PyRSB: Portable Performance on Multithreaded Sparse BLAS Operations

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Abstract—This article introduces PyRSB, a Python interface to the LIBRSB library. LIBRSB is a portable performance library offering so-called Sparse BLAS (Sparse Basic Linear Algebra Subprograms) operations for modern multicore CPUs. It is based on the Recursive Sparse Blocks (RSB) format, which is particularly well suited for matrices of large dimensions. PyRSB allows LIBRSB usage with an interface styled after that of SciPy’s sparse matrix classes, and offers the extra benefit of exploiting multicore parallelism. This article introduces the conceptsbehind the RSB format and LIBRSB, and illustrates usage of PyRSB. It concludes with a user-oriented overview of speedup advantage of rsb_matrix over scipy.sparse.csr_matrix running general sparse matrix-matrix multiplication on a modern shared-memory computer.

Introduction
Sparse linear systems solving is one of the most widespread problems in numerical scientific computing. The key to timely solution of sparse linear systems by means of iterative methods resides in fast multiplication of sparse matrices by dense matrices. More precisely, we mean the update: \[ C = C + \alpha AB \] (at the element level, equivalent to \[ C_{i,k} \leftarrow C_{i,k} + \alpha A_{i,j}B_{j,k} \]) where \( B \) and \( C \) are dense rectangular matrices, \( A \) is a sparse rectangular matrix, and \( \alpha \) a scalar. If \( B \) and \( C \) are vectors (i.e. have one column only) we call this operation SpMV (short for Sparse Matrix-Vector product); otherwise SpMM (short for Sparse Matrix-Matrix product).

PyRSB [PYRSB] is a package suited for problems where: i) much of the time is spent in SpMV or SpMM, ii) one wants to exploit multicore hardware, and iii) sparse matrices are large (i.e. occupy a significant fraction of a computer’s memory).

The PyRSB interface is styled after that of the sparse matrix classes in SciPy [Virtanen20]. Unlike certain similarly scoped projects ([Abbasi18], [PyDataSparse]), PyRSB is restricted to 2-dimensional matrices only.

Background: LIBRSB
LIBRSB [LIBRSB] is a LGPLv3-licensed library written primarily to speed up solution of large sparse linear systems using iterative methods on shared-memory CPUs. It takes its name from the Recursive Sparse Blocks (RSB) data layout it uses. The RSB format is geared to execute multithreaded SpMV and SpMM as fast as possible. LIBRSB is not a solver library, but provides most of the functionality required to build one. It is usable via several languages: C, C++, Fortran, GNU Octave [SPARSERSB], and now Python, too. Bindings for the Julia language have been authored by D.C. Jones [RSB_JL].

LIBRSB has been reportedly used for: Plasma physics [Stegmeir15], sub-atomic physics [Klos18], data classification [Lee15], eigenvalue computations [Wu16], meteorology [Browne15T], and data assimilation [Browne15M].

It is available in pre-compiled form in popular GNU/Linux distributions like Ubuntu [UBUNTU], Debian [DEBIAN], OpenSUSE [OPENSUSE]; this is the best way to have a LIBRSB installation to familiarize with PyRSB. However, pre-compiled packages will likely miss compile-time optimizations. For this reason, the best performance will be obtained by building on the target computer. This can be achieved using one of the several source-based code distributions offering LIBRSB, like Spack [SPACK], or EasyBuild [EASYBUILD], or GIIX [GIIX]. LIBRSB has minimal dependencies, so even building by hand is trivial.

PyRSB [PYRSB] is a thin wrapper around LIBRSB based on Cython [Behnel11]. It aims at bringing native LIBRSB performance and most of its functionality at minimal overhead.

Basic Sparse Matrix Formats
The explicit (dense) way to represent any numerical matrix is to list each of its numerical entries, whatever their value. This can be done in Python using e.g. scipy.matrix.

```
>>> from scipy import matrix
>>> A = matrix([[11., 12.], [ 0., 22.]])
>>> A.shape
tuple (2, 2)
```

This matrix has two rows and two columns; it contains three non-zero elements and one zero element in the second row. Many scientific problems give rise to systems of linear equations with many (e.g. millions) of unknowns, but relatively few coefficients which are different than zero (e.g. <1%) in their matrix-form representation. It is usually the case that representing these zeroes in memory and processing them in linear algebraic operations does not impact the results, but takes compute time nevertheless. In these cases the matrix is usually referred as sparse, and appropriate sparse data structures and algorithms are sought.

The most straightforward sparse data structure for a numeric matrix is one listing each of the non-zero elements, along with its coordinate location, by means of three arrays. This is called COO.
It’s one of the classes in scipy.sparse; see the following listing, whose output also illustrates conversion to dense:

```python
>>> from scipy.sparse import coo_matrix
>>> V = [11.0, 12.0, 22.0]
>>> I = [0, 0, 1]
>>> J = [0, 1, 1]
>>> A = coo_matrix((V, (I, J)))
<2x2 sparse matrix of type '<class 'numpy.float64'>'
  with 3 stored elements in COOrdinate format>
>>> B = A.todense()
>>> B
matrix([[11., 12.],
        [ 0., 22.]])
```

Even if yielding the same results, the algorithms beneath differ considerably. To carry out the \( C_{jk} \leftarrow C_{jk} + \alpha A_{ik} B_{jk} \) updates the scipy.coo_matrix implementation will get the matrix coefficients from the \( V \) array, its coordinates from the \( I \) and \( J \) arrays, and use those (notice the indirect access) to address the operand’s elements.

In contrast to that, a dense implementation like scipy.matrix does not use any index array: the location of each numerical value (including zeroes) is in direct relation with its row and column indices.

Beyond the \( V, I, J \) arrays, COO has no extra structure. COO serves well as an exchange format, and allows expressing many operations.

The second most straightforward format is CSR (Compressed Sparse Rows). In CSR, non-zero matrix elements and their column indices are laid consecutively row after row, in the respective arrays \( V \) and \( J \). Differently than in COO, the row index information is compressed in a row pointers array \( P \), dimensioned one plus rows count. For each row index \( i, P[i] \) is the count of non-zero elements (nonzeros) on preceding rows. The count of nonzeros at each row \( i \) is therefore \( P[i+1] - P[i] \), with \( P[0]==0 \). SciPy offers CSR matrices via scipy.csr_matrix:

```python
>>> import scipy
>>> from scipy.sparse import csr_matrix
>>> V = [11.0, 12.0, 22.0]
>>> P = [0, 2, 3]
>>> J = [0, 1, 1]
>>> A = csr_matrix((V, (I, J)))
>>> A.todense()
array([[11., 12.],
       [ 0., 22.]])
```

CSR’s \( P \) array allows direct access of each sparse row. This helps in expressing row-oriented operations. In the case of the SpMV operation, CSR encourages accumulation of partial results on a per-row basis.

Notice that indices’ occupation with COO is strictly proportional to the non-zeroes count of a matrix; in the case of CSR, only the \( J \) indices array. Consequently, a matrix with more nonzeros than rows (as usual for most problems) will use less index space if represented by CSR. But in the case of a particularly sparse block of such a matrix, that may not be necessarily true. These considerations back the usage choice of COO and CSR within the RSB layout, described in the following section.

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**From RSB to PyRSB**

Recursive Sparse Blocks in a Nutshell

The Recursive Sparse Blocks (RSB) format in LIBRSB [Martono14] represents sparse matrices by exploiting a hierarchical data structure. The matrix is recursively subdivided in halves until the individual submatrices (also: sparse blocks or simply blocks) occupy approximately the amount of memory contained in the CPU caches. Each submatrix is then assigned the most appropriate format: COO if very sparse, CSR otherwise.

Any operation on an RSB matrix is effectively a polyalgorithm, i.e. each block’s contribution will use an algorithm specific to its format, and the intermediate results will be combined. For a more detailed description, please consult [Martono14] and further references from there.

The above details are useful to understand, but not necessary to use PyRSB. To create an rsb_matrix object one proceeds just as with e.g. coo_matrix:

```python
>>> from pyrsb import rsb_matrix
>>> V = [11.0, 12.0, 22.0]
>>> I = [0, 0, 1]
>>> J = [0, 1, 1]
>>> A = rsb_matrix((V, (I, J)))
>>> A.todense()
array([[11., 12.],
       [ 0., 22.]])
```

Direct conversion from scipy.sparse classes is also supported. Instancing an RSB structure is computationally more demanding than with COO or CSR (in both memory and time). Exploiting multiple cores and the savings from faster SpMM’s shall make the extra construction time negligible.
Multi-threaded Sparse Matrix-Vector Multiplication with RSB

The following sequence of pictures schematizes eight states of a two-threaded SpMV on an RSB matrix consisting of four (non-empty sparse) blocks. At any moment, up to two blocks are being object of concurrent SpMV (active). Here each active block has a gray background; its rows and column ranges are highlighted. For each of the active blocks, the corresponding active range (corresponding to the rows) is highlighted on the vector. Similarly, right of the matrix, the (out-of-horizontal-scale) operand vector is shown; its active ranges (corresponding to each blocks’ column range) are highlighted.

The idea behind the algorithm is that a thread won’t write to a portion of the result array which is currently being updated by another thread. Beyond that, there is no further synchronization of threads.

This algorithm applies to square as well as non-square matrices. It supports transposed operation (in which case the ranges of each block are swapped). Symmetric operation is supported, too; in this case, an additional transposed contribution is considered for each block.

As depicted in the first RSB illustration (Fig. 1), the order of the sparse blocks in memory proceeds along a space-filling curve. That order of processing the individual blocks can help to deliver data from the memory to the cores faster. For this reason the individual cores attempt to follow that order whenever possible.

To have enough work for each thread, RSB arranges to have more blocks than threads. For this and other trade-offs involved, as well for a formal description of the multiplication algorithm, see [Martone14] and further literature about RSB listed there.

The SpMV algorithm sketched above is what happens under the hood in PyRSB. In practice, rsb_matrix is used in SpMV just as with scipy.sparse classes seen earlier:

```python
>>> from numpy import ones
>>> B = ones([2], dtype=A.dtype)
>>> C = A * B
```

Multi-threaded Sparse Matrix-Matrix Multiplication with RSB

With multiple column operands (in jargon, multiple right hand sides), the operation result is equivalent to that of performing correspondingly many SpMVs.

In these cases it comes naturally to lay the columns one after the other (consecutively) in memory, and have the resulting rectangular dense matrix as operand to the SpMM. Also here the same notation of the previous section is supported; see this example with 2 right hand sides:

```python
>>> from numpy import ones
>>> B = ones([2,2], dtype=A.dtype)
>>> C = A * B
```

Let’s look at how to deal with this when using the RSB layout. As anticipated, the individual right hand sides may lay after each other, as columns of a rectangular dense matrix. See Fig. 3, where a broken line follows the two operands’ layout in memory, also by columns.

A straightforward SpMM implementation may run two individual SpMV over the entire matrix, one column at a time. That would have the entire matrix (with all its blocks) being read once per column.

A first RSB-specific optimization would be to run all the per-column SpMVs at a block level. That is, given a block, repeat the SpMVs over all corresponding column portions. This would increase chance of reusing cached matrix elements as the operands are visited. This reuse mechanism is being exploited by LIBRSB-1.2. The by columns layout (or order) is the recommended one for SpMM there.

The most convenient thing though, would be to read the entire matrix only once. That is the case for LIBRSB-1.3 (scheduled for release in summer 2021): for small column counts, block-level
SpMM goes through all the columns while reading a block exactly once.

The aforementioned SpMM algorithm is to be regarded as LIBRSB-specific internals, with not much user-level control over it.

But there is another factor instead, that plays a certain role in the efficiency of SpMM, where the PyRSB user has a choice: the layout of the SpMM operands.

**SpMM with different Operands Layout**

The by-columns layout described earlier and shown in Fig. 3 appears to be the most natural one if one thinks of the columns as laid in successive multiple arrays. However, one may instead opt to choose a by-rows layout instead, shown in figure 4.

A by-rows layout can be thought as interspersing all the columns, one index at a time. Here in the figure, the blue line follows their order in memory. At SpMM time, given one of the input columns, an element at a given index is multiplied by nonzeros located at that column index. Similarly, given one of the output columns, an element at a given index receives a contribution from the nonzeros located at that row coordinate. With a by-rows layout of the operands, SpMM may proceed by reading a nonzero once, read all right hand sides at that row index (they are adjacent), and then update the corresponding left hand sides’ elements (which are also adjacent). On current cache- and register-based CPUs, the locality induced by this layout leads often to a slightly faster operation than with a by-columns layout.

The by-columns and by-rows layouts go by the respective names of Fortran (’F’) and C (’C’) order. A user can choose which dense layout to use when creating operands for SpMM. Their physical layouts differ, but NumPy makes their results are equivalent here. In the following, we will often refer to right-hand sides count as by NRHS.

### Using PyRSB: Environment Setup and Autotuning

Usage of PyRSB requires no knowledge beyond its documentation. However, the underlying LIBRSB library can be configured in a variety of ways, and this affects PyRSB. To begin using PyRSB, a distribution-provided installation shall suffice. To expect best performance results, a native LIBRSB build is recommended. The next section comments some basic facts to control LIBRSB and make the most out of PyRSB.

#### Environment Variables

PyRSB does not use any environment variable directly; it is affected via underlying LIBRSB and Python. By default, LIBRSB it is built with shared-memory parallelism enabled via OpenMP [OPENMP]. As a consequence, a few dozen OpenMP environment variables (all prefixed by OMP_) apply to LIBRSB as well. Of these, the most important is the one setting the active threads count: OMP_NUM_THREADS. Administrators of HPC (High Performance Computing) systems customarily set this variable to recommended values. Even if unset, chances are good the OpenMP runtime will guess the right value for this. Most other OpenMP variables will be of less use to PyRSB, except one: setting OMP_DISPLAY_ENV=TRUE will get current defaults printed at program start (very useful when debugging a configuration).

In addition to the above, there are environment variables affecting specifically LIBRSB. All of those are prefixed by RSB_, so to avoid any clash. One recommended to end users is RSB_USER_SET_MEM_HIERARCHY_INFO, and is used to override cache hierarchy information detected at runtime or hard-coded at build time. Essentially, one can use it to force a finer or coarser blocking. For its usage, and for verification of further LIBRSB defaults, please see its documentation (accessible from [LIBRSB]). Modifying the variables mentioned in this section will be mostly useful on very new or not fully configured systems, or for tuning a bit over the defaults.

#### RSB Autotuning Procedure for SpMM

Cores count, cache sizes, operands data layout, and matrix structure all play a role in RSB performance. The default blocks layout chosen when assembling an RSB instance may not be the most efficient for the particular SpMM to follow. In practice, given an RSB instance and an SpMM context (vector and scalar operands info, transposition parameter, run-time threads count), it may be the case that a better-performing layout can be found by exploring slightly coarser or finer blockings. An automated (autotuning)
Fig. 5: Rendering of an RSB instance matrix audikw_1 (for this and other matrices, see table) as dtype=numpy.float32 (or S) after autotune(order='C', nrhs=1) on our setup. Autotuning merged an initial 766 blocks guess into 295, bringing a 1.56× speedup to rsb_matrix SpMV time. With rsb_matrix it now takes 1/34th of (1-threaded) csr_matrix time; before autotuning, it took 1/22th. Autotuning itself took the time of 1.5 csr_matrix SpMV iterations, or 34 pre-autotuning rsb_matrix SpMV iterations.

procedure for this exists and is accessible via autotune. The following example shows how to use it on matrix audikw_1 from [SSMC].

```python
>>> import sys, rsb, numpy
>>> dtype=numpy.float32

>>> A = rsb.rsb_matrix("audikw_1.mtx", dtype=dtype)
>>> print(A) # original blocking printed out

>>> sf = A.autotune(verbose=False)
>>> print("autotune speedup for SpMV : %.2e x" %sf )
>>> print(A) # updated blocking printed out

>>> A = rsb.rsb_matrix("audikw_1.mtx", dtype=dtype)
>>> print(A) # original blocking printed out

>>> sf = A.autotune(verbose=False, transA='N', order='C', nrhs=8)
>>> print("autotune speedup for SpMM-8: %.2e x" %sf )
>>> print(A) # updated blocking printed out
```

In scenarios where SpMM is to be iterated many times, time spent autotuning an instance shall amortize over the now faster iterations. See the comments of instances of autotuning on Fig. 5, Fig. 6, and Fig. 7 for realistic use cases.

The reader impatient to see further speedup figures achievable by autotune can already peek at Fig. 10.

Fig. 6: Same matrix as Fig. 5, but autotuned with nrhs=2. Here the initial 766 blocks have been merged into 406, with 1.14× speedup. Before autotuning, it took 1/22th of a (1-threaded) csr_matrix SpMV time; now it’s 1/31th. Here too, it took the time of 1.5 csr_matrix SpMV iterations, or 34 with the pre-autotuning rsb_matrix instance.

Fig. 7: Differently than with nrhs=1 or nrhs=2, autotune(nrhs=8) did not find a better blocking than the original 766 blocks. Still, the procedure costed the time of 11 csr_matrix SpMM’s, or 234 rsb_matrix ones. Though not autotuned, (threaded) RSB takes merely 1/22th the time of CSR here.

Experiments with SpMM and Autotuning

Purpose of this section is to present statistics of speedups one may encounter by using PyRSB instead of SciPy CSR in practical usage. In our choice of experiments, and in the exposition, we favour breadth over depth. So differently than in a paper with HPC in focus, we focus on the achievable speedup, and not on performance. We also take shortcuts which we would not take otherwise, like mixing statistics from single precision computations with double precision ones, or real-valued and complex-valued ones. Also the very focus of the article, namely comparing directly threaded RSB to serial CSR in SciPy would be ill-posed, were we interested to compare the parallelism grade of the two implementations. On the plots that will follow, samples are grouped by matrix; for each one, a five-number summary (minimum and maximum, first quartile, second (median) and third quartiles) is drawn with a boxes and whiskers representation.

Experimental Setup

We use a AMD Epyc 7742 node with 64 cores. Scaling of memory bandwidth in STREAM-like loops here is around 10×. Considering we are dealing with memory-bound operations, we chose OMP_NUM_THREADS=24, OMP_PROC_BIND=spread, and OMP_PLACES=cores. RSB_USER_SET_MEM_HIERARCHY_INFO was set to "L2:4/64/16000K,L1:8/64/32K". We use CSR from csr_matrix in SciPy e171a1 from Feb 20, 2021, PyRSB 8a6d603 from Jun 08, 2021, pre-release LIBRSB-1.3. For both, we use -Ofast -march=native -mtune=native flags and gcc version 10.2.1 20210110 (Debian 10.2.1-6). We use matrices which were also used in
see the table below. Many of these are symmetric; differently than rsb_matrix, csr_matrix does not support symmetric SpMM; therefore in both cases we expand their symmetry and perform only unsymmetric (general) SpMM. Before starting any measurement, we run autotune on a temporary matrix to warm-up the OpenMP environment, once. Then we do one non-timed warm-up SpMM before iterating for 0.2s and taking the fastest sample. We repeat this for each of the 28 matrices, right-hand-sides (NRHS) in 1, 2, 4, 8, order among 'C' and 'F', BLAS numerical types in C, D, S, Z. When using rsb_matrix, we measure both non-autotuned, and autotuned with autotune(nrhs=...,order=...,tmax=0). So the above totals to 28 · 4 · 2 · 4 = 896 records with samples in SpMM and tuning timing. To avoid also timing repeated allocation of the SpMM result (C=A*B), we allocate it once, and then instead of the * operator, we use the functions underneath it, which take C as argument (this can be of interest to many performance-conscious users).

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Figure 8 summarizes the speed ratio of non-autotuned rsb_matrix over csr_matrix. Speedup without RSB autotuning ranges from 4× to 64×, with median 15×. Half of observed speedup cases falls between 11× and 20×. A streaming memory access benchmark we ran on this machine scaled up to circa 10×, which just less than the observed median speedup (remember rsb_matrix is running with multiple cores, but csr_matrix cannot exploit that).

For the reader who is not practical of SpMM performance: the memory access pattern of SpMM is typically very irregular, and largely dependent on the sparsity structure of the matrix. For this reason, for most layouts the multicore scaling of SpMM performance (in particular SpMV) tends to be worse than a streaming memory access scaling. But here we are comparing speed ratios of different algorithms, and these ratios differ as well. That reflects the better or worse aptness of a given format to a given matrix. For instance, matrix 17 has nonzeros scattered quite regularly over the entire matrix, not much clustered: this favours RSB and the cache blocking induced by its structure rather than CSR (serial or not). Conversely, matrix 9 has most of its nonzeros adjacent to some other, which is more CSR-friendly, and a contribution to the lesser improvement when switching to RSB here. See [Martone14] for more RSB-vs-CSR commentary.

The speedups shown so far and those in Fig. 8 rely on default RSB layouts. As said earlier, the RSB format is suited best to scenarios with large matrices and repeated SpMM applications. These are also the scenarios where the usage of autotune, which refines the default layout according to the operands at hand, is most convenient.

Figure 9 shows results with autotuned instances. Here autotune has been called for each combination of matrix, operands layout, NRHS, and numerical type. The median speedup over CSR here (circa 28.8×) is almost twice the one before autotuning.

With respect to non-autotuned RSB samples, the application of autotune brought a median improvement of 1.6×. This includes all samples, inclusive of the lower quartile, with speedup between 1× (no speedup) and 1.2×, which we nevertheless regard as ineffective (see next subsection’s discussion). An overview of which matrix benefited more, and which less from autotuning is given by Fig. 10. There is no clear trend to see here. We observe that most of the cases (70%) benefited from RSB here. It’s worth mentioning that the longer the time limit chosen to run SpMM before taking each performance sample, the less the fluctuation we would have encountered here, and times we chose were quite tight.

Speedups of tuned RSB vs CSR have median 29× with the ‘C’ layout, and 28.6× with ‘F’ layout; also within RSB the ‘C’ layout performs a few percentage points better than ‘F’.

As seen in this section, autotuning can speedup RSB a further bit, but not always. The next section quantifies the cost of autotun-
The Cost of RSB Autotuning

As introduced earlier, autotune adapts the structure of an RSB matrix, seeking instances which execute a specified operation (here, SpMM) faster. A consistent fraction of the autotuning time is spent measuring SpMM timings of prospective RSB instances. It’s important to remark: what one wants here is not merely faster execution of SpMM after autotuning. What one wants is that autotuning plus all following SpMM iterations shall take less time than the same count of iterations with a non-autotuned matrix. In other words, if the time savings of faster SpMM’s cannot cover the autotuning duration, autotuning time is lost. For this reason it is convenient to quantify the number of iterations to reach the first SpMM bringing actual time saving (amortization); this is the duration of autotune divided by the time saved at each iteration (that is, slow time with old RSB blocking, minus faster time with new RSB blocking).

For the purpose of this article, we chose to declare autotuning as effective if it brings a speedup of 20% or more. With this threshold set, while 94.5% of the cases get some speedup, it is 70% that qualify also as effective.

What one observes among effectively autotuned cases (see Fig. 11) is that in 75% of those cases, merely 2.5 CSR iterations are needed to amortize the autotuning time. This is thanks to the large speedup going from (serial) CSR to (parallel) RSB.

If as cost unit we consider going from non-autotuned to autotuned RSB instead, then the relative gain is less (because threaded non-autotuned RSB is already much faster than serial CSR), and consequently, it takes more to amortize it; see Fig. 12.

When autotuning was ineffective (30% of the cases with our 1.2× threshold, though only 5.5% exhibit no speedup at all), we regard its time as lost; in our test setup this was from a few dozen to a few hundred RSB iterations, with median 33; see Fig. 13. If expressed in terms of serial CSR iterations, this would be < 2.8 iterations in half of the cases, < 8 in 75% of the cases.

These results shall convince users that using autotune is a good option most of the times.

Conclusions and Future Work

Full utilization of the parallelism potential is important in achieving efficient operations on current CPUs. PyRSB does that by giving Python users transparent access to the shared-memory parallel performance library LIBRSB. Differently than classes in current scipy.sparse, but with a very similar usage interface, PyRSB’s rsb_matrix readily exploits shared-memory parallelism. This article’s results section gave a wide sample of speedup statistics with respect to SciPy’s csr_matrix, on the SpMM operation. Observed median speedup with respect to csr_matrix exceeded the known memory bandwidth speedup on the machine; with autotuning, it doubled that, speaking for the good implementation in LIBRSB. Trade-off considerations in
using PyRSB effectively by means of autotuning have also been delineated.

SpMM and autotuning are the workhorses of PyRSB and we addressed their use here. Follow-up studies may address or reflect improvements on the LIBRSB side, special use cases, as well as mostly usability-related aspects on the PyRSB side, especially in striving for SciPy interoperability in the user interface. Comparing symmetric SpMM of PyRSB to that of specific symmetric formats in SciPy may also be of interest.

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