Newly Released Capabilities in Distributed-memory SuperLU Sparse Direct Solver

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We present the new features available in the recent release of SuperLU_DIST, Version 8.0.0. SuperLU_DIST is a distributed-memory parallel sparse direct solver. The new features include (1) a 3D communication-avoiding algorithm framework which trades off inter-process communication for selective memory duplication, (2) multi-GPU support for both NVIDIA GPUs and AMD GPUs, and (3) mixed precision routines that perform single precision LU factorization and double precision iterative refinement. Apart from the algorithm improvements, we also modernized the software build system to use CMake and Spack package installation tools to simplify the installation procedure. Throughout the paper, we describe in detail the pertinent performance-sensitive parameters associated with each new algorithm feature, show how they are exposed to the users, and give general guidance of how to set these parameters. We illustrate that the solvers performance both in time and memory can be greatly improved after systematic tuning of the parameters, depending on the input sparse matrix and underlying hardware.

CCS Concepts: • **Mathematics of computing → Solvers**.

Additional Key Words and Phrases: Sparse direct solver, communication-avoiding, GPU, mixed-precision

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1 OVERVIEW OF SUPERLU AND SUPERLU_DIST

SuperLU contains a set of sparse direct solvers for solving large sets of linear equations $AX = B$ [5]. Here A is a square, nonsingular, $n \times n$ sparse matrix, and X and B are dense $n \times nrhs$ matrices, where $nrhs$ is the number of right-hand sides and solution vectors. The matrix A need not be symmetric or definite; indeed, SuperLU is particularly appropriate for unsymmetric matrices, and it respects both the unsymmetric values as well as the unsymmetric sparsity pattern. The routines appear in three different libraries: sequential (`SuperLU`), multithreaded (`SuperLU_MT`) and distributed-memory parallel (`SuperLU_DIST`). They can be linked together in a single application. All three libraries use variations of Gaussian elimination (LU factorization) optimized to take advantage of the sparsity of the matrix and modern high performance computer architectures (specifically memory hierarchy and parallelism). The `SuperLU_DIST` library is implemented in ANSI C, using MPI for communication, OpenMP for multithreading, and CUDA (or HIP) for NVIDIA (or AMD) GPUs. The library includes routines to handle both real and complex matrices in single and double precisions, and some functions with mixed precisions. The parallel algorithm consists of the following major steps.

(1) Preprocessing
(2) Sparse LU factorization (SpLU)
(3) Sparse triangular solutions (SpTRSV)
(4) Iterative refinement (IR) (optional)

The preprocessing in Step 1 transforms the original linear system $Ax = b$ into $\bar{A}x = \bar{b}$, so that the latter one has more favorable numerical properties and sparsity structures. In `SuperLU_DIST`, typically A is first transformed into $\bar{A} = P_c P_r D_r A D_c P_c^T$. Here D_r and D_c are diagonal scaling matrices to equilibrate the system, which tends to reduce condition number and avoid over/underflow. P_r and P_c are *permutation matrices*. The role of P_r is to permute rows of the matrix to make diagonal elements large relative to the off-diagonal elements (numerical pivoting). The role of P_c is to to permute rows and columns of the matrix to minimize the fill-in in the L and U factors (sparsity reordering). Note that we apply P_c symmetrically so that the large diagonal entries remain on the diagonal. With these transformations, the linear system to be solved is: $(P_c P_r D_r A D_c P_c^T)(P_c D_c^{-1})x = P_c P_r D_r b$. In the software configuration, each transformation can be turned off, or can be achieved with different algorithms. Further algorithm details and user interfaces can be found in [5, 7]. After these transformations, the last preprocessing step is symbolic factorization which computes the distributed nonzero structures of the L and U factors, and distributes the nonzeros of $\bar{A}$ into L and U.

This release paper focuses on the new capabilities in Steps 2-4 in SuperLU_DIST. Throughout the paper, when there is no ambiguity, we simply refer to the library SuperLU_DIST as SuperLU.

Before the new Version-7 release (2021), the distributed memory code had been largely built upon the design in the first SuperLU_DIST paper [6]. The main ingredients of the parallel SpLU algorithm are:

- supernodal fan-out (right-looking) based on elimination DAGs,
- static pivoting with possible half-precision perturbations on the diagonal (GESP) [6],
- 2D logical process arrangement for non-uniform block-cyclic mapping, based on the supernodal block partition, and
- loosely synchronous scheduling with lookahead pipelining [12].

The parallel SpTRSV uses a block-cyclic layout for the L and U matrices as in the results of SpLU. It also uses a message-driven asynchronous and dynamically scheduled algorithm—designed to reduce the communication and latency costs. The user can optionally invoke a few steps of iterative refinement to improve the solution accuracy.

The routines in SuperLU are divided into *driver routines* and *computational routines*. The routine names are inspired by the LAPACK and ScaLAPACK naming convention. For example, the 2D linear solver driver is pdgssvx, where 'p' means parallel, 'd' means double precision,[1] 'gs' means general sparse matrix format, and 'svx' means solving a linear system. Below is a list of double precision user-callable routines.

- Driver routines: pdgssvx (driver for the old 2D algorithms), pdgssvx3d (driver for the new 3D algorithms in Section 2).
- Computational routines: pdgstrf and pdgstrs are respectively triangular factorization SpLU and triangular solve in the 2D process grid. pdgstrf3d is triangular factorization SpLU in the 3D process grid. These routines take a *preprocessed* linear system as an input. An experienced user can use them directly in the application code as they can provide greater flexibility. For a new user, however, using them can be cumbersome and error-prone. We recommend using driver routines, which are easier to use.
- The pddrive and pddrive3d examples in the EXAMPLE/ directory call the respective drivers pdgssvx and pdgssvx3d to solve linear systems. Other examples in the same directory, such as pddrive1, pddrive2, etc., illustrate how to reuse the preprocessing results for a sequence of linear systems with similar structures.

The Doxygen generated documentation for all the routines is available at https://portal.nersc.gov/project/sparse/superlu/superlu_dist_code_html/. Each routine begins with a comment that breaks down input/output arguments and explains the functions of the routine. Although the original User's Guide contains comprehensive description of various internal data structures and algorithms [5], it does not contain the new features presented here.

In the sections that follow, we will describe the new features which are available since Version-7. This includes the new 3D communication-avoiding algorithm framework, multi-GPU support, mixed precision routines and support for new build tools. Throughout the paper, we discuss all the parameters that may influence the code performance. These parameters can be set in a compile-time "options" structure, or by environment variables (with capitalized names), the latter of which take precedence. Section 6 gives a summary of the parameters.

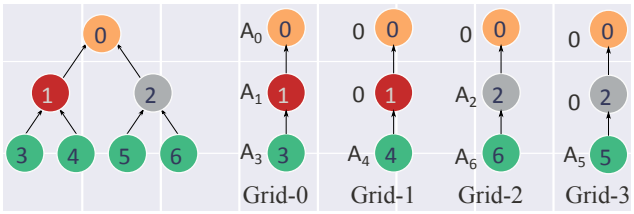
[1] We support four datatypes: 's' (FP32 real), 'd' (FP64 double), 'c' (FP32 complex) and 'z' (FP64 complex). Throughout the paper, we use the 'd' version of the routine names.

2 3D COMMUNICATION-AVOIDING ROUTINES

We developed a novel 3D algorithm framework for sparse factorization and triangular solutions. This new approach is motivated by the strong scaling requirement from exascale applications. Our novel 3D algorithm framework for sparse factorization and triangular solutions alleviates communication costs by taking advantage of the three-dimensional MPI process grid, the elimination tree parallelism, and the communication-memory tradeoff—inspired from communication-avoiding algorithms for dense linear algebra in the last decade.

The 3D processes grid, configured as $P = P_x \times P_y \times P_z$ (see Fig. 3a), can be considered as P_z sets of 2D processes layers. The distribution of the sparse matrices is governed by the supernodal elimination tree-forest (etree-forest): the standard etree is transformed into an etree-forest which is binary at the top $\log_2(P_z)$ levels and has P_z subtree-forests at the leaf level (see Fig. 1a). The description of the tree partition and mapping algorithm is described in [11, Section 3.3]. The matrices A, L, and U corresponding to each subtree-forest are assigned to one 2D process layer. The 2D layers are referred to as Grid-0, Grid-1, ..., up to $(P_z - 1)$ grids. Fig. 1b shows the submatrix mapping to the four 2D process grids.

(a) 2-level etree partition



(b) Matrix view on 4 process grids

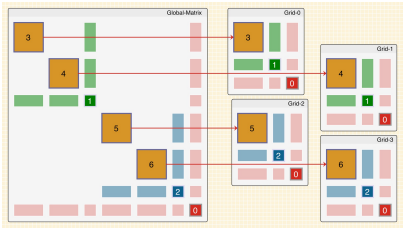


Fig. 1. Illustration of the 3D parallel SpLU algorithm with 4 process grids. Note that, here A_i refers to $A[i{:}, i{:}]$

```
typedef struct {
    MPI_Comm comm;        /* MPI communicator */
    superlu_scope_t rscp; /* row scope */
    superlu_scope_t cscp; /* column scope */
    superlu_scope_t zscp; /* scope in third dimension */
    gridinfo_t grid2d;    /* for using 2D functions */
    int iam;              /* my process number in this grid */
    int nprow;            /* number of process rows */
    int npcol;            /* number of process columns */
    int npdep;            /* number of replication factor in Z-dimension  */
    int rankorder;        /* = 0: Z-major ( default )
                           * = 1: XY-major (need set environment variable: SUPERLU_RANKORDER=XY)
                           */
} gridinfo3d_t;
```

Fig. 2. 3D process grid definition.

An example for calling the 3D algorithm to solve a sparse linear system is provided by the sample program `EXAMPLE/pddrive3d.c`. As an initialization step, the user needs to call

```
superlu_gridinit3d (MPI_COMM_WORLD, nprow, npcol, npdep, &grid);
```

The SuperLU routines use a separate process group—part of the `grid` structure, for the MPI communication. This prevents other communications from interfering with the MPI messages in SuperLU. In this example, a new process group for SuperLU is built upon the MPI default communicator `MPI_COMM_WORLD`. In general, it can be built upon any MPI communicator. Fig. 2 shows the C structure defining the 3D process grid.

2.1 The 3D Process layout and its performance impact

In SuperLU, a 3D process grid can be arranged in two formats: XY-major or Z-major, see Fig. 3. In XY-major format, processes with the same XY-coordinate and different Z-coordinate have consecutive global ranks. Consequently, when spawning multiple processes on a node, the spawned processes will have the same XY coordinate (except for cases where P_z is not a multiple of the number of processes spawned on the node). Alternatively, We can arrange the 3D process grid in Z-major format where processes with the same Z coordinate have consecutive global ranks. This is the default ordering in SuperLU.

The Z-major format can be better for performance as it keeps processes in a 2D grid closer. Hence it may provide higher bandwidth for 2D communication, typically the bottleneck in communication. On the other hand, the XY-major format can be helpful when using GPU acceleration. This can happen since the XY-major ordering will keep more GPUs active during ancestor factorizations. In some cases, e.g. sparse matrices from non-planar graphs, ancestor factorization can become compute dominant, and XY-major ordering helps by keeping more GPUs active. For example, on 16 Haswell nodes of the NERSC Cori Cray XC40, the Z-major ordering was .85-1.3× faster than the XY major ordering. Haswell compute nodes have dual-socket 16-core 2.3 GHz Intel Xeon E5-2698v3 CPUs. Note that this performance difference is system-dependent, depending on the hardware topology as well as the job scheduler policy of the parallel machine.

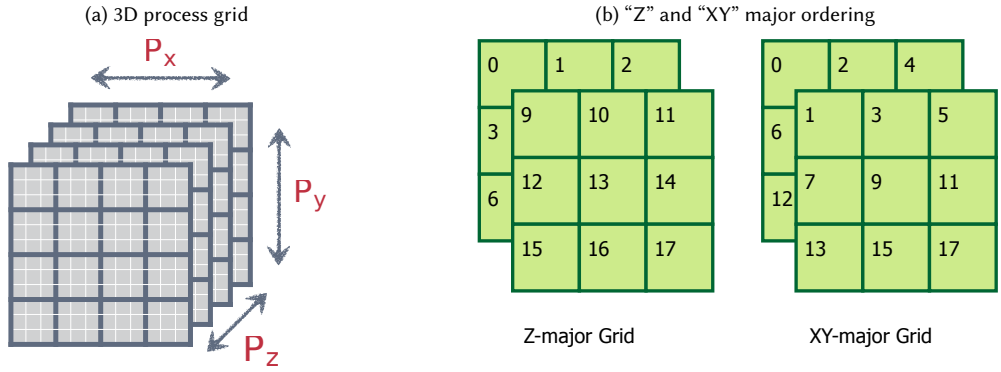


Fig. 3. A logical 3D process grid and process configuration for two types of process arrangements.

The driver routine is `pdgssvx3d`, with the following calling API:

```
void pdgssvx3d (superlu_dist_options_t *options, SuperMatrix *A,
                dScalePermstruct_t *ScalePermstruct,
                double B[], int ldb, int nrhs, gridinfo3d_t *grid,
                /* following are output */
                dLUstruct_t *LUstruct, dSOLVEstruct_t *SOLVEstruct,
                double *berr, SuperLUStat_t *stat, int *info);
```

The first argument is input, making the algorithm choices in the `options` structure. Section 6 describes all possible options and how to change each option. Table 3 tabulates the default values. The second argument is the input matrix A stored in the SuperMatrix metadata structure. The third argument is an input/output structure storing all the transformation vectors obtained from the preprocessing steps. The input right-hand sides are given by the `{B, ldb, nrhs}` tuple. The `grid` structure defines the 3D process grid, including the MPI communicator for this grid. All the precision-independent structures are defined in `superlu_defs.h`, and the precision-dependent structures are defined in `superlu_ddef.h` (for double precision). The sparse LU factors and the triangular solve structures are output. In addition the `berr` argument returns an array of componentwise relative backward error of each solution vector.

The sparse LU factorization progresses from leaf level $l = \log_2 P_z$ to the root level 0. The two main phases are local factorization and Ancestor-Reduction.

(1) *Local factorization.* In parallel and independently, every 2D process grid performs the $2D$ factorization of its locally owned submatrix of A. This is the same algorithm as the one before Version-7 []. The only difference is that each process grid will generate a partial Schur complement update, which will be summed up with the partial updates from the other process grids in the next phase.

(2) *Ancestor-Reduction.* After the factorization of level-i, we reduce the partial Schur complement of the ancestor nodes before factorizing the next level. In the i-th level's reduction, the receiver is the $k2^{l-i+1}$-th process grid and the sender is the $(2k+1)2^{l-i}$-th process grid, for some integer k. The process in the 2D grid which owns a block $A_{i,j}$ has the same (x,y) coordinate in both sender and receiver grids. So communication in the ancestor-reduction step is point-to-point pair-wise and takes places along the z-axis in the 3D process grid.

We analyzed the asymptotic improvements for planar graphs (e.g., those arising from 2D grid or mesh discretizations) and certain non-planar graphs (specifically for 3D grids and meshes). For a planar graph with n vertices, our algorithm reduces communication volume asymptotically in n by a factor of $O\left(\sqrt{\log n}\right)$ and latency by a factor of $O(\log n)$. For non-planar cases, our algorithm can reduce the per-process communication volume by 3× and latency by $O\left(n^{\frac{1}{3}}\right)$ times. In all cases, the extra memory needed to achieve these gains is a small constant factor of the L and U memory. We implemented our algorithm by extending the 2D data structure used in `SuperLU`. Our new 3D code achieves empirical speedups up to 27× for planar graphs and up to 3.3× for non-planar graphs over the baseline 2D `SuperLU` when run on 24,000 cores of a Cray XC30 (Edison at NERSC). Please see [11] for comprehensive performance tests with a variety of real-world sparse matrices.

Remark. The algorithm structure requires that the z-dimension of the 3D process grid P_z must be a power-of-two integer. There is no restriction on the shape of the 2D grid P_x and P_y. The rule of thumb is to define it as square as possible. When square grid is not possible, it is better to set the row dimension P_x slightly smaller than the column dimension P_y. For example, the following are good options for the 2D grid: 2x3, 2x4, 4x4, 4x8.

Inter-grid Load-balancing in the 3D SpLU Algorithm. The 3D algorithm provides two strategies for partitioning the elimination tree to balance the load between different 2D grids. The `SUPERLU_LBS` environment variable specifies which one to use.

- **Nested Dissection (ND)** strategy uses the partitioning provided by a nested dissection ordering. It works well for regular grids. The ND strategy can only be used when the elimination tree is binary, i.e., when the column order is also ND, and it cannot handle cases where the separator tree has nodes with more than two children.

- **Greedy Heuristic (GD)** strategy uses a greedy algorithm to divide one level of the elimination tree. It seeks to minimize the maximum load imbalance among the children of that node; if the imbalance in children is higher than 20%, it further subdivides the largest child until the imbalance falls below 20%. The GD strategy works well for arbitrary column ordering and can handle irregular graphs; however, if it is used on heavily imbalanced trees, it leads to bigger ancestor sizes and, therefore, more memory than ND. GD strategy is the default strategy unless `SUPERLU_LBS=ND` is specified.

In summary, two parameters are specific to the 3D SpLU algorithm:

- `superlu_rankorder` (`SUPERLU_RANKORDER`) defines the arrangement of the 3D process grid (default is Z-major);
- `superlu_lbs` (`SUPERLU_LBS`) defines the inter-grid load-balancing strategy (default is GD).

3 OPENMP INTRA-NODE PARALLELISM

SuperLU can use shared-memory parallelism in two ways. First, is by using the multithreaded BLAS library for linear-algebraic operations. This is independent of the implementation of SuperLU itself. Second, SuperLU can use OpenMP pragmas for explicitly parallelizing some of the computations.

OpenMP is portable across a wide variety of CPU architectures and operating systems. OpenMP offers a shared-memory programming model, which can be easier to use than a message-passing programming model. In this section, we discuss the advantages and limitations of using OpenMP, and offer some performance considerations.

Advantage of `OpenMP` *Parallelism.* We have empirically observed that hybrid programming with MPI+OpenMP often requires less memory than pure MPI. This is because OpenMP does not require additional memory for message passing buffers. In most cases, correctly tuned hybrid programming with MPI+OpenMP provides better performance than pure MPI.

Limitations of `OpenMP` *Parallelism.*

- The performance of OpenMP parallelism is often less predictable than pure MPI parallelism. This is due to non-determinism in the threading layer, the CPU hardware, and thread affinities.
- OpenMP threading may cause a significant slowdown if parameters are chosen incorrectly. Performance slowdown is often not entirely transparent. Slow-down can be due to false-sharing, NUMA effects, hyperthreading, incorrect or suboptimal thread affinities, or underlying threading libraries.
- Performance variation can be observed between compilers and threading libraries.
- Performance can be difficult to model or predict. Performance tuning may require some trial and error. Performance tuning is also dependent on the CPU architecture, the number of cores, and the underlying operating system.

3.1 OpenMP Performance tuning

Performance tuning of OpenMP applications is critical to get the desired performance. In this section, we list some of the most important environment variables that impact the performance of SuperLU and indicate how they should be set to achieve maximum performance.

- OMP_NUM_THREADS: controls the number of OpenMP threads. To avoid resource over-subscription, the product of MPI processes per node and OpenMP threads should be less than or equal to available physical cores.

- OMP_PLACES: Defines where OpenMP threads may run. Possible values are cores, threads, or socket. A generally good choice is "threads". You might want to test both "cores" and "threads" values on older processor models.
- OMP_PROC_BIND: The `OMP_PROC_BIND` directive determines whether threads may be moved between processors. When set to TRUE, OpenMP threads should not be moved; when FALSE they may be moved. A good setting of OMP_PROC_BIND is TRUE when OMP_PLACES is set and FALSE otherwise. You might want to test both "close" and "spread" values on some older processor models.
- OMP_NESTED: The number of levels of OpenMP parallelism desired. Typically, setting it to FALSE gives the best performance—in fact, setting it to TRUE may degrade performance due to over-subscription to threads.
- OMP_DYNAMIC: decides whether to dynamically change any of the numbers of thread/ threads groups for better performance. Typically, FALSE gives the best performance. Setting it to TRUE can lead to degraded performance.

In Figure 4, we show the impact of different OpenMP variables and hybrid MPI-OpenMP configurations on Cori Haswell nodes. Figure 4a shows the best performance achieved for different OpenMP and NUMA settings variables for purely threaded configurations. Figure 4b shows the performance for different MPI×OpenMP threads on four Haswell nodes of Cori. It should be noted that, hybrid configurations, i.e. configurations with more than one OpenMP threads per MPI process, tends to require far less memory for MPI's internal buffers[10]. In general, using 2-8 OpenMP threads per MPI process gives good performance across a wide range of matrices.

(a) Best performance for OMP variables (b) Performance w.r.t MPI× OMP threads

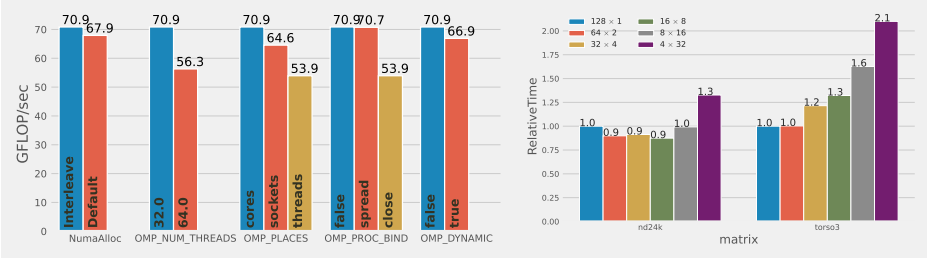


Fig. 4. OpenMP peformance tuning on Cori Haswell node.

The OpenMP API lets you control these variables programmatically. This becomes useful when the application and SuperLU require different OpenMP configurations. For best performance, the user can use our autotuner GPTune to tune these variables automatically, see Section 6.

4 GPU-ENABLED ROUTINES

In the current release, the SpLU factorization routines can offload certain computations to GPUs, which is mostly in each Schur complement update (SCU) step. We support both NVIDIA and AMD GPUs. We are actively developing code for the Intel GPUs. To enable GPU offloading, first a compile-time CMake variable needs to be defined: `-DTPL_ENABLE_CUDALIB=TRUE` (for NVIDIA GPU with CUDA programming) or `-DTPL_ENABLE_HIPLIB=TRUE` (for AMD GPU with HIP programming). Then, a runtime environment variable `SUPERLU_ACC_OFFLOAD` is used to control whether to use GPU or not. By default, `SUPERLU_ACC_OFFLOAD=1` is set. ('ACC' denotes ACCelerator.)

4.1 2D SpLU GPU algorithm and tuning parameters

The first sparse LU factorization algorithm capable of offloading the matrix-matrix multiplication to the GPU was published in [10]. The panel factorization and the Gather/Scatter operations are performed on the CPU. This algorithm has been available since SuperLU_DIST version 4.0 of the code (October 2014); however, many users are uncertain about using it correctly due to limited documentation. This paper provides a gentle introduction to GPU acceleration in SuperLU_DIST and its performance tuning.

Performing SCU requires some temporary storage to hold dense blocks. In an earlier algorithm, at each elimination step, the SCU is performed block by block. After performing updates on a block, the temporary storage can be reused for the next block. A conspicuous advantage of this approach is its memory efficiency, since the temporary storage required is bounded by maximum block size. The maximum block size is a tunable parameter that trades off local performance of matrix-matrix multiplication (GEMM) with inter-process parallelism. A typical setting for the maximum block size is 512 (or smaller). However, a noticeable disadvantage of this approach is that it fails to fully utilize the abundance of local fine-grained parallelism provided by GPUs because each GEMM is too small.

In [10], we modified the algorithm in the SCU step. At each step k, we first copy the individual blocks (in skyline storage) in the kth block row of U into a consecutive buffer $\mathtt{U}(k,:)$. The $L(:,k)$ is already in consecutive storage thanks to the supernodal structure. We then perform a single GEMM call to compute $V \leftarrow L(:,k) \times U(k,:)$. The matrix V is preallocated and the size of V needs to be sufficiently large to achieve close to peak GEMM performance. If the size of $L(:,k) \times U(k,:)$ is larger than V, then we partition the product into several large chunks such that each chunk requires temporary storage smaller than V. Given that modern GPUs have considerably more memory than earlier generations, this extra memory can enable a much faster runtime.

Now, each step of SCU consists of the following substeps:

(1) Gather sparse blocks $U(k,:)$ into a dense BLAS compliant buffer $\mathtt{U}(k,:)$;
(2) Call dense GEMM $V \leftarrow L(:,k) \times \mathtt{U}(k,:)$ (leading part on CPU, trailing part on GPU); and
(3) Scatter $V[]$ into the remaining $(k{+}1:N, k{+}1:N)$ sparse L and U blocks.

It should be noted that the Scatter operation can require indirect memory access, and therefore, it can be as expensive as the GEMM cost. The Gather operation, however, has a relatively low overhead compared to other steps involved. The GEMM offload algorithm tries to hide the overhead of Scatter and data transfer between the CPU and GPU via software pipelining. Here, we discuss the key algorithmic aspects of the GEMM offload algorithm:

- To keep both the CPU and GPU busy, we divide the $\mathtt{U}(k,:)$ into a CPU part and GPU part, so that the GEMM call is split into [cpu : gpu] parts: $L(:,k) \times \mathtt{U}(k,[cpu])$ and $L(:,k) \times \mathtt{U}(k,[gpu])$. To hide the data transfer cost, the algorithm further divides the GEMM into multiple streams. Each stream performs its own sequence of operations: CPU-to-GPU transfer, GEMM, and GPU-to-CPU transfer. Between these streams, these operations are asynchronous. The GPU matrix multiplication is also pipelined with the Scatter operation performed on the CPU.
- To offset the memory limitation on the GPU, we devised an algorithm to divide the SCU into smaller chunks as $\{[cpu:gpu]_1 \mid [cpu:gpu]_2 \mid \dots\}$. These chunks depend on the available memory on the GPU and can be sized by the user. A smaller chunk size will result in many iterations of the loop.

There are three environment variables that can be used to control the memory and performance in the GEMM offload algorithm:

- `superlu_n_gemm` (`SUPERLU_N_GEMM`) is the minimum value of the product *mnk* for a GEMM call to be worth offloading to GPU (default is 5000);
- `superlu_num_gpu_streams` (`SUPERLU_NUM_GPU_STREAMS`) defines the number of GPU streams to use (default is 8); and
- `superlu_max_buffer_size` (`SUPERLU_MAX_BUFFER_SIZE`) defines the maximum buffer size on GPU that can hold the GEMM output matrix V (default is 256M in floating-point words).

This simple GEMM offload algorithm has limited performance gains. We observed a roughly 2-3× speedup over the CPU-only code for a range of sparse matrices.

4.2 3D SpLU GPU algorithm and tuning parameters

We extend the 3D algorithm for heterogeneous architectures by adding the Highly Asynchronous Lazy Offload (Halo) algorithm for co-processor offload [9]. Compared to the GPU algorithm in the 2D code (Section 4.1), this algorithm also offloads the Scatter operations of each SCU step to the GPU (in addition to the GEMM call).

On 4096 nodes of a Cray XK7 (Titan at ORNL) with 32,768 CPU cores and 4096 Nvidia K20x GPUs, the 3D algorithm achieves empirical speedups up to 24× for planar graphs and 3.5× for non-planar graphs over the baseline 2D SuperLU with co-processor acceleration.

The performance related parameters are:

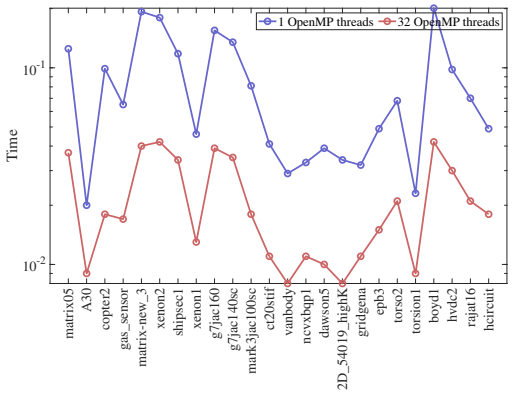
- `superlu_num_lookaheads` (`SUPERLU_NUM_LOOKAHEADS`), number of lookahead levels in the Schur-complement update (default is 10)
  In order to reduce the critical path of the sequence of panel factorizations, we devised a *software pipelining* method to overlap the panel factorization of the processes at step $k + 1$ with the Schur-complement update of the other processes at step k. When there are multiple remaining supernodes in the Schur complement, the lookahead window (i.e. pipeline depth) can be greater than 1 [12]. This environment variable defines the width of the lookahead window.
- `superlu_mpi_process_per_gpu` (`MPI_PROCESS_PER_GPU`) (default is 1).
  The Halo algorithm uses GPU memory based on its availability. To do this correctly, the SuperLU Halo algorithm needs to know how many MPI processes are running on a GPU, which can be difficult to determine on some systems. This environment variable can be set to inform SuperLU that there are N ranks on each GPU so that it can limit its memory usage of each GPU to 90% of available memory shared among all MPI processes, which will, in turn, limit the amount of memory used by each rank.

4.3 2D SpTRSV GPU algorithm

When the 2D grid has one MPI rank, SpTRSV in SuperLU is parallelized using OpenMP for shared-memory processors and CUDA or HIP for GPU. Both versions of the implementations are based on an asynchronous level-set traversal algorithm that distributes the computation workload across CPU threads and GPU threads/blocks [4]. The CPU implementation uses OpenMP taskloops and tasks for dynamic scheduling, while the GPU implementation relies on static scheduling. Fig. 5a shows the performance of SpTRSV (L and U solves) on 1 Cori Haswell node with 1 and 32 OpenMP threads with a number of matrices.

Fig. 5b shows the performance of L-solve using SuperLU (8 ORNL Summit IBM POWER9 CPU cores or 1 Summit V100 GPU) and cuSPARSE (1 Summit V100 GPU). The GPU SpTRSV in SuperLU consistently outperforms cuSPARSE

(a) L and U solve (in seconds) with 1 and 32 OpenMP threads on Cori Haswell



(b) L solve of SuperLU and cuSparse on CPU and GPU

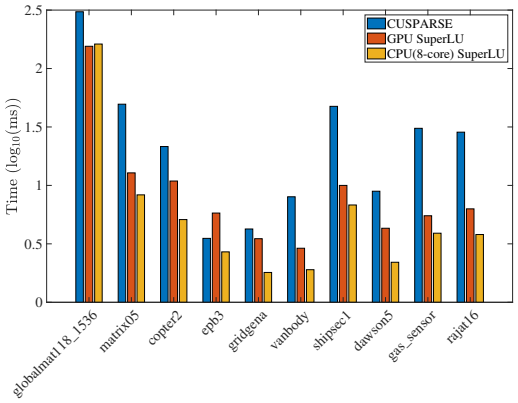


Fig. 5. Performance of SpTRSV with 1 MPI rank for a variety of sparse matrices.

and is comparable to the 8-core CPU results. Here we choose 8 CPU cores as there are on average 7 CPU cores per GPU on Summit, and 8 is the closest power of 2 number. Note that GPU performance of the U-solve requires major improvements and is not available in the current release. That said, we compare the performance of SpTRSV (both L and U solves) on one Summit node using three configurations: 1. (baseline) 1-core L solve and 1-core U solve, 2. (GPU) 1-GPU L solve and 1-core U solve, and 3. (GPU+OpenMP) 1-GPU L solve and 8-core U solve. The speedups comparing to the baseline configuration are shown in Table 1.

When the 2D grid has more than 1 MPI rank, SpTRSV also supports OpenMP parallelism with less speedups. In addition, the multi-GPU SpTRSV in SuperLU is under active development and will be available in future releases.

The number of OpenMP threads can be controlled by the environment variable OMP_NUM_THREADS, and the GPU SpTRSV can be turned on with the -DGPU_SOLVE compiler flag. *The user needs to make sure that only 1 MPI rank is used for the 2D grid when GPU SpTRSV is employed.*

	copter2	epb3	gridgena	vanbody	shipsec1	dawson5
GPU vs. Baseline	1.6	1.7	1.6	1.6	1.54	1.6
GPU+OpenMP vs. Baseline	5.3	5.7	5.3	4.4	4.1	5.2

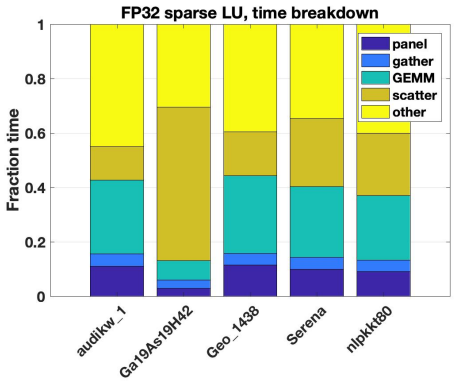
Table 1. Speedup of GPU SpTRSV compared with sequential CPU SpTRSV.

5 MIXED-PRECISION ROUTINES

SuperLU has long supported four distinct floating-point types: IEEE FP32 real and complex, IEEE FP64 real and complex. Furthermore, the library allows all four datatypes to be used together in the same application. This is often not supported by other libraries.

Recent hardware trends have motivated increased development of *mixed-precision* numerical libraries, mainly because hardware vendors have started designing special-purpose units for low precision arithmetic with higher performance. For direct linear solvers, a well understood method is to use lower precision to perform factorization (expensive) and

(a) Time breakdown of various steps of FP32 SpLU, "Other" mostly consists of MPI communication



(b) Comparison of SpLU time between the FP32 and FP64 versions

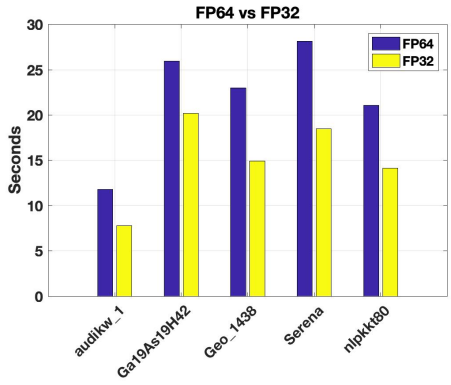


Fig. 6. Times of FP32 and FP64 SpLU for 5 matrices. All are measured on 10 nodes of ORNL Summit with 6 MPI ranks and 6 GPUs per node.

higher precision to perform iterative refinement (IR) to recover accuracy (cheap). For a typical sparse matrix resulting from the 3D finite difference discretization of a regular mesh, the SpLU needs $O\left(n^2\right)$ flops while each IR step needs only $O\left(n^{4/3}\right)$ flops (including sparse matrix-vector multiplication (SpMV) and SpTRSV).

For dense LU and QR factorizations, the benefit of lower precision format comes mainly from accelerated GEMM speed. But in the sparse case, the dimensions of the GEMM are generally smaller and of non-uniform size throughout factorization. Therefore, the speed gain from GEMM alone is limited. In addition to GEMM, a nontrivial cost is the Scatter operation. In Figure 6 we tally the time of various steps in SpLU and the time comparison of using FP32 vs. FP64. These are measured times for five real matrices of dimension on the order of 1 million. As can be seen, depending on the matrix sparsity structure, the fraction of time in GEMM varies, and usually is less than 50% (left plot). Because of this, the Tensor Core version of GEMM calls led to a less than 5% speedup for the whole SpLU. When comparing FP32 with the FP64 versions, we observed about 50% speedup with the FP32 version (right plot).

The simplest mixed precision sparse direct solver is to use lower precision for the expensive LU and QR factorizations, and higher precision in the cheap residual and solution update in IR. We recall the IR algorithm using three precisions in Algorithm 1 [2, 3]. This algorithm is already available as **x**GERFSX functions in LAPACK, where the input matrix is dense and so is LU. Potentially, the following three precisions may be used:

- ε_w is the working precision; it is used for the input data A and b, and output x.
- ε_x is the precision for the computed solution $x^{(i)}$. We require $\varepsilon_x \leq \varepsilon_w$, possibly $\varepsilon_x \leq \varepsilon_w^2$ if necessary for componentwise convergence.
- ε_r is the precision for the residuals $r^{(i)}$. We usually have $\varepsilon_r \leq \varepsilon_w^2$, i.e., at least twice the working precision.

Algorithm 1 converges with small normwise (or componentwise) error and error bound if the normwise (or componentwise) condition number of A does not exceed $1/(\gamma\varepsilon_w)$, where $\gamma \stackrel{\text{def}}{=} \sqrt{max_i(nnz(A(i,:))}$. Moreover, this IR procedure can return to the user both normwise and componentwise reliable error bounds. The error analysis in [2] should carry through to the sparse cases.

We implemented Algorithm 1 in SuperLU, using two precisions in IR:

Algorithm 1 Three-precisions Iterative Refinement (IR) for Direct Linear Solvers

1: Solve $Ax^{(1)} = b$ using the basic solution method (e.g., LU or QR) ▷ (ε_w)
2: $i = 1$
3: **repeat**
4: $r^{(i)} \leftarrow b - Ax^{(i)}$ ▷ (ε_r)
5: Solve $A\,dx^{(i+1)} = r^{(i)}$ using the basic solution method ▷ (ε_w)
6: Update $x^{(i+1)} \leftarrow x^{(i)} + dx^{(i+1)}$ ▷ (ε_x)
7: $i \leftarrow i + 1$
8: **until** $x^{(i)}$ is "accurate enough"
9: **return** $x^{(i)}$ and error bounds

(a) audikw_1 convergence history (b) Ga19As19H2 convergence history

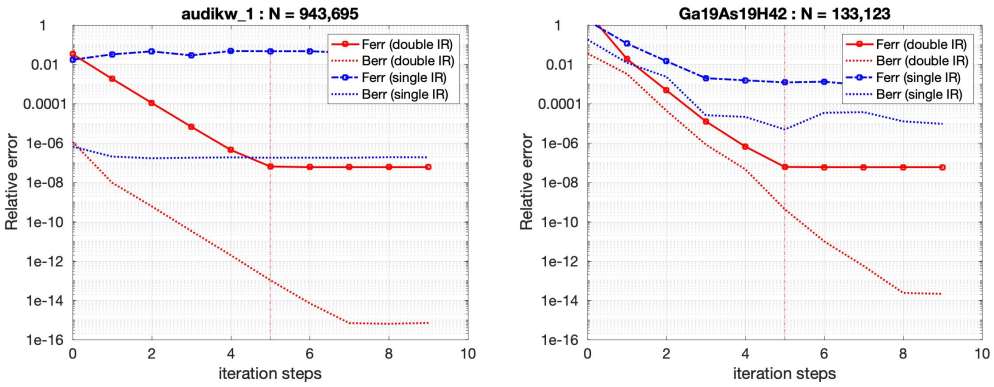


Fig. 7. Convergence history of Algorithm 1 when applied to two sparse linear systems. The vertical line in each plot corresponds to the IR steps taken when our stopping criteria are satisfied.

- $\varepsilon_w = 2^{-24}$ (IEEE-754 single precision), $\varepsilon_x = \varepsilon_r = 2^{-53}$ (IEEE-754 double precision)

In Figure 7, the left two plots show the convergence history of two systems, in both normwise foward and backward errors, F_{err} and B_{err}, respectively (defined below). We perform two experiments: one using single precision IR, the other using double precision IR. As can be seen, single precision IR does not reduce much F_{err}, while double precision *IR* delivers F_{err} close to ε_w. The IR time is usually under 10% of the factorization time. Overall, the mixed-precision speed is still faster than using pure FP64, see Table 2.

Table 2. Parallel solution time (seconds) (including SpLU and IR): purely double precision, purely single precision, and mixed precision (FP32 SpLU + FP64 IR). ORNL Summit using up to 8 nodes, each node uses 6 CPU Cores (C) and 6 GPUs (G).

Matrix	Precision	6 C+G	24 C+G	48 C+G	Matrix	Precision	6 C+G	24 C+G	48 C+G
audikw_1	Double	65.9	21.1	18.9	Ga19As19H42	Double	310.9	62.4	34.3
	Single	45.8	13.8	10.5		Single	258.1	48.2	25.8
	Mixed	49.2	13.9	11.4		Mixed	262.8	48.8	26.1

The 2D driver routine for this mixed-precision approach is `psgssvx_d2`, where the suffix "d2" denotes that the intermediate x vector and r vector internal to the IR routine are carried in double precision. The API of this routine is as follows. To use double precision IR, we need to set: `options->IterRefine = SLU_DOUBLE`.

```
void psgssvx_d2(superlu_dist_options_t *options, SuperMatrix *A,
                sScalePermstruct_t *ScalePermstruct,
                float B[], int ldb, int nrhs, gridinfo_t *grid,
                sLUstruct_t *LUstruct, sSOLVEstruct_t *SOLVEstruct,
                float *err_bounds, SuperLUStat_t *stat, int *info)
```

The only difference from the one-precision routine `psgssvx` is the output array `err_bounds[]`. For each right-hand side, we return the following three quantities:

- `err_bounds[0]`: normwise forward error bound: $B_{norm} = \max\left(\frac{\|dx^{(i+1)}\|_\infty/\|x^{(i)}\|_\infty}{1-\rho_{max}}, \gamma\varepsilon_w\right) \approx \frac{\|x^{(i)}-x\|_\infty}{\|x\|_\infty}$
  where, $\rho_{\max} \stackrel{\text{def}}{=} \max_{j\le i} \frac{\|dx^{(j+1)}\|_\infty}{\|dx^{(j)}\|_\infty}$ is the estimate of the convergence rate of $x^{(i)}$.
- `err_bounds[1]`: componentwise forward error bound: $\max\left(\frac{\|C^{-1}dx^{(i)}\|_\infty}{1-\hat{\rho}_{max}}, \gamma\varepsilon_w\right) \approx \max_k \left|\frac{x_k^{(i)}-x_k}{x_k}\right|$
  where, $C = diag(x)$, $\hat{\rho}_{\max} = \max_{j\le i} \frac{\|Cdx^{(j+1)}\|_\infty}{\|Cdx^{(j)}\|_\infty}$ is the estimate of the convergence rate of $C^{-1}x^{(i)}$
- `err_bounds[2]`: componentwise backward error: $\max_k \left(\frac{|b-Ax^{(i)}|_k}{(|A||x^{(i)}|+|b|)_k}\right)$

The detailed error analysis can be found in [2].

6 SUMMARY OF PARAMETERS, ENVIRONMENT VARIABLES AND PERFORMANCE IMPACT

Throughout all phases of the solution process, a number of algorithm parameters can influence the solver's performance. These parameters can be modified by the user. For each user-callable routine, the first argument is usually an input "`options`" argument, which points to the structure containing a number of algorithm choices. These choices are determined at compile time. The second column in Table 3 lists the named fields in the `options` argument. The fourth column lists all the possible values and their corresponding C's enumerated constant names. The user should call the following routine to set up the default values.

```
superlu_dist_options_t options;
set_default_options_dist(&options);
```

After setting the defaults, the user can modify each default, for example:

```
options.RowPerm = LargeDiag_HWPM;
```

For a subset of these parameters, the user can change them at runtime via environment variables. These parameters are listed in the third column in Table 3. At various places of the code, an environment inquiry function SRC/sp_ienv.c is called to retrieve the values of the environment variables.

Two algorithm blocking parameters can be changed at runtime: `SUPERLU_MAXSUP` and `SUPERLU_RELAX`. `SUPERLU_MAXSUP` sets the maximum size of a supernode. That is, if the number of columns in a supernode exceeds this value, we will split this supernode into two supernodes. Setting this parameter to a large value results in larger blocks and generally better performance for threaded and GPU GEMM. Increasing it limits the number of available parallel tasks across MPI processes. Figure 8a illustrates how performance, as measured in Gflops, varies with `SUPERLU_MAXSUP` on a single node of Cori Haswell when using 32 OpenMP threads. For smaller matrices, such as this one (torso3), performance is near its peak when `SUPERLU_MAXSUP` equals 128, which is over 50× faster than when this value is set to 4. However, above this value, the performance starts to taper off.

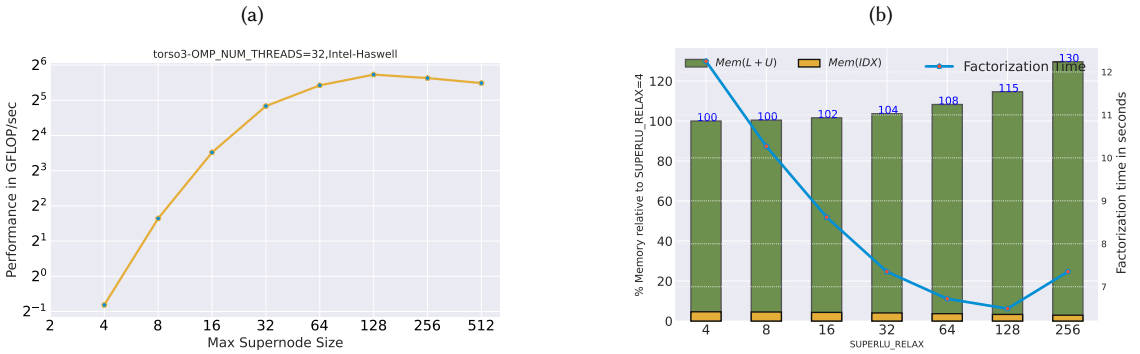


Fig. 8. Impact of maximum supernode size (SUPERLU_MAXSUP) and supernodal relaxation (SUPERLU_RELAX) on performance and memory. The machine is NERSC Cori Haswell node. The matrix is torso3 from SuiteSparse.

SUPERLU_RELAX is a relaxation parameter: if the number of nodes (columns) in a subtree of the elimination tree is less than this value, this subtree is treated as one supernode, regardless of the row structures. That means, we pad explicit zeros to enforce that all the columns within this relaxed supernode have the same row structure. The advantage of this padding is to mitigate many small supernodes at the bottom of the elimination tree. On the other hand, a large value of SUPERLU_RELAX may introduce too many zeros which in turn propagate to the ancestors of the elimination tree, resulting in a large number of fill-ins in the L and U factors. Figure 8b shows the impact of this parameter on the memory use (left axis) and factorization time. A value of 32 or 64 represents a good tradeoff between memory and time.

The optimal settings of these parameters are matrix-dependent and hardware-dependent. Additionally, several other parameters and environment variables listed in Table 3 are performance critical for the 2D and 3D, CPU and GPU algorithms described in Sections 2, 4.1 and 4.2. It is a daunting task for manual tuning to find the optimal setting of these parameters. Now in Sections 6.1 - 6.3 we show how an autotuner can significantly simplify this task. Here we leverage an autotuner called GPTune [8] to tune the performance (time and memory) of SpLU. We consider two example matrices from the Suitesparse matrix collection, G3_circuit from circuit simulation and H2O from quantum chemistry simulation. For all the experiments, we consider a two-objective tuning scenario and generate a Pareto front from the samples demonstrating the tradeoff between memory and CPU requirement of SpLU.

6.1 3D CPU SpLU parameter tuning

For the 3D CPU SpLU algorithm (2), we use 16 NERSC Cori Haswell nodes and the G3_circuit matrix. The number of OpenMP threads is set to 1, so there are a total of $P_x P_y P_z = 512$ MPI ranks. We consider the following tuning parameters [SUPERLU_MAXSUP, SUPERLU_RELAX, num_lookaheads, P_x, P_z]. We set up GPTune to generate 100 samples. All samples and the Pareto front are plotted in Fig. 9a. The samples on the Pareto front and the default one are shown in Table 4, one can clearly see that by reducing the computation granularity (SUPERLU_MAXSUP, SUPERLU_RELAX) and increasing P_z, one can significantly improve the SpLU time while using slightly more memory.

6.2 2D GPU SpLU parameter tuning

For the 2D GPU SpLU algorithm (4.1), we use 2 NERSC Perlmutter GPU compute nodes with 4 MPI ranks per node and the H2O matrix. Perlmutter GPU compute nodes consist of a single 64-core 2.45 GHz AMD EPYC 7763 CPU and four

Table 3. List of algorithm parameters used in various phases of the linear solver. The third column lists the environment variables that can be reset at runtime. parameters must be set in the `options{}` structure input to a driver routine.

phase	`options` **(compile-time)**	env variables **(runtime)**	values (enum constants)	in 2D or 3D algo.
Pre-process	Equil		NO, YES (default)	2d, 3d
	RowPerm		0: NOROWPERM	2d, 3d
			1: `LargeDiag_MC64` (default)	2d, 3d
			2: `LargeDiag_HWPM`	2d, 3d
			3: `MY_PERMR`	2d, 3d
	ColPerm		0: NATURAL	2d, 3d
			1: `MMD_ATA`	2d, 3d
			2: `MMD_AT_PLUS_A`	2d, 3d
			3: COLAMD	2d, 3d
			4: `METIS_AT_PLUS_A` (default)	2d, 3d
			5: PARMETIS	2d, 3d
			6: ZOLTAN	2d, 3d
			7: `MY_PERMC`	2d, 3d
	ParSymbFact		YES, NO (default)	2d, 3d
SpLU	ReplaceTinyPivot		YES, NO (default)	2d, 3d
	Algo3d		YES, NO (default)	3d
	DiagInv		YES, NO (default)	2d
	num_lookaheads	`SUPERLU_NUM_LOOKAHEADS`	default 10	2d, 3d (Section 4.2)
	superlu_maxsup	`SUPERLU_MAXSUP`	default 256	2d, 3d (Section 6)
	superlu_relax	`SUPERLU_RELAX`	default 60	2d, 3d
	superlu_rankorder	`SUPERLU_RANKORDER`	default Z-major	3d (Section 2.1)
	superlu_lbs	`SUPERLU_LBS`	default GD	3d (Section 2.1)
	superlu_acc_offload	`SUPERLU_ACC_OFFLOAD`	0, 1 (default)	2d, 3d (Section 4)
	superlu_n_gemm	`SUPERLU_N_GEMM`	default 5000	2d (Section 4.1)
	superlu_max_buffer_size	`SUPERLU_MAX_BUFFER_SIZE`	default 250M words	2d, 3d (Section 4.1)
	superlu_num_gpu_streams	`SUPERLU_NUM_GPU_STREAMS`	default 8	2d (Section 4.1)
	superlu_mpi_process_per_gpu	`SUPERLU_MPI_PROCESS_PER_GPU`	default 1	3d (Section 4.2)
		`OMP_NUM_THREADS`	default system dependent	2d, 3d (Section 3)
		`OMP_PLACES`	undefined	2d, 3d
		`OMP_PROC_BIND`	undefined	2d, 3d
		`OMP_NESTED`	undefined	2d, 3d
		`OMP_DYNAMIC`	undefined	2d, 3d
SpTRSV	IterRefine (Section 5)		0: NOREFINE (default)	2d, 3d
			1: `SLU_SINGLE`	
			2: `SLU_DOUBLE`	
Others	PrintStat		NO, YES (default)	2d, 3d

NVIDIA A100 (40GB HBM2) GPUs. The number of OpenMP threads is set to 16. We consider the following tuning parameters [ColPerm, `SUPERLU_MAXSUP`, `SUPERLU_RELAX`, `SUPERLU_N_GEMM` , `SUPERLU_MAX_BUFFER_SIZE`, P_x]. We set up GPTune to generate 100 samples. All samples and the Pareto front are plotted in Fig. 9b. The samples on the Pareto front and the default one are shown in Table 5. Compared to the default configuration, both the time and memory can be significantly improved by increasing the computation granularity (larger `SUPERLU_MAXSUP`, `SUPERLU_RELAX`). Also, less GPU offload (larger `SUPERLU_N_GEMM`) leads to better performance.

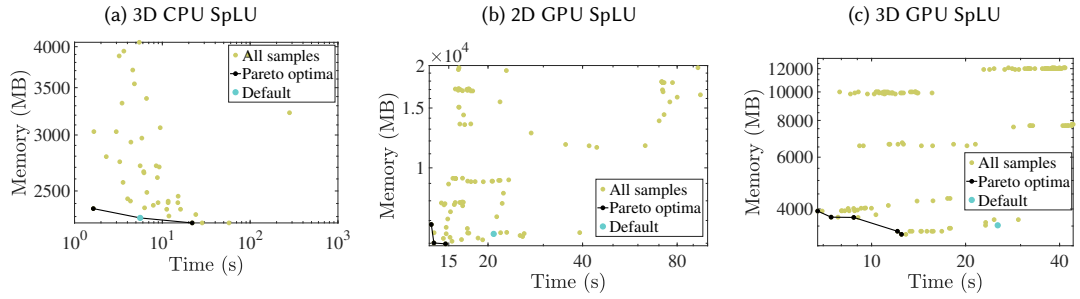


Fig. 9. Samples generated by GPTune for the three tuning experiments. Only valid samples are plotted.

6.3 3D GPU SpLU parameter tuning

For the 3D GPU SpLU algorithm in Section 4.2, we use 2 NERSC Perlmutter GPU nodes with 4 MPI ranks per node and the H2O matrix. The number of OpenMP threads is set to 16, and $P_x P_y P_z = 8$. We consider the following tuning parameters [ColPerm, SUPERLU_MAXSUP, SUPERLU_RELAX SUPERLU_MAX_BUFFER_SIZE, P_x, P_z]. We set up GPTune to generate 200 samples. All samples and the Pareto front are plotted in Fig. 9c. The samples on the Pareto front and the default one are shown in Table 6. Compared to the default configuration, both the time and memory utilization can be significantly improved by increasing the computation granularity and decreasing GPU buffer sizes. ColPerm='4' (METIS_AT_PLUS_A) is always preferable in terms of memory usage. The effects of P_x and P_z are insignificant as only 8 MPI ranks are used.

	SUPERLU_MAXSUP	SUPERLU_RELAX	num_lookaheads	P_x	P_z	Time (s)	Memory (MB)
Default	256	60	10	16	1	5.6	2290
Tuned	31	25	17	16	1	21.9	2253
Tuned	53	35	7	4	4	1.64	2360

Table 4. Default and optimal samples returned by GPTune for the 3D CPU SpLU algorithm. Note that P_y is derived by $P_y = 512/(P_x P_z)$, as the total MPI count is fixed at 512.

	ColPerm	SUPERLU_MAXSUP	SUPERLU_RELAX	SUPERLU_N_GEMM	SUPERLU_MAX_BUFFER_SIZE	P_x	Time (s)	Memory (MB)
Default	'4'	256	60	1000	2.5E8	4	20.8	6393
Tuned	'4'	154	154	2048	2.68E8	2	13.5	6011
Tuned	'4'	345	198	262144	6.7E7	2	13.2	6813
Tuned	'4'	124	110	8192	1.3E8	2	14.6	5976

Table 5. Default and optimal samples returned by GPTune for the 2D GPU SpLU algorithm. Note that P_y is derived by $P_y = 8/P_x$, as the total MPI count is fixed at 8.

7 FORTRAN 90 INTERFACE

In the FORTRAN/ directory, there are Fortran 90 module files that implement the wrappers for Fortran programs to access the full functionality of the C functions in SuperLU. The design is based on object-oriented programming concept:

	ColPerm	SUPERLU_MAXSUP	SUPERLU_RELAX	SUPERLU_MAX_BUFFER_SIZE	P_x	P_z	Time (s)	Memory (MB)
Default	'4'	256	60	2.5E8	4	1	25.3	3520
Tuned	'4'	176	143	1.34E8	2	1	12.1	3360
Tuned	'4'	327	182	1.34E8	4	2	7.4	3752
Tuned	'4'	610	200	3.34E7	8	1	12.5	3280
Tuned	'4'	404	187	3.34E7	1	2	8.76	3744
Tuned	'4'	232	199	3.34E7	4	2	6.7	3936

Table 6. Default and optimal samples returned by GPTune for the 3D GPU SpLU algorithm. Note that P_z is calculated from P_x and P_y as the total MPI count is fixed.

define *opaque objects* in the C space, which are accessed via *handles* from the Fortran space. All SuperLU objects (e.g., process grid, LU structure) are opaque from the Fortran side. They are allocated, deallocated and operated at the C side. For each C object, we define a Fortran handle in Fortran's user space, which points to the C object and implements the access methods to manipulate the object. All handles are 64-bit integer type. For example, consider creating a 3D process grid. The following code snippet shows what are involved from the Fortran and C sides.

- Fortran side

```
/* Declare handle: */
integer(64)::f_grid3d
/* Call C wrapper routine to create 3D grid pointed to by "f_grid3d": */
call f_superlu_gridinit3d(MPI_COMM_WORLD, nprow, npcol, npdep, f_grid3d)
```

- C side

```
 /* Fortran-to-C interface routine: */
void f_superlu_gridinit3d(int *MPIcomm, int *nprow, int *npcol,int *npdep, int64_t *f_grid3d)
 {
     /* Actual call to C routine to create grid3d structture in *grid3d{} */
  superlu_gridinit3d(f2c_comm(MPIcomm),*nprow, *npcol, *npdep, (gridinfo3d_t *) *f_grid3d);
 }
```

Here, the Fortran handle `f_grid3d` essentially acts as a 64-bit pointer pointing to the internal 3D grid structure, which is created by the C routine `superlu_gridinit3d()`. This structure (see Fig. 2) sits in the C space and is invisible from the Fortran side.

For all the user-callable C functions, we provide the corresponding Fortran-to-C interface functions, so that the Fortran program can access all the C functionality. These interface routines are implemented in the files `superlu_c2f_wrap.c` (precision-independent) and `superlu_c2f_dwrap.c` (double precision). The Fortran-to-C name mangling is handled by CMake through the header file `SRC/superlu_FCnames.h`. The module file `superlupara.f90` defines all the constants matching the enum constants defined in the C side (see Table 3). The module file `superlu_mod.f90` implements all the access methods (set/get) for the Fortran side to access the objects created in the C user space.

8 INSTALLATION WITH CMAKE OR SPACK

8.1 Dependent external libraries

One can have a bare minimum installation of SuperLU without any external dependencies, although the following external libraries are useful for high performance: BLAS, (Par)METIS (sparsity-preserving ordering), CombBLAS (parallel numerical pivoting) and LAPACK (for inversion of dense diagonal block).

8.2 CMake installation

You will need to create a build tree from which to invoke CMake. The following describes how to define the external libraries.

BLAS (highly recommended)

If you have a fast BLAS library on your machine, you can link it using the following CMake definition:

`-DTPL_BLAS_LIBRARIES="<BLAS library name>"`

Otherwise, the `CBLAS/` subdirectory contains the part of the C BLAS (single threaded) needed by SuperLU, but it is not optimized for performance. You can compile and use this internal BLAS with the following CMake definition:

`-DTPL_ENABLE_INTERNAL_BLASLIB=ON`

ParMETIS (highly recommended)

http://glaros.dtc.umn.edu/gkhome/fetch/sw/parmetis/parmetis-4.0.3.tar.gz

You can install ParMETIS and define the two environment variables as follows:

```
export PARMETIS_ROOT=<Prefix directory of the ParMETIS installation>
export PARMETIS_BUILD_DIR=${PARMETIS_ROOT}/build/Linux-x86_64
```

Note that by default, we use serial METIS as the sparsity-preserving ordering, which is available in the ParMETIS package. You can disable ParMETIS during installation with the following CMake definition: `-DTPL_ENABLE_PARMETISLIB=OFF`. In this case, the default ordering is set to be `MMD_AT_PLUS_A`.

See Table 3 for all the possible ColPerm options.

In order to use parallel symbolic factorization function, you need to use ParMETIS ordering.

LAPACK (highly recommended)

In the triangular solve routine, we may use LAPACK to explicitly invert the dense diagonal block to improve the performance. You can use it with the following CMake option:

`-DTPL_ENABLE_LAPACKLIB=ON`

CombBLAS (optional)

https://people.eecs.berkeley.edu/~aydin/CombBLAS/html/index.html

In order to use parallel weighted matching HWPM (Heavy Weight Perfect Matching) for numerical pre-pivoting [1], you need to install CombBLAS and define the environment variables:

```
export COMBBLAS_ROOT=<Prefix directory of the CombBLAS installation>
export COMBBLAS_BUILD_DIR=${COMBBLAS_ROOT}/_build
```

Then, install with the CMake option:

`-DTPL_ENABLE_COMBBLASLIB=ON`

Use GPU

You can enable (NVIDIA) GPU with CUDA with the following CMake option:

```
-DTPL_ENABLE_CUDALIB=TRUE
```

You can enable (AMD) GPU with HIP with the following CMake option:

```
-DTPL_ENABLE_HIPLIB=TRUE
```

For a simple installation with default settings:

```
mkdir build ; cd build;
cmake .. \
  -DTPL_PARMETIS_INCLUDE_DIRS="${PARMETIS_ROOT}/include;\
       ${PARMETIS_ROOT}/metis/include" \
  -DTPL_PARMETIS_LIBRARIES="${PARMETIS_BUILD_DIR}/libparmetis/libparmetis.a;\
       ${PARMETIS_BUILD_DIR}/libmetis/libmetis.a" \
```

There are a number of example build scripts in the `example_script/` directory, with filenames `run_cmake_build_*.sh` that target various machines.

To actually build (compile), type: 'make'.

To install the libraries, type: 'make install'.

To run the installation tests, type: 'test'. (The outputs are in file: 'build/Testing/Temporary/LastTest.log') or, 'ctest -D Experimental', or, 'ctest -D Nightly'.

Note that the parallel execution in `ctest` is invoked by the "mpiexec" command, which is from the MPICH environment. If your MPI is not MPICH/mpiexec based, the test execution may fail. You can pass the definition option `-DMPIEXEC_EXECUTABLE` to CMake. For example on Cori at NERSC, you will need the following: `cmake .. -DMPIEXEC_EXECUTABLE=/usr/bi`

Or, you can always go to `TEST/` directory to perform testing manually.

The following list summarizes the commonly used CMake definitions. In each case, the first choice is the default setting. After running a 'cmake' installation, a configuration header file is generated in `SRC/superlu_dist_config.h`, which contains the key CPP definitions used throughout the code.

```
-DTPL_ENABLE_INTERNAL_BLASLIB=OFF | ON
-DTPL_ENABLE_PARMETISLIB=ON | OFF
-DTPL_ENABLE_LAPACKLIB=OFF | ON
-DTPL_ENABLE_COMBBLASLIB=OFF | ON
-DTPL_ENABLE_CUDALIB=OFF | ON
-DCMAKE_CUDA_FLAGS=<...>
-DTPL_ENABLE_HIPLIB=OFF | ON
-DHIP_HIPCC_FLAGS=<...>
-Denable_complex16=OFF | ON        (double-complex datatype)
-Denable_single=OFF | ON           (single precision real datatype)
-DXSDK_INDEX_SIZE=32 | 64          (integer size for indexing)
-DBUILD_SHARED_LIBS= OFF | ON
-DCMAKE_INSTALL_PREFIX=<...>
-DCMAKE_C_COMPILER=<MPI C compiler>
```

```
-DCMAKE_C_FLAGS=<...>
-DCMAKE_CXX_COMPILER=<MPI C++ compiler>
-DCMAKE_CXX_FLAGS=<...>
-DXSDK_ENABLE_Fortran=OFF | ON
-DCMAKE_Fortran_COMPILER=<MPI F90 compiler>
```

8.3 Spack installation

Spack installation of SuperLU_DIST is a fully automated process. Assume that the develop branch of Spack (https://github.com/spack/spack) is used. You can find available compilers via: `spack compilers`. In the following, let's assume the available compiler is gcc@9.1.0. The installation supports the following variants:

Use 64-bit integer

You can enable 64-bit integer with:

```
spack install superlu-dist@master+int64%gcc@9.1.0
```

Use GPU

You can enable (NVIDIA or AMD) GPUs with:

```
spack install superlu-dist@master+cuda%gcc@9.1.0
spack install superlu-dist@master+rocm%gcc@9.1.0
```

Test installation

You can run a few smoke tests of the spack installation via

```
spack test run superlu-dist@master    (pick the appropriate installation if multiple variants available)
```

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