

RESEARCH ARTICLE

On the parallel solution of dense saddle-point linear systems arising in stochastic programming

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We present a novel approach for solving dense saddle-point linear systems in a distributed memory environment. This work is motivated by an application in stochastic optimization problems with recourse, but the proposed approach can be used for a large family of dense saddle-point systems, in particular those arising in convex programming. Although stochastic optimization problems have many important applications, they can present serious computational difficulties. In particular, sample average approximation (SAA) problems with a large number of samples are often too big to solve on a single shared-memory system. Recent work has developed interior point methods and specialized linear algebra to solve these problems in parallel. A Schur-complement technique is used to obtain a scenario-based decomposition that allows the data and the work to be distributed across computational nodes. Even when sparse SAA problems are solved, combining the results from the scenarios in many cases produces a very large dense saddle-point linear system, which must be solved repeatedly. We developed a specialized parallel factorization procedure for these systems, together with a streamlined method for assembling the distributed dense matrix. Strong scaling tests indicate over 90% efficiency on 1024 cores on a stochastic unit commitment problem with 57 million variables. Stochastic unit commitment problems with up to 189 million variables are solved efficiently on up to 2048 cores.

Keywords: stochastic programming, parallel computing, parallel dense linear algebra, saddle-point

AMS Subject Classification: 90C15; 65F05; 68W10

1. Introduction

In this paper we consider two-stage stochastic convex problems with recourse of the form:

$$\min \left(\frac{1}{2} x_0^T Q_0 x_0 + c_0^T x_0 \right) + \mathbb{E}[G(x_0, \xi)] \quad \text{subject to} \quad T_0 x_0 = b_0, \quad x_0 \geq 0, \quad (1)$$

where, for a given realization $\tilde{\xi}$ of the random vector ξ , the recourse function $G(x_0, \tilde{\xi})$ is the optimal value of the second-stage problem (2) parameterized by the realization $\tilde{\xi}$. The expectation $\mathbb{E}[\cdot]$ is taken with respect to the density function of ξ . The matrix Q_0 is symmetric positive definite and the matrix T_0 has full rank.

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The second-stage problem is a convex quadratic programming problem of the form:

$$\min \frac{1}{2}y^T Qy + c^T y \quad \text{subject to} \quad Wy = b - Tx_0, \quad y \geq 0. \quad (2)$$

The problem is parameterized by ξ in the sense that the random entries of the data (Q, c, T, W) form the random vector ξ . We assume that Q is symmetric positive semidefinite, and that the technology matrix T and recourse matrix W have full rank for any realization of ξ .

The convexity of the second-stage quadratic problem implies that the recourse function is convex [3]. Also, the recourse function $G(x_0, \tilde{\xi})$ is nonlinear in general. Therefore, the problem (1) is a nonlinear convex optimization problem, although in the literature the problem (1) is called a two-stage stochastic convex quadratic problem with recourse (TCQP) [12] and we adopt this terminology. In addition to the fact that the second-stage problem is a QP, the term TCQP is also used because any TCQP can be reformulated as an equivalent convex QP when the support of ξ is finite, or it is approximated by a convex QP when the support of ξ is not finite, as we show below.

Sampling methods such as Monte Carlo, Latin Hypercube sampling, importance sampling, etc. are used to make the computation of the expected value term and its derivative(s) tractable from a computational point of view. Once a finite sample $(\xi_1, \xi_2, \dots, \xi_N)$ of N realizations of the random vector ξ is obtained, the recourse term $\mathbb{E}[G(x_0, \xi)]$ is approximated by the average of the values $G(x_0, \xi_i)$, $i = 1, 2, \dots, N$. This is the sample average approximation (SAA) approach, with which one obtains a convex quadratic deterministic approximation to the TCQP (1), which has the form:

$$\begin{aligned} \min & \left(\frac{1}{2}x_0^T Q_0 x_0 + c_0^T x_0 \right) + \frac{1}{N} \sum_{i=1}^N \left(\frac{1}{2}x_i^T Q_i x_i + c_i^T x_i \right) \\ \text{subj to} & \quad T_0 x_0 & & = b_0, \\ & \quad T_1 x_0 + W_1 x_1 & & = b_1, \\ & \quad T_2 x_0 + & W_2 x_2 & = b_2, \\ & \quad \vdots & & \vdots \\ & \quad T_N x_0 + & & W_N x_N = b_N, \\ & \quad x_0 \geq 0, x_1 \geq 0, x_2 \geq 0, \dots, x_N \geq 0. \end{aligned} \quad (3)$$

The SAA problems are usually extremely large and even in the sparse case they can be solved only by means of distributed computing. Recently we implemented PIPS, a parallel solver in C++ for stochastic SAA problems using interior-point methods (based on OOQP[8]). We were able to achieve very good strong scaling from 80 to 1000 cores (77% efficiency) on a problem with 29 million variables. The parallelization is achieved by using a Schur complement technique that allows the computations of the second stage recourse objective and its derivatives to be performed independently on different nodes, using a decomposition based on the sample points.

The main obstacle to solving larger problems on a larger number of cores was a memory usage bottleneck caused by the number of variables in the first stage problem. This type of bottleneck is not specific to the use of interior-point methods; it also occurs in L-shaped and related methods. It is caused by solving the optimization in the space of the first stage variables in serial. For large problems, this becomes impossible due to the memory requirements. The present work removes this bottleneck by performing the linear algebra related to the first stage problem

in a parallel, distributed memory MPI-based framework.

In the context of interior-point methods applied to SAA problems of the form (3), the linear algebra operations associated with the first stage consist of solving symmetric indefinite systems of the form

$$C = \begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix}, \quad (4)$$

where Q is a *dense* symmetric positive definite matrix and A is a full rank rectangular matrix. Systems of this form are also known as saddle-point linear systems.

The size of the matrix Q can be very large; for example, it can approach 100,000 by 100,000 in the case of the stochastic unit commitment problem with wind power generation presented in Section 4.1. Such large dense linear systems can be solved efficiently by using existing libraries for parallel dense linear algebra: e.g. ScaLAPACK, PLAPACK and Elemental. This is the approach that we follow; however, there are two issues which we address and solve in this paper.

The first issue is the lack of a parallel solver for symmetric indefinite linear systems. Instead, one must use an LU-based solver for general matrices, which is twice as expensive. We overcome this drawback by implementing a specialized Cholesky-based LDL^T factorization. Most work on solving saddle-point systems is in a *sparse* context; for example, the well-known review article by Benzi et. al. [2] focuses on the sparse case. To our knowledge, this is the first specialized solver for dense saddle-point systems in a distributed memory environment.

The second difficulty is specific to stochastic optimization problems and comes from assembling the distributed saddle-point linear system (4). More specifically, C needs to be distributed across processors as required by the particular parallel solver, but all processors contribute to all of the elements of the Q block. Therefore a large amount of inter-process communication (in the form of “reduce” operations) is required in the assembly operation. This can incur a significant cost, possibly greater than the cost of factorization. We describe a technique that yields good large-scale performance. It uses efficient `Reduce_scatter` operations that maximize network bandwidth given the available memory on each node.

The paper is organized as follows. In Section 2 we outline the linear algebra required by interior-point methods for the solution of the stochastic SAA problems and present the Schur complement-based decomposition used to parallelize the computation of Q . In Section 3 we describe the parallel dense linear solvers ScaLAPACK and Elemental and our LDL^T factorization based on Elemental. We also give the implementation details of the specialized reduce operations we use to distribute the saddle-point dense linear system. In Section 4 we investigate and report on the large-scale performance of our code (up to 2,048 cores). The conclusions of this work and related future research directions are given in Section 5.

2. Schur complement decomposition of SAA problems

In this section we present the linear algebra needed to solve convex quadratic SAA problems of the form (3) by interior-point methods. We refer the reader to [9], [10], [11], or [13] for more details on how the linear algebra is derived.

The deterministic SAA problem (3) has a staircase structure that can be exploited to produce highly parallelizable linear algebra. The linear system that needs to be solved at each iteration of the interior-point algorithm has an arrow shape of

the form

$$K := \begin{bmatrix} K_1 & & & B_1 \\ & \ddots & & \vdots \\ & & K_N & B_N \\ B_1^T & \dots & B_N^T & K_0 \end{bmatrix}. \quad (5)$$

Here we used the following simplifying notation,

$$K_i := \begin{bmatrix} \frac{1}{N}\bar{Q}_i & \frac{1}{N}W_i^T \\ \frac{1}{N}W_i & 0 \end{bmatrix}, \quad K_0 := \begin{bmatrix} \bar{Q}_0 & W_0^T \\ W_0 & 0 \end{bmatrix},$$

$$B_i := \begin{bmatrix} 0 & 0 \\ \frac{1}{N}T_i & 0 \end{bmatrix}, \quad i = 1, 2, \dots, N,$$

where $\bar{Q}_i = Q_i + D_i$, $i = 0, 1, \dots, N$, with each D_i being a diagonal matrix with positive diagonal entries occurring from the use of interior-point algorithms.

Solving linear systems of the form $K\Delta z = r$ is the main computational effort at each iteration of the interior-point algorithm. Since K is symmetric, it can be factorized as LDL^T , where L is a unit lower triangular matrix and D is a diagonal matrix. One can easily verify that L and D have the following particular structures,

$$L = \begin{bmatrix} L_1 & & & \\ & \ddots & & \\ & & L_N & \\ L_{N1} & \dots & L_{NN} & L_c \end{bmatrix}, \quad D = \begin{bmatrix} D_1 & & & \\ & \ddots & & \\ & & D_N & \\ & & & D_c \end{bmatrix},$$

where

$$L_i D_i L_i^T = K_i, \quad i = 1, \dots, N, \quad (6)$$

$$L_{Ni} = B_i^T L_i^{-T} D_i^{-1}, \quad i = 1, \dots, N, \quad (7)$$

$$L_c D_c L_c^T = C := K_0 - \sum_{i=1}^N B_i^T K_i^{-1} B_i. \quad (8)$$

Observe that C defined above is the Schur complement of the first-stage Hessian block K_0 in the entire Hessian matrix K and that the terms in the sum can be computed concurrently in separate processes. This observation is the core of the so-called Schur complement scenario-based decomposition we employed in PIPS to perform an implicit factorization of the matrix K in parallel.

Let $\Delta z_i := [\Delta x_i^T \quad -\Delta y_i^T]^T$, $i = 0, 1, \dots, N$, $\Delta z := [\Delta z_1^T \quad \dots \quad \Delta z_N^T \quad \Delta z_0^T]^T$, and let r be of the form $[r_1^T \quad \dots \quad r_N^T \quad r_0^T]^T$. The following steps are needed to solve

$K\Delta z = r$:

$$w_i = L_i^{-1}r_i, \quad i = 1, \dots, N, \quad (9)$$

$$w_0 = L_c^{-1} \left(r_0 - \sum_{i=1}^N L_{N_i} w_i \right), \quad (10)$$

$$v_i = D_i^{-1}w_i, \quad i = 0, 1, \dots, N, \quad (11)$$

$$\Delta z_0 = L_c^{-1}v_0, \quad (12)$$

$$\Delta z_i = L_i^{-T}(v_i - L_{N_i}\Delta z_0), \quad i = 1, \dots, N. \quad (13)$$

Steps (9), (11), and (13) can be done in parallel, while the steps (10) and (12) have to be performed serially.

As shown in [13], C has the following simplified form,

$$C = \begin{bmatrix} Q & T_0^T \\ T_0 & 0 \end{bmatrix}, \quad (14)$$

where $Q := \bar{Q}_0 + \frac{1}{N} \sum_{i=1}^N T_i^T (W_i \bar{Q}_i^{-1} W_i^T)^{-1} T_i$. Note that Q is positive definite. The terms in the sum can be computed independently, in parallel, by partitioning the second stage scenarios and distributing them across nodes, using load balancing techniques when necessary. Then, each node computes the $T_i^T (W_i \bar{Q}_i^{-1} W_i^T)^{-1} T_i$ terms for its assigned scenarios by means of triangular solves (“backsolves”) with the factors of K_i . The results are combined across all processors, adding \bar{Q}_0 at the end.

Each of the $T_i^T (W_i \bar{Q}_i^{-1} W_i^T)^{-1} T_i$ terms become dense even when all the second-stage matrices are sparse. This adverse behavior is somehow expected since, formally speaking, two matrices are inverted and it is well known that matrix inversion destroys sparsity. Consequently, the (1, 1) block Q of the Schur complement matrix C becomes dense. This is a square block of the size of the number of first stage variables. Before our recent work, C had been stored as a dense matrix on each processor, and operations related to the first stage linear algebra, *i.e.*, the factorization of C and steps (10) and (12) had been performed *in serial* identically on all processors using LAPACK. This approach led to a memory bottleneck when solving SAA problems with a large number of first stage variables. That is, C becomes too large to store completely on each node for some real-life problems with many first stage variables (more than $\sim 10,000$).

3. Factorization and distribution of the dense system

Here, we present our solutions to the issues arising in the parallelization of the dense linear algebra required in the first stage, whose details were just described above. In Section 3.1 we provide an overview of existing parallel distributed-memory linear algebra libraries, followed by our specialized factorization procedure in Section 3.2. In Section 3.3 we describe the procedure for assembling the distributed matrix.

3.1. Parallel solvers for dense linear systems

As described in Section 2, the linear system we must factorize and solve at each iteration is a symmetric indefinite system with the following block form:

$$C = \begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix} \quad (15)$$

where Q is fully dense, symmetric positive definite and $A (= T_0)$ is sparse and of full rank. This is known as a standard saddle-point system. In the initial versions of PIPS, we used the symmetric indefinite solver in LAPACK[1] (DSYSV), which is based on the Bunch-Kaufman decomposition[5]. As mentioned above, for the large scale problems that PIPS is designed to solve, storing the system entirely in local memory in order to solve it using LAPACK is simply infeasible. Our solution is to solve the system in parallel in a distributed memory environment.

A review of the literature yielded a single parallel dense symmetric indefinite solver by Strazdins and Lewis[15], however the code has not been maintained in the last 10 years and was not incorporated into any major library. Strazdins confirmed in correspondence that he was unaware of any other efforts. Also we are not aware of any solver specialized for dense saddle-point systems, either in serial or in parallel.

Historically, the most important and most widely used parallel dense linear algebra packages are ScaLAPACK[4] and PLAPACK[16]. A package currently under development is Elemental[14], which claims significant performance improvements over ScaLAPACK and PLAPACK. We chose to focus on ScaLAPACK and Elemental; PLAPACK did not offer any particular advantages, and one may consider Elemental as its successor. In sections 3.1.1 and 3.1.2, we describe these packages and their particular methods of distributing the dense matrix across nodes. The matrix distributions are the important, if not defining, characteristic of these packages.

While all of these packages provide routines for LU and Cholesky decompositions, none provides routines for symmetric indefinite systems. Cholesky decomposition is not directly applicable to our linear system, since it is indefinite, and LU decomposition requires double the number of operations than are necessary. In light of the lack of an existing symmetric indefinite solver, we developed a specialized Cholesky-based LDL^T factorization procedure which exploits saddle-point structure of the matrix; it is described in Section 3.2.

3.1.1. ScaLAPACK

ScaLAPACK (Scalable LAPACK), is a library designed to present an LAPACK-like interface to dense distributed linear algebra. The procedures follow LAPACK naming and calling conventions; however, not all LAPACK functions have been implemented. In particular, while there is a PDGESV for solving general linear systems, there is no “PDSYSV” procedure for solving symmetric indefinite systems, as mentioned above.

For load balancing concerns, ScaLAPACK uses a *block-cyclic* distribution so that all processors “own” all parts of the matrix. We describe this distribution below.

First, a block size b is fixed, and the available processors are arranged into an $n_p \times m_p$ processor grid. The matrix is partitioned into blocks of size $b \times b$. Irregular, smaller sized blocks are permitted at the boundaries of the matrix. Using zero-based indexing, the block-cyclic distribution arises by assigning block (i, j) to processor $(i \bmod n_p, j \bmod m_p)$. Each processor has a single column-oriented local storage buffer, where the blocks are stored in their original shape, *as if* there were no blocks of the matrix between them. See Figure 1 for an example.

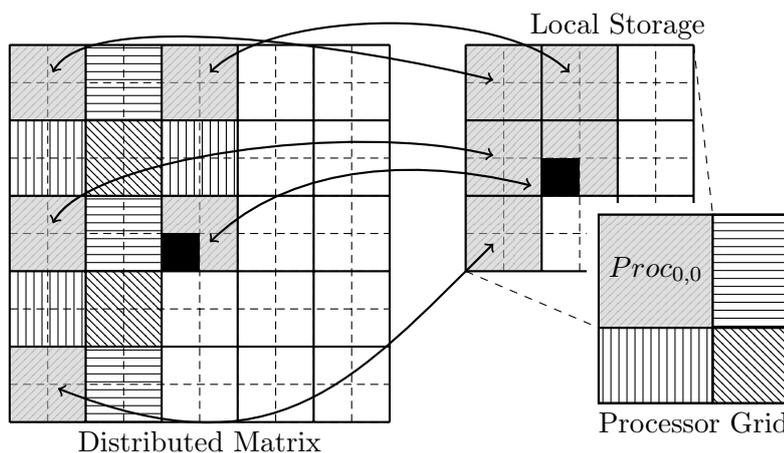


Figure 1. An illustration of the block-cyclic distribution used in ScaLAPACK, with blocksize 2 on a 2×2 processor grid, 10×10 matrix. The mapping is shown between the blocks of the distributed matrix and the local storage on processor (0,0). The blocks belonging to each processor are marked with a pattern. The highlighted square in black illustrates the element-to-element mapping. The size of blocks in the processor grid indicates the size of the local storage; note that it need not be uniform.

The above is a fairly complete description of the block-cyclic distribution at a high level. Additionally, one may consider non-square blocks, but these are only supported for some operations in ScaLAPACK. The formulas for calculating the exact index mappings become somewhat complex. They are covered in full detail in [4].

A particularity of ScaLAPACK is that these storage blocks are the same blocks used algorithmically. In the ScaLAPACK implementations of direct factorizations (LU and Cholesky), large algorithmic blocks achieve optimal cache performance, while small storage blocks yield the best load balancing. Hence, there is an inevitable compromise when choosing the optimal block size. We also found that the coupling of the storage and algorithmic blocks imposes other severe restrictions. For example, ScaLAPACK has the ability to perform operations on sub-matrices of the distributed matrix, but the sub-matrices must be completely aligned with the storage blocks. In Section 3.2 we will describe how this restriction prevented implementing our specialized LDL^T factorization in ScaLAPACK.

3.1.2. Elemental

Elemental is a new library which is intended as a replacement for ScaLAPACK and PLAPACK. It is currently under active development.

The distinguishing characteristics of Elemental are the *element-cyclic* matrix storage distribution, that is precisely the block-cyclic ScaLAPACK distribution with a blocksize of 1 (see Figure 2), and the separation of the storage and algorithmic sizes. In Elemental it is possible to use large algorithmic block sizes to obtain the best cache performance without compromising the load balancing, which actually is the best possible since the storage blocks are of size 1. The element-cyclic distribution requires Elemental to use more elaborate and possibly more costly communication patterns than ScaLAPACK. However, the abovementioned benefits of the element-cyclic distribution prevails over the communication overhead and Elemental outperforms ScaLAPACK as shown in [14]. Other important feature of the “elemental” matrix distribution is the ability to perform operations on arbitrary sub-matrices, which we exploited in our specialized LDL^T factorization.

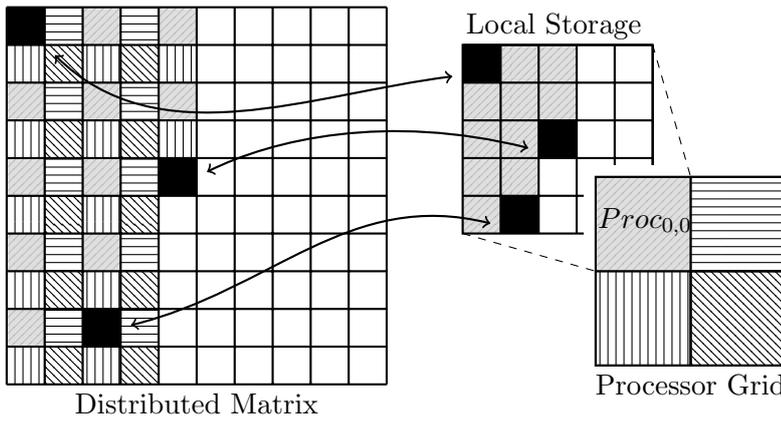


Figure 2. Illustration of the element-cyclic distribution used in Elemental on a 2×2 processor grid, 10×10 matrix. The mapping is shown between elements of the distributed matrix and the local storage on processor $(0,0)$. The blocks belonging to each processor are marked with a pattern.

3.2. Specialized Cholesky-based LDL^T factorization

Although using a general LU factorization routine to solve the linear system C given by (15) presents a practicable solution, it is not ideal. We would expect to be able to gain a two times increase in performance by using an algorithm that at least exploited the symmetric structure. We describe below a specialized LDL^T factorization algorithm which exploits both the symmetric and saddle point structure of C , and proceed to analyze the flop count.

3.2.1. Algorithm

Every symmetric indefinite matrix whose diagonal is not all zeros has a decomposition LDL^T where L is lower triangular and D is diagonal[6]. This decomposition is usually avoided in practice because of the numerical instabilities that may arise when the elements of the diagonal of the matrix all approach zero. Instead, a slightly modified decomposition is used, taking D to be a block-diagonal matrix with blocks of size 1 or 2. This is used in the Bunch-Kaufman[5] and Bunch-Parlett[6] methods.

However, in the case of the saddle point system C , the LDL^T factorization with D strictly diagonal always exists because the Q block is positive definite. Furthermore, we can derive the exact form of the LDL^T factorization using the block structure of the matrix,

$$\begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix} = \begin{bmatrix} M & 0 \\ AM^{-T} & \widetilde{M} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \begin{bmatrix} M^T & M^{-1}A^T \\ 0 & \widetilde{M}^T \end{bmatrix}, \quad (16)$$

where M and \widetilde{M} are lower triangular Cholesky factors satisfying $MM^T = Q$ and $\widetilde{M}\widetilde{M}^T = AQ^{-1}A^T$. These factors necessarily exist because Q is positive definite, and therefore $AQ^{-1}A^T$ is positive definite as well because A has full rank. Note there is a close connection between the factorization and the Schur complement $(-AQ^{-1}A^T)$, which is used in the interior-point community in the “reduced system” or “normal equations” approach.

Computationally, we need only calculate the lower triangular L factor. What makes this factorization practical is that it can be performed *in-place* on the distributed matrix!

Let us denote the four logical blocks of the distributed matrix as follows:

$$B = \begin{bmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{bmatrix} \quad (17)$$

where $B = C$ initially, that is $B_{00} = Q, B_{10} = A, B_{01} = A^T, B_{11} = 0$; in fact, only the lower triangle must be filled. We perform a sequence of standard linear algebra operations on B , after which B contains the lower triangular L factor. See Figure 3 for the procedure.

Specialized LDL^T Procedure

In-place factorization

1. $B_{00} \leftarrow \text{Cholesky}(B_{00})$ ($= \text{Cholesky}(Q) = M$)
2. $B_{10} \leftarrow B_{10}B_{00}^{-T}$ ($= AM^{-T}$) (*trsm*)
3. $B_{11} \leftarrow (B_{10})(B_{10})^T$ ($= (AM^{-T})(AM^{-T})^T = AQ^{-1}A^T$) (*syrk*)
4. $B_{11} \leftarrow \text{Cholesky}(B_{11})$ ($= \text{Cholesky}(AQ^{-1}A^T) = \tilde{M}$)

Solving $Sx = b$

5. $b \leftarrow L^{-1}b$ (*trsv*)
 6. $b \leftarrow D^{-1}b$ (*ad-hoc*)
 7. $b \leftarrow L^{-T}b$ (*trsv*)
-

Figure 3. Specialized procedure for solving the saddle point system S . After the factorization, the lower triangle of B contains L . The name of the operations is in parentheses. The operations are described in the text.

The operations used are Cholesky factorization, triangular solve (*trsm*, *trsv*), and symmetric rank-k update (*syrk*). On line 2, *trsm* is used to solve a matrix triangular system of the form $XY^T = Z$ for X , overwriting Z with the answer. On line 3, a symmetric rank-k update performs the operation $Z \leftarrow \alpha XX^T + \beta Z$, where we take $\alpha = 1, \beta = 0$. The sequence of operations is very similar to a step of blocked right-looking Cholesky factorization[16].

In the solution phase, the *trsv* operation solves a simple triangular system $Zx = b$ or $Z^T x = b$. Finally, note that $D = D^{-1}$. Then, multiplication by D^{-1} can be performed *ad-hoc* by simply negating the lower part of the right hand side vector.

Cholesky factorization, triangular solve, and symmetric rank-k update are standard operations which, in principle, are provided by both ScaLAPACK and Elemental. In both ScaLAPACK and Elemental, these operations can also operate on sub-matrices of a distributed matrix, a property which is fully exploited above. However, ScaLAPACK has an important caveat: the sub-matrices must align with the storage blocks; that is, the top left element of a sub-matrix must be the top left element of a storage block. Given that Q may be of arbitrary size, and that there is a practical limit on the size of a storage block, this restriction is effectively impossible to satisfy in the given context without extensively modifying ScaLAPACK's source code. Therefore, this procedure was only implemented using Elemental, requiring just five lines of code in C++ to perform the factorization.

3.2.2. Flop count

We analyze here the number of operations required by the algorithm above, in order to confirm the desired theoretical two times decrease in operation count over LU factorization. Only the higher order terms are counted.

Note first that for an $n \times n$ matrix, LU decomposition requires $\frac{2}{3}n^3$ floating-point operations, and both Cholesky and Bunch-Kaufman (symmetric indefinite)

decompositions require $\frac{1}{3}n^3$. Both LU and Bunch-Kaufman require an additional $O(n^2)$ comparisons to perform pivoting[5].

Now let n be the size of Q and m be the number of rows in A ($Q \in \mathbb{R}^{n \times n}$, $A \in \mathbb{R}^{m \times n}$). Then the entire matrix is $(n+m) \times (n+m)$. We verify that $trsm$ requires mn^2 operations and $syrk$ requires m^2n operations.

For $trsm(B_{10}B_{00}^{-T})$: one may verify that a triangular solve requires n^2 operations; this is performed m times, resulting in mn^2 operations. For $syrk((B_{10})(B_{10})^T)$: this is a normal matrix-matrix multiplication, but only the lower triangle is calculated. Each of the $\frac{1}{2}m^2$ elements requires n multiplications and $n-1$ additions, resulting in m^2n operations.

The specialized LDL^T factorization therefore requires $\frac{1}{3}n^3 + m^2n + mn^2 + \frac{1}{3}m^3 = \frac{1}{3}(n+m)^3$ floating point operations. This is the same number of flops as Bunch-Kaufman and half those of an LU decomposition, confirming that we have achieved the goal of a factorization routine that requires half the operations of LU , and in theory, should deliver twice the performance. Also note that no comparisons are required in this case, unlike both LU and general symmetric indefinite factorization routines.

As a final observation, recall that the A block is in reality sparse, although it has been treated as a block of a dense matrix. We implemented it as such, but one may be able to significantly reduce communication costs and flops in the $trsm$ stage by storing A as a sparse matrix on each processor and implementing a specialized triangular solve routine. However, since the number of rows of A is less than the the number of rows of Q , usually much more smaller, this would likely be a minor optimization.

3.2.3. As a saddle point solver

Benzi et al.[2] is a well-known work that provides a thorough review of methods for saddle point problems. The factorization (16) appears, and direct solution methods based on it are discussed; however, only sparse methods are mentioned. They note that using this factorization can be more efficient than Bunch-Kaufman because no pivoting is required; in addition, it is sufficiently numerically stable. To our knowledge, there has been no previous attempt to solve dense saddle point systems in parallel using the LDL^T factorization or any other specialized approach.

We note that the method proposed applies with only a slight modification to a more general saddle point system of the form:

$$C = \begin{bmatrix} Q & A^T \\ A & -S \end{bmatrix} \quad (18)$$

where S is symmetric positive semidefinite, and Q and A are symmetric positive definite and of full rank, respectively, as above. The LDL^T factorization for this more general case is provided in [2]. We will not cover it in detail, but we note that the only modification necessary to the algorithm in Figure 3 is on the $syrk$ step to include S in the Schur complement. This saddle point system has applications outside of constrained optimization, which are referenced in [2].

3.3. Assembling the matrix

We have assumed up to this point that the linear system is already distributed across processors as required by Elemental or ScaLAPACK. However, assembling the matrix and distributing it as required can be a costly operation, possibly more costly than the factorization itself. This operation must be streamlined to obtain

acceptable large-scale performance.

We present a simplified version of the summation which was more fully described in Section 2. Let B refer to the distributed matrix, partitioned as in (17). Let \mathcal{P} be the set of processors. The distribution operation we must perform can be described simply as:

$$B_{00} = \sum_{p \in \mathcal{P}} M_p \quad (19)$$

where M_p is calculated locally on processor p , and B_{00} is distributed across processors. Here M_p is the local contribution to the sum discussed in Section 2.

In the serial case where LAPACK is used to solve the entire system on each processor, this operation maps directly to an `Allreduce` in MPI. In the distributed case, we have two important considerations which make the distribution problem significantly more complicated:

- M_p is too large to fit entirely in a node's local memory.
- Every node owns different, non-contiguous, elements in B_{00} ; however, all nodes contribute to all elements.

To address the first issue, we assume M_p may be calculated in blocks of columns. This is trivial during the “backsolve” step described in Section 2. Then, repeated communication operations are performed to build B_{00} by blocks of columns.

For the second issue, we observe that the communication pattern required maps closely to a `Reduce_scatter` operation in MPI, in which a large array is “reduced” (summed) across all processors, and then its pieces are partitioned and “scattered”, distributed to processors.

However, `Reduce_scatter` requires that each processor receive a single contiguous part of the send buffer. Considering the distribution of the matrix across processors, a single contiguous column of the matrix can not be partitioned such that the elements belonging to a given processor are in contiguous memory. Some intermediate steps are therefore necessary.

We first present a method to distribute the entire B_{00} block (“full reduce”), followed by a method to distribute only the lower triangle of B_{00} (“lower triangular reduce”). We only describe these methods for the matrix distribution corresponding to Elemental, but a “full reduce” was also implemented for ScaLAPACK.

3.3.1. Full reduce

In order to apply LU decomposition, the entire distributed matrix must be filled with the corresponding elements, disregarding the symmetry of the matrix. This is not the case for the LDL^T procedure, which requires only the lower triangle. Nevertheless, we will compare our approach empirically to LU decomposition, so a method to fill the entire B_{00} block is necessary. This method is also a starting point for the lower triangular procedure which will be described next.

Figure 4 contains a high level description of the procedure. While it is generally straightforward, special care is needed at some points to ensure an efficient implementation.

As mentioned above, we build the matrix in blocks of columns. The size of the blocks is governed by the parameter b . This should be as large as possible to maximize the communication bandwidth, given the available memory on each node.

The **Pack** step fills the send buffer for `Reduce_scatter`. The send buffer must be arranged such that the elements destined for a processor are in a single contiguous block, and the blocks must be ordered according to processor number. For fast

“Full reduce” procedure

Initialization

1. Let n be the size of B_{00} .
2. Fix buffer size b .
3. **Allocate** b doubles for column buffer and b doubles for send buffer.
4. **Allocate** recv buffer (sufficiently large).
5. $step \leftarrow b/n$

Main loop

6. **For** $i = 0$ to $n - 1$, **step**
 7. $endCol \leftarrow \min(i + step - 1, n - 1)$
 8. **Compute columns** i to $endCol \rightarrow$ column buffer
 9. **Pack** column buffer \rightarrow send buffer
 10. **MPI_Reduce_scatter**(send buffer) \rightarrow recv buffer
 11. **Unpack** recv buffer \rightarrow local matrix storage
 12. **End For**
-

Figure 4. Overall procedure for distributing the full B_{00} block.

unpacking, we also require that inside a block, the order of elements match their order in the local matrix storage. We have fully specified a one-to-one map between the location of the elements in the column buffer and their location in the send buffer, and theoretically only a permutation of the column buffer is necessary. An in-place permutation would have very poor cache performance, so we allocate a separate array and copy the elements into their positions.

The key to streamlining this copying procedure is to avoid expensive division and modulus operations that one would naively use to calculate the required positions of the elements. Instead, one should loop over continuous memory in the send buffer and copy the corresponding elements of the column buffer, using only addition operations to calculate the addresses. The following loop implicitly copies the elements into the correct order in the send buffer: loop over each processor p in order, and in an inner loop pick out the elements from the column buffer belonging to processor p , copying them to the send buffer, in order. The offsets between elements is known, so this inner loop may be performed just by incrementing the counters correctly. Recall that all buffers store elements in column-major order.

Once the send buffer is filled, `Reduce_scatter` is called. The entries are summed across all processors and the result is partitioned and distributed to the receive buffers on the desired processors. We have arranged the elements so that they are in the correct order for unpacking, so this step is straightforward. Note that we can not use the local storage directly as the receive buffer, because the local storage has additional rows for the rest of the distributed matrix.

3.3.2. Lower triangular reduce

For the LDL^T factorization procedure, we would be performing unnecessary work by distributing the entire symmetric B_{00} block, when only the lower triangle is required. Also, in initial experiments we noticed that the communication in the reduce step can take a significant amount of time. Therefore, we set out to design a “lower triangular reduce” which should take nearly exactly half the time of the “full reduce” procedure above, excluding computing the columns. We arrived at a procedure that can effectively guarantee requiring only half of the communication time, with little extra overhead.

With this goal in mind, we must fix the size b of the send buffer as above, and design a procedure that calls `Reduce_scatter` half the number of times. We only

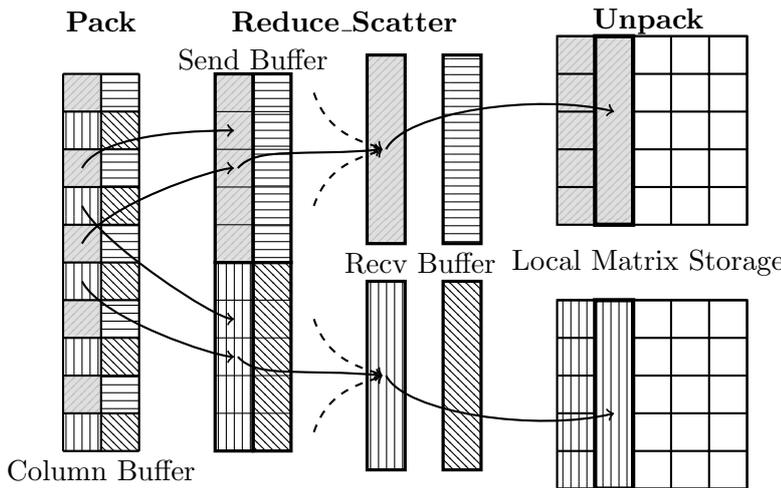


Figure 5. Illustration of a step of the “full reduce” procedure. The 3rd and 4th columns are sent of a 10×10 B_{00} block on a 2×2 processor grid. Note that the local storage contains more rows and columns than displayed; only the elements belonging to B_{00} are shown. Dashed lines indicate communication from other processes. In general, processors will receive more than one column, unlike shown here.

need to send half the number of elements, so this is certainly possible. In a more naive approach, one might be led to loop over fixed-sized blocks of columns as before, and only send the lower triangular elements. This approach can not deliver the performance desired, because it results in the same number of **Reduce_scatter** calls as before, and so does not decrease the communication overhead.

The solution for a fixed send buffer size is to vary the number of columns calculated in each iteration, taking exactly as many as whose lower triangular elements fit in the send buffer. This number will increase with each iteration. We may count the lower triangular elements as follows. Let n be the size of the B_{00} block, then the block of columns starting at column s and ending at column $e - 1$ (inclusive, zero indexed) has the following number of elements:

$$\sum_{i=s}^{e-1} (n - i) = -\frac{1}{2}e^2 + \left(n + \frac{1}{2}\right)e + \frac{1}{2}s^2 - \left(n + \frac{1}{2}\right)s =: f(e; n, s) \quad (20)$$

At each iteration, n and s are fixed, and the problem is to find the largest integer e satisfying $f(e; n, s) \leq b$ and $e \leq n$. This is an easy and inexpensive calculation, given that $f(e; n, s)$ is quadratic.

Besides varying the number of columns at each iteration, the overall procedure is the same as in Figure 4. The **Pack** and **Unpack** operations require a small overhead in addressing, but only in calculating offsets. Instead of describing these in detail, we provide an illustration in Figure 6, which indicates the operations required.

4. Numerical experiments

Numerical experiments were performed on the Fusion cluster at Argonne National Laboratory. Each node has a large 36GB of RAM and dual quad-core Intel[®] Xeon[®] 2.53Ghz CPUs, for a total of 8 cores per node. In further discussion, we treat each core itself as a node or processor with its own local memory. The cluster has an

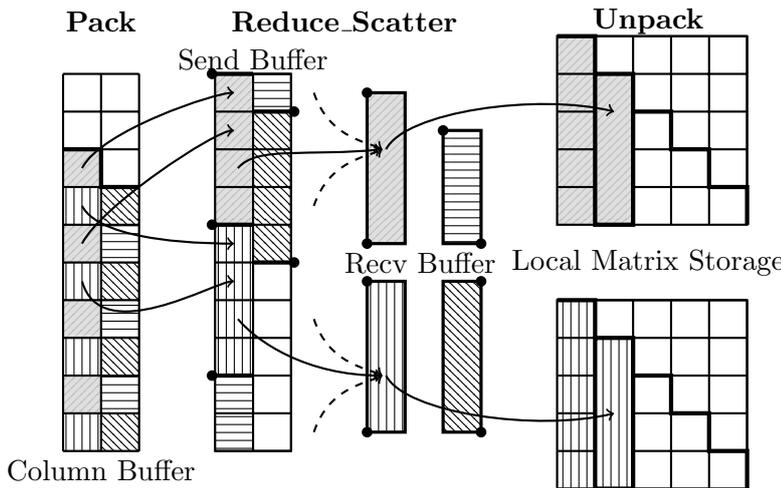


Figure 6. Illustration of a step of the “lower triangular reduce” procedure. The 3rd and 4th columns are sent of a 10×10 B_{00} block on a 2×2 processor grid. Note that the local storage contains more rows and columns than displayed; only the elements belonging to B_{00} are shown, and the lower triangular elements are indicated. Dashed lines indicate communication from other processes. Dots indicate the partitions of the column-major send buffer. In the illustrated case, only two columns fit in the send buffer. Note that in general, not each processor will receive an equal number of elements, due to the properties of the matrix distribution.

Infiniband interconnect. A storage blocksize of 32 is used for ScaLAPACK and an algorithmic blocksize of 96 is used for Elemental, optimized respectively by empirical observation. Additionally, 250MB is used for buffers during the reduce stage.

We first describe the test problem, and proceed to present strong and weak scaling results.

4.1. The test problem

We use a formulation of the stochastic unit commitment problem with wind power generation in the tests for PIPS. For brevity, we do not present the full model. Instead, we provide an overview of the problem and the terminology used to describe it, and direct the interested reader to [7] for a complete presentation.

Unit commitment refers to committing power generation *units* to either produce electricity or remain idle. In our problem there are two types of power units: thermal power plants using fossil fuels, and wind farms using renewable energy. The thermal power generation units are costly to operate, both economically and environmentally. And so, they should not be operating in large excess of demand. Each unit has startup, shutdown, and running costs, and can not change state instantaneously.

The stochastic component arises from considering electricity produced by wind farms, which highly is variable. The optimization problem is to minimize operation costs *subject to* satisfying the demand with some safety margin. Solving such problems, we may realize the economic and environmental benefits of wind power while ensuring that it is safely integrated with the power grid.

Each second stage *scenario* is a possible realization of weather patterns, which corresponds to a different amount of electricity produced by the wind farms. These scenarios are generated by simulation using the state-of-the-art Weather Research and Forecast (WRF) model. In the formulation proposed by [7], this is a two-

stage stochastic mixed-integer linear program with recourse, and the problem is solved over a 24-hour time frame with a *recourse* stage to reallocate units at the end of the period. The problem solved by PIPS has one (large) simplification: the mixed-integer problem is relaxed to a continuous problem. However, the problems solved are realistically sized, in both the number of variables and the number of second-stage scenarios.

Problems of various sizes that are used in the experiments of this section are obtained by replicating a (small) real-life unit commitment problem (10 thermal units, 12 wind farms) set up for the State of Illinois [7]. We were forced to do this because of the lack of data for a larger area. We mention that our implementation is not tuned in any way to take advantage of any special structure that may be introduced by replications.

4.2. Solvers

We compare here the first-stage factorization times for the three solvers tested, LU with ScaLAPACK, LU with Elemental, and LDL^T with Elemental. A fixed problem size of 300 thermal units is used and we vary the number of processors used by PIPS. The Q block of C is of size 23436 and the A block has 1224 rows. This is not an especially large first stage problem, and so we would expect the solver to be less efficient with a larger number of processors. To verify this, we include cases where only a subset of the processors is used for factoring the matrix. See Table 1.

Table 1. Factorization times. In some cases, a subset of the total CPUs is used for the factorization. (S) indicates ScaLAPACK and (E) indicates Elemental. The LDL^T factorization is performed with Elemental. Values are averages over 5 iterations. There was insufficient memory to run with 32 processors.

# Procs.		Factor (sec)		
	# Factoring	LU (S)	LU (E)	LDL^T
32	32	*	*	*
64	64	55.14	89.18	29.94
256	256	15.63	17.68	9.78
1024	256	22.34	25.54	11.48
	1024	16.59	20.04	6.71
2048	256	35.20	42.48	16.86
	1024	31.25	41.43	10.81
	2048	38.45	56.19	14.08

In all cases, the LDL^T factorization is the fastest, and in many taking less than half of the best LU time. We note that ScaLAPACK LU times are better than Elemental LU times. This was a surprising result, given Elemental's claims of improved performance. After discussions with the author, we concluded that the poor performance is most likely related to the characteristics of the Fusion cluster. Elemental makes liberal use of advanced MPI collective operations, while ScaLAPACK primarily uses broadcast operations. This communication pattern may be relatively more efficient on Fusion, whose interconnect is not designed for all-to-all communications. In spite of this issue, the LDL^T factorization, which uses Elemental, does deliver the expected 2x increase in performance over even the LU solver in ScaLAPACK.

We observe that 1024 processors appears to be an optimal number for this problem size; this is clear in the case of 2048 total processors, where factorization time

decreases from 256 to 1024 and increases from 1024 to 2048 for all solvers. It is curious that factorization times appear to worsen for a fixed number of factoring processors when the total number of processors is increased. We did not have the opportunity to fully investigate this.

4.3. Reduce

As the reader will later see, the factorization times above are small compared to the total execution time. In fact, the reduce times are more significant. The performance of the “full reduce” procedure is generally independent of the ScaLAPACK or Elemental matrix distribution, with most of the time spent in the `Reduce_scatter` step. Therefore, the benefit of ScaLAPACK is minor, and only when we compare between LU factorizations. For simplicity and due to a lack of CPU time, from this point on we present strong scaling results only from Elemental. We will further justify this decision in Section 4.4.

The times for the full and lower triangular reduce operations are compared below in Table 2. In all cases, the lower triangular reduce takes about half the time. Note that these times are bigger than the factorization times themselves. Also, reducing onto a subset of processors is slower than reducing onto all processors, because of the load imbalance that arises from the uneven communication costs. This slowdown appears to be greater than the possible improvement in factorization time.

Table 2. Time spent assembling Q block of the distributed matrix, excluding calculating the columns. The operation involves summing contributions from all processors to each of the 549,246,096 elements, and scattering the elements to their required place in the distributed matrix. Values are averages over 5 iterations. There was insufficient memory to run with 32 processors.

# Procs.	# Factoring	Reduce (sec)	
		LU	LDL^T
32	32	*	*
64	64	28.31	12.96
256	256	37.55	17.18
1024	256	110.45	45.21
	1024	54.32	26.35
2048	256	167.73	89.50
	1024	100.40	50.80
	2048	82.41	43.93

The reduction step presents a difficulty for strong scaling. With a fixed problem size, the reduce time increases with the number of processors. This can be explained easily by an increase in communication overhead. Because the lower triangular reduce grows more slowly than the full reduce in absolute terms, we will see that in addition to being faster, the lower triangular reduce also provides the best strong scaling results.

4.4. Strong scaling

For the fixed problem size chosen (300 thermal units), the “backsolve” procedure to generate the columns of the terms in the sum of the Q block (14) takes approximately 140 seconds per scenario, independently of the total number of processors. This itself is large compared to the reduction and factorization steps, which are the only significant operations that are not “embarrassingly parallel”. With 4096

scenarios, we would expect very good strong scaling, until the point where each processor is assigned a very small number of scenarios. This is the exact behavior we observed. The results are reported in Table 3.

Table 3. Total walltime for 5 interior-point iterations. Fixed problem size with 4096 scenarios, divided evenly across processors. All processors are used for factoring. Elemental is used for both LU and LDL^T . The execution time for 64 processors is used as the baseline, and we calculate speedup and efficiency.

Procs.	Tot. Walltime (min)		Speedup (Efficiency)		Peak Mem. (MB)
	LU	LDL^T	LU	LDL^T	
64	759.01	735.37	64 (100%)	64 (100%)	1818
256	195.62	193.12	248.3 (97.0%)	243.7 (95.2%)	770
1024	55.76	50.99	871.1 (85.1%)	922.9 (90.1%)	533
2048	37.9	30.48	1282.05 (62.6%)	1534.9 (75.4%)	523

The LDL^T solver has the best strong scaling, due primarily to the smaller increases in reduce times. We observe very good scaling (90%) up to 1024 processors, where each processor is assigned 4 scenarios. Scaling degrades to 75% efficiency with 2048 processors, where each processor is assigned only two scenarios, and the reduction and factorization steps become more significant. The peak memory usage per node decreases with the number of processors, because the size of the local matrix storage decreases and less scenarios are assigned. Note that memory usage includes the fixed 250MB used during the reduce step.

Currently, the number of processors is limited by the total number of scenarios. This is not an unreasonable limitation, given that the computational difficulty with SSA problems generally arises from the large number of scenarios. However, splitting scenarios across processors is a possibility, and could be accomplished using parallel sparse libraries to perform the linear algebra in the second stage.

Earlier we disregarded ScaLAPACK, claiming that the benefit over Elemental's LU solver is insignificant. For 1024 processors, the difference in factor times was about 3.5 seconds (20.04 versus 16.59). Recalling that the reduction process is the same, over five iterations, this amounts to about a 17.5 second difference in total execution time. This is, in fact, not very significant compared to the 5 minute difference between LU full reduce and LDL^T lower triangular reduce.

4.5. Weak scaling

Strong scaling is more difficult on smaller problems, and so above we used a first stage matrix with size 24660. By itself, this matrix requires about 4.5GB to store, which does not exceed the capabilities of a modern computer; in the tests above, most of the memory on each node was in fact used to store the data associated with the scenarios. Here, we present weak scaling results, solving larger problems with a fixed number of processors. We solve the unit commitment problem described earlier, now with 640 and 1000 thermal units on a fixed 1024 processors with 4096 scenarios. Table 4 contains the reduce and factorization time, and Table 5 contains the average iteration times. Because of the very large CPU time requirements, we ran three interior-point iterations for 640 and 1000 thermal units (with 5 iterations for 300); for ScaLAPACK we can only present factorization times.

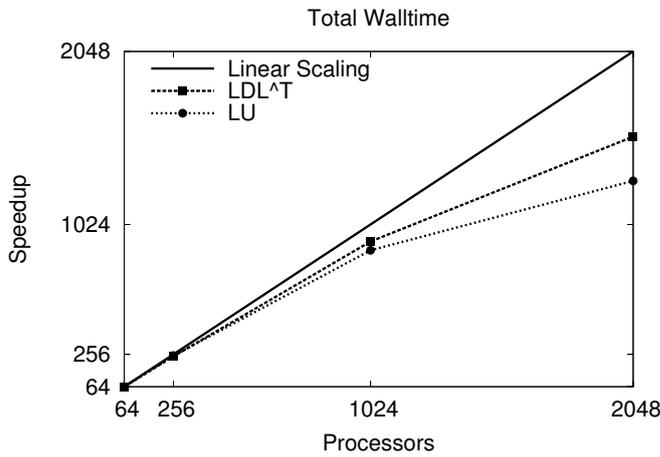


Figure 7. Plot of strong scaling results. See Table 3 for numerical values.

Table 4. Factorization and reduce times. 1024 processors with all used for factorization, 4096 scenarios. (S) indicates ScaLAPACK and (E) indicates Elemental.

Thermal Units	1st Stage Size ($Q+A$)	Factor (Sec.)			Reduce (Sec.)	
		$LU(S)$	$LU(E)$	LDL^T	LU	LDL^T
300	23436+1224	16.59	20.04	6.71	54.32	26.35
640	49956+2584	60.67	83.24	36.77	256.95	128.59
1000	78030+4024	173.67	263.53	90.82	565.36	248.22

Table 5. Average iteration times and “backsolve” times per second stage scenario. 1024 processors with all used for factorization, 4096 scenarios. Elemental used for LU .

Thermal Units	Total Variables	Per Scenario		Min./Iter.		Peak Mem. (MB)
		Vars.	Sec.	LU	LDL^T	
300	57,677,508	14,076	139.55	11.15	10.19	533
640	121,764,108	29,716	689.35	53.49	50.44	722
1000	189,620,508	46,276	1711.29	132.72	122.74	954

Both the factorization and reduce times for LDL^T continue to be about half of the times for LU . These are promising weak scaling results. The reduce times scale quadratically with the size of the Q block, since the operation is a function of the number of elements. The factorization time should scale with the cube of the size of the 1st stage matrix, but as the matrix size increases, the factorization routines become more efficient, and so we observe less than cubic scaling at these problem sizes. The matrix of the largest problem has a size of over 82,000, which would take approximately 50GB to store, and the LDL^T routine factors it in only 90 seconds. This translates to over two teraFLOPS of performance (20% of peak). Large matrices that would be very difficult if not impossible to solve in serial present no problem to solve efficiently in parallel.

None of these problems could have been solved previously by PIPS using LAPACK to factor the dense matrices. Problems of this size are real-life problems. For example, 1000 thermal units and 1200 wind farms covers the entire Midwest region of the United States. To our knowledge, problems such as these with nearly 80,000 first stage variables and 190 million total variables have not been previously solved.

5. Conclusions and future work

We presented a specialized LDL^T factorization procedure for solving dense saddle-point linear systems in parallel. In numerical experiments, this procedure obtains the desired two times increase in performance over a general LU factorization. Our procedure applies to an entire class of saddle-point systems and requires only five lines of C++ code to implement using an actively maintained parallel dense linear algebra library, Elemental. Currently, it is the only such procedure available. For saddle-point systems, it is likely more efficient than general parallel symmetric-indefinite solvers, if any are implemented in the future, because no comparisons or pivoting is required. The procedure scales well to very large systems, and performance will improve with improvements in the Elemental core.

We also presented an efficient method to assemble the matrix in the context of a parallel solver for two-stage stochastic optimization problems with recourse using the SAA approach. These problems are highly parallelizable by distributing the calculation for the second stage scenarios, but one must also solve a large dense linear system in the first stage variables. This work demonstrated how to parallelize solving this system as well. The overhead of parallelization arises in the assembly phase of the matrix, and we were able to reduce this cost by half by assembling only the lower triangle, significantly increasing strong scaling efficiency. The communication overhead would likely be greatly reduced on a system with tightly-coupled nodes and a dedicated collectives network, such as the Blue Gene/P at Argonne National Laboratory. We intend to test PIPS on this system as well as investigate efficient hybrid programming approaches (MPI plus shared-memory parallelization) which has become increasingly important for current and next generation supercomputers.

By parallelizing the dense factorization, we removed the memory bottleneck that prevented PIPS from solving problems with a large number of first stage variables. Now, PIPS is capable of solving very large real-life sized problems. This is an important problem for the integration of wind-generated power with the electricity grid, and this work is a necessary step forward in order to be able to solve it and similarly sized large-scale stochastic optimization problems.

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