and $ID_{\mathcal{J}}^{(\mathcal{K})}$ correspond to the updates from the diagonal block of \mathcal{K} to those two supernodes in \mathcal{C}' . Data dependencies from previously computed values of A^{-1} are denoted with solid arrows. Data dependencies from values in LU factors are indicated using dashed arrows.

ways to divide the tasks for the inner product stage. One way is to treat each matrix product $A_{\mathcal{K},\mathcal{I}'}^{-1} \hat{L}_{\mathcal{I},\mathcal{I}'}$ as a separate task, where $A_{\mathcal{K},\mathcal{I}'}^{-1} \neq 0$ and $\hat{L}_{\mathcal{I},\mathcal{I}'} \neq 0$. However, all such tasks will update a common matrix block $A_{\mathcal{K},\mathcal{I}'}^{-1}$, resulting in a “write conflict” that must be resolved to maintain thread safety. The conflict can potentially be resolved by using a thread blocking strategy, but this will potentially hinder parallel efficiency. Our numerical experience indicates that an alternative solution with a coarser granularity is a more effective strategy. Since the update to $A_{\mathcal{K},\mathcal{I}'}^{-1}$ can be regarded as a single task and performed by a single thread, the update of $A_{\mathcal{K},\mathcal{I}'}^{-1}$ for different \mathcal{I}' can be performed concurrently without conflict. Such tasks are denoted $I_{\mathcal{I}'}^{(\mathcal{K})}$ in Figure 2.

Because $A_{\mathcal{K},\mathcal{I}'}^{-1}$ becomes available long before $A_{\mathcal{K},\mathcal{K}}^{-1}$ is computed for $\mathcal{I}' > \mathcal{K}$, we decouple the task that involves using $A_{\mathcal{K},\mathcal{K}}^{-1}$ from other tasks that do not depend on the completion of the $A_{\mathcal{K},\mathcal{K}}^{-1}$ block. This allows the latter tasks, denoted by $I_{\mathcal{I}'}^{(\mathcal{K})}, \mathcal{I}' \in \mathcal{C}'$, to be executed while $A_{\mathcal{K},\mathcal{K}}^{-1}$ is being updated in task $D_{\mathcal{K},\mathcal{K}}$. Tasks that depend on $A_{\mathcal{K},\mathcal{K}}^{-1}$ are denoted by $ID_{\mathcal{I}'}^{(\mathcal{K})}, \mathcal{I}' \in \mathcal{C}'$.

We rely on task dependency analysis to prevent write conflicts between task $I_{\mathcal{I}'}^{(\mathcal{K})}$ and task $ID_{\mathcal{I}'}^{(\mathcal{K})}$ by adding a dependency between these two tasks. Therefore, task $ID_{\mathcal{I}'}^{(\mathcal{K})}$ depends on both the completion of tasks $D_{\mathcal{K},\mathcal{K}}$ and $I_{\mathcal{I}'}^{(\mathcal{K})}$.

A summary of task dependencies is depicted in Figure 3

for two supernodes \mathcal{K} and \mathcal{I} . It should be noted that the outer product stage is completely independent of the inner product as well as the diagonal block update stages.

In all three phases above, each task uses the level-3 GEMM operation to exploit cache and memory locality. All tasks can then be dynamically scheduled for execution. The sequence of execution is determined by the dependencies among the tasks and the availability of computational resources. In that sense the execution of the algorithm is performed by asynchronously scheduling the tasks without imposing explicit barriers. This leads to good load balance and parallel scalability.

B. OpenMP implementation

In order to describe the tasks and their dependencies, we exploit the latest features of OpenMP 4.0, which enables tasks to be described by the `task` clause, and dependencies described by the additional `depend` clause. Simply speaking, the `depend` clause consists of a list of input and output dependencies for each task, which can be seen as a list of variables or memory addresses from which a given task will read its input data, and to which a task will write its output data. In order to start the execution of a particular task, all dependencies previously submitted to the OpenMP dynamic task queue must have been finished. This restriction allows the program to dynamically set barriers to certain tasks without hindering the execution of the rest of the tasks. A pseudo code for describing the task and task dependencies in step 3-7 of Alg. 2 is given in Alg. 3. For instance, the task associated with `depend (out: \mathcal{K})` means that upon the finish of the task of diagonal block update operations, all tasks that has a dependency clause `depend (in: \mathcal{K})` can be executed. In the case when multiple dependency clauses are present, the task can only be executed after all tasks in the dependency list are complete.

For each supernode \mathcal{K} , we submit all tasks at the beginning. Note that the tasks are just *described* rather than really executed. In particular, the order of which the tasks are submitted do not reflect the order in which the tasks are executed in the OpenMP task scheduling procedure. After all tasks have been submitted, each task will be executed dynamically according to their dependencies. When multiple routes of parallelism are possible, we do not attempt to arrange *a priori* the order in which the tasks are performed. This strategy tends to enhance parallel performance.

In the future hybrid MPI+OpenMP version of the left looking selected inversion algorithm, each MPI process will be expected to handle multiple supernodes. The use of barrier can hinder the parallel performance in that scenario as well. In order to eliminate the usage of `omp barrier`, task dependencies must be expressed between communication tasks (to receive data from a remote process for instance) and local computation tasks. If a set of computations is completely local to an MPI process, OpenMP will allow to exploit as much concurrency as possible between these local computations.

Algorithm 3: Task based OpenMP implementation of the left-looking selected inversion algorithm.

```

for  $\mathcal{K} = \mathcal{N}, \mathcal{N} - 1, \dots, 1$  do
  #pragma omp parallel{
    #pragma omp single nowait{
      #pragma omp task depend (out:  $\mathcal{K}$ ) {
        Diagonal block update operations
      }
      for  $\mathcal{I}' \in \mathcal{C}'$  do
        #pragma omp task {
          Outer product operations
        }
        #pragma omp task depend (out:  $\mathcal{I}'$ ) {
          Inner product operations
        }
        #pragma omp task depend (in:  $\mathcal{K}$ , in:  $\mathcal{I}'$ ) {
          Inner product from Diagonal block
          operations
        }
      end
    }
  }
end

```

IV. NUMERICAL RESULTS

Numerical tests are performed on two platforms from the National Energy Research Scientific Computing Center (NERSC). The first one is the Cori supercomputer. Cori computing nodes are each equipped with two 2.3 GHz 16-core Intel Haswell processors and 128 GB of memory [22]. Each core has its own 64 KB L1 and 256 KB L2 caches; and there is also a 40 MB shared L3 cache per socket.

The second platform is an Intel Knight's Corner (KNC) testbed. Each computing node is equipped with two Manycore Integrated Core (MIC) architecture card [23]. Each MIC card has an Intel KNC processor containing 60 cores, with 4 hardware threads per core and 8 GB memory per card. The 60 MIC cores are interconnected in a high-speed bidirectional ring. Each MIC core has a 512 KB L2 cache locally with high speed access to all other L2 caches. All experiments are conducted in "native" mode, meaning that the host processor is not involved in any way in the computations (as opposed to the "offload" mode).

We evaluate the performance of the left-looking selected inversion on two sets of matrices. The first group of matrices consists of practical electronic structure computation problems generated from the SIESTA [24] and DGDFT [25], [26] software. The second set of matrices is a selection of problems from the widely used University of Florida Matrix Collection [27]. A description of these matrices is given in Table I.

The *LU* factorization is performed by using the SuperLU_DIST software package [11]. SuperLU_DIST does not use dynamic pivoting, and as we focus first on the

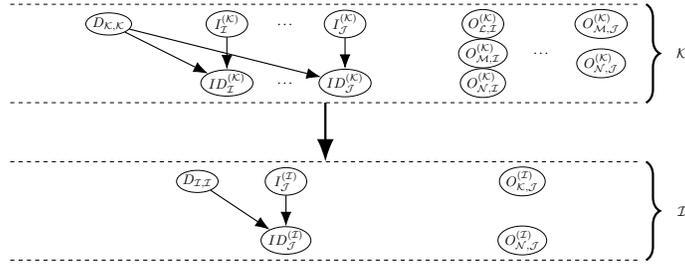


Fig. 3: Task dependencies for supernode \mathcal{K} . \mathcal{I} is the next supernode that will be processed.

Matrices from Electronic structure computations				
Name	Type	n	$nnz(A)$	$nnz(L+U)$
DGDFT_ACPNR4_60	Phospherene nanoribbon with 1080 atoms from DGDFT	16000	12800000	24115200
DGDFT_ACPNR4_120	Phospherene nanoribbon with 2160 atoms from DGDFT	40000	40000000	76400000
DGDFT_Graphene180	Graphene with 180 atoms from DGDFT	3600	4480000	8040000
DGDFT_Graphene720	Graphene with 720 atoms from DGDFT	14400	17640000	58480000
SIESTA_MoS2	MoS2 with 147 atoms from SIESTA	2401	1800995	4616651
SIESTA_DNA	DNA with 715 atoms from SIESTA	7752	2430642	8980372
Matrices from UFL sparse matrix collection				
Name	Type	n	$nnz(A)$	$nnz(L+U)$
nd3k	ND problem set, matrix nd3k.	9000	3279690	30659502
nd12k	ND problem set, matrix nd12k.	36000	14220946	342223280
raefsky4	Buckling problem for container model.	19779	1328611	13337337
ship_001	DNV-Ex 2 : Ship structure, predesign model.	34920	4644230	31845572
smt	3D model, thermal stress analysis of surface mounted transistor.	25710	3753184	29208900

TABLE I: Characteristics of matrices used in the experiments

symmetric case, our matrices are permuted in a symmetric way without taking into account the values of matrix entries.

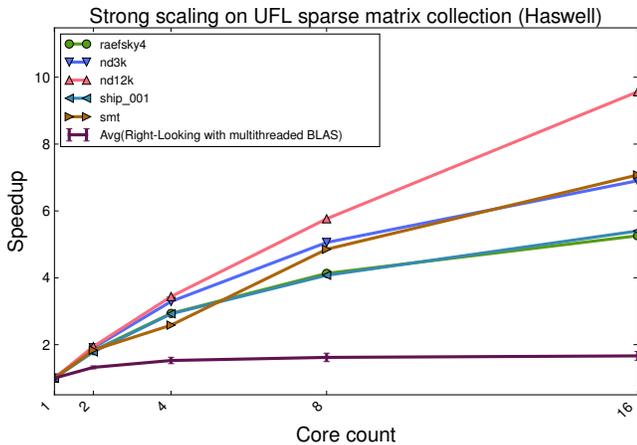


Fig. 4: Strong scaling of left-looking selected inversion on Cori (Intel Haswell) for matrices from the University of Florida Sparse Matrix Collection.

On the Cori platform, which uses Intel Haswell Xeon processors, we observe good strong scalability when using up to 16 threads. Speedups achieved by the left-looking selected inversion algorithm for various core counts on general sparse matrices are depicted on Figure 4. As a reference, we also provide the average speedup for the original right-looking selected inversion algorithm. The associated standard deviation is represented using error bars. Note that this algorithm only leverage parallelism within BLAS calls. Left-looking selected

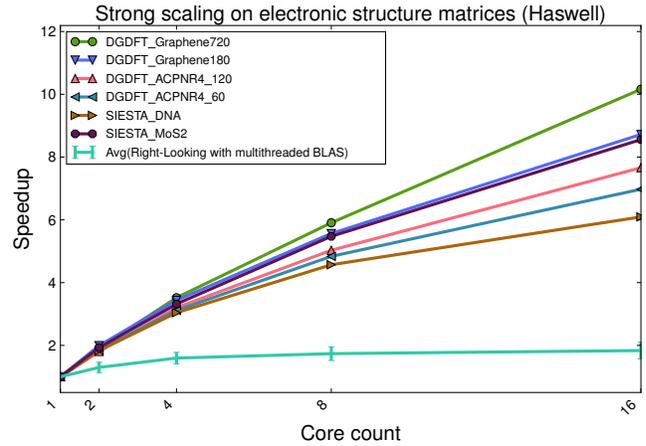


Fig. 5: Strong scaling of left-looking selected inversion on Cori (Intel Haswell) for matrices from electronic structure computations.

inversion achieves speedups ranging from 5.25x to 9.56x using all 16 cores, with an average of 6.84x.

Speedups achieved on matrices coming from electronic structure computations are depicted in Figure 5. Here, speedups range from 6.09x to 10.15x, and an average of 8.02x using all 16 cores, thus reaching an average parallel efficiency of 50%, which is relatively good given the fact that it is a sparse matrix computation.

On the Babbage testbed, which uses Intel Knights Corner (KNC) processors, we observe a similar behavior for each class of matrices. Results are depicted in Figures 6 and 7. On

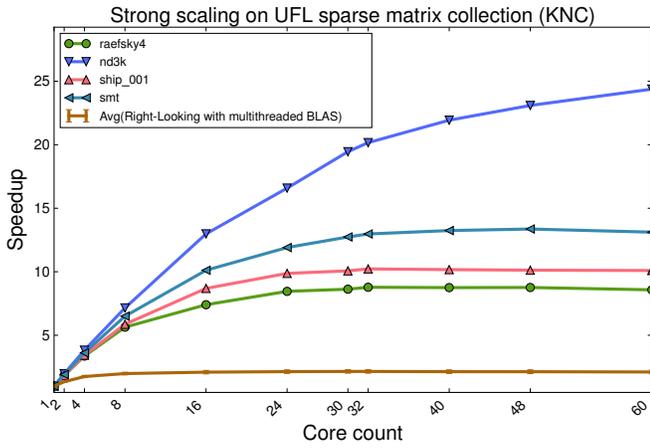


Fig. 6: Strong scaling of left-looking selected inversion on Babbage (Intel KNC) for matrices from the University of Florida Sparse Matrix Collection.

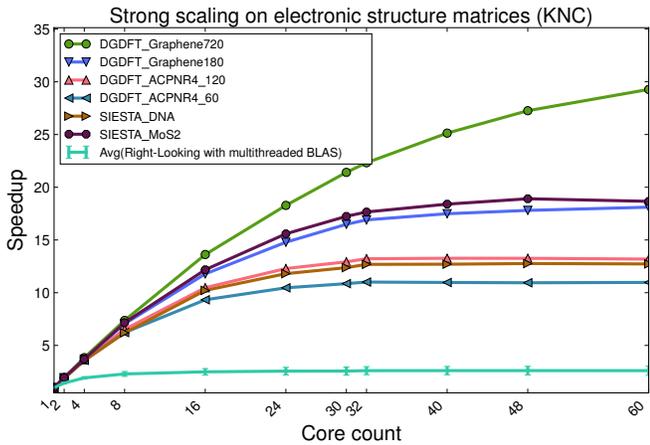


Fig. 7: Strong scaling of left-looking selected inversion on Babbage (Intel KNC) for matrices from electronic structure computations.

matrices from the University of Florida collection, the speedup results from a 60-core run ranges from 8.58x to 24.38x. The average speedup of is 14.04x. Note that only one thread per core was used in the experiments.

On matrices generated with SIESTA or DGDFT, the speedup results from a 60-core run ranges from 10.98x to 29.28x. The average speedup is 17.15x. The average parallel efficiency is 28.5% while the maximum efficiency is close to 50%.

Altogether, our numerical experiments demonstrate the practical validity of our approach. Left-looking selected inversion is able to leverage the parallelism offered by modern multicore and manycore processors in an efficient way. As such, it is a good candidate for a hybrid MPI + OpenMP implementation that would allow to handle larger systems.

V. CONCLUSION

We have developed a left-looking variant of selected inversion algorithm, which can also be viewed as analogous to the right-looking factorization algorithm in terms of the sequence of operations. The left-looking selected inversion algorithm simplifies task scheduling when multiple tasks are executed simultaneously on a parallel machine. As a first step, we have developed an efficient implementation of the left-looking selected inversion algorithm for shared memory machines. We demonstrate that, with the task scheduling features provided by OpenMP 4.0, the left-looking selected inversion algorithm can scale well both on the Intel Haswell multicore architecture and on the Intel Knights Corner (KNC) architecture. The hybrid MPI/OpenMP implementation of the left-looking selected inversion algorithm on multicore and manycore architecture will be our immediate future work.

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