



LIBRSB: Multicore Sparse Matrix Performance across Languages and Architectures



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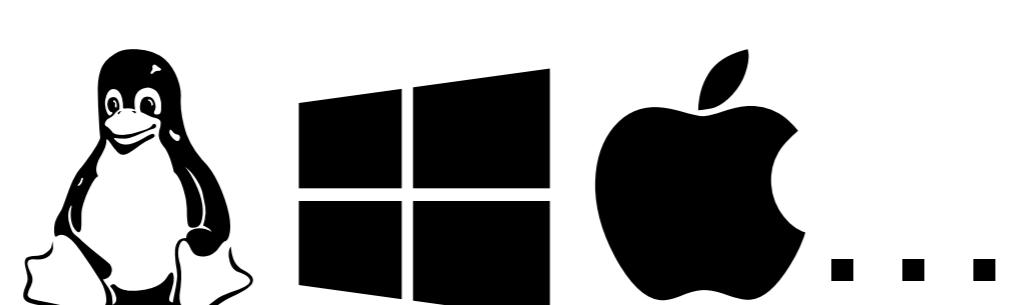
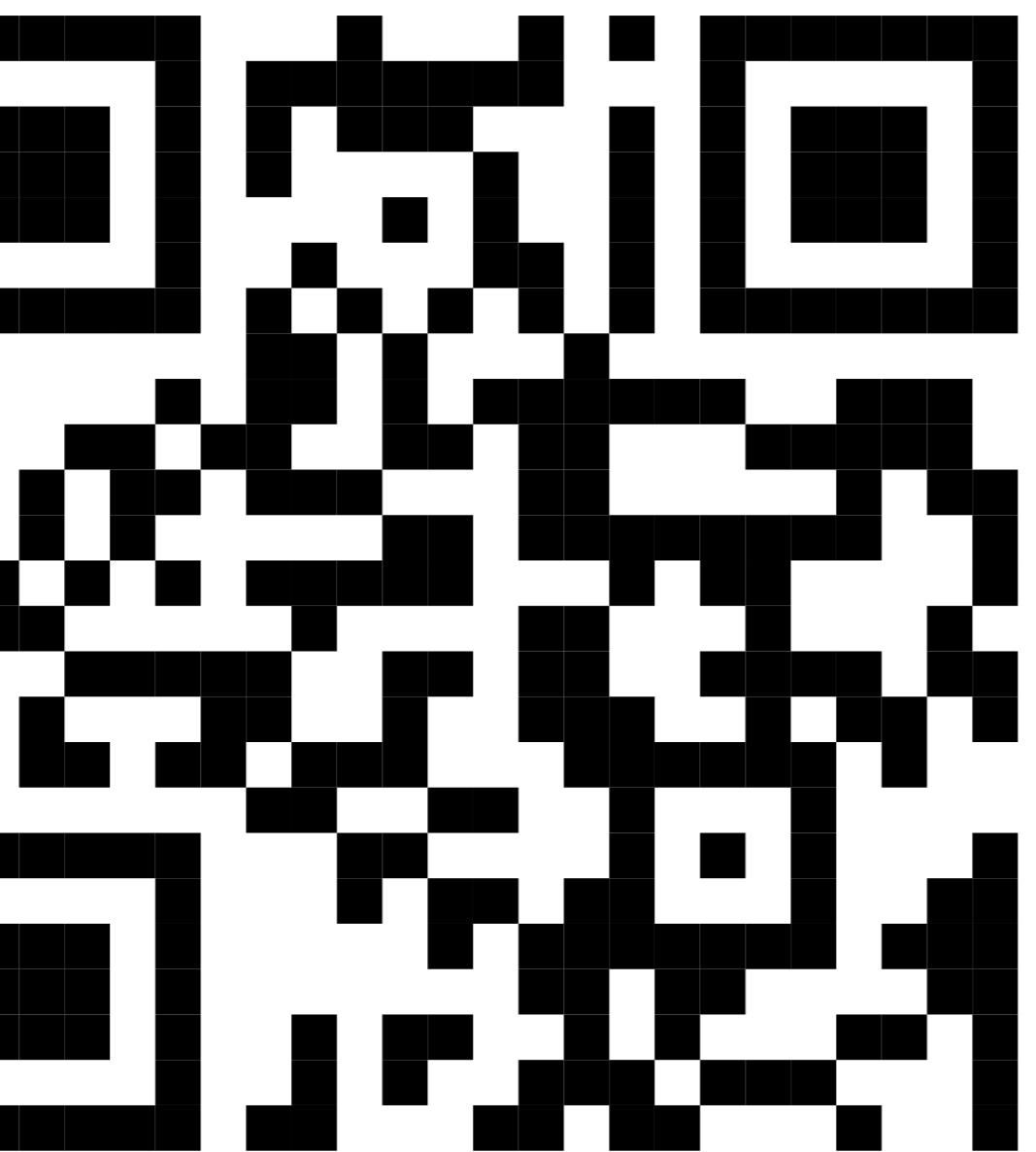
Leibniz Supercomputing Centre, Garching bei München, Germany

$$C = A \cdot B \rightarrow C = \underbrace{\begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix} \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}}_{\text{sparse } A} \cdot B \rightarrow C = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix} \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix} \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \end{bmatrix} \cdot B = \begin{bmatrix} \cdot & \begin{pmatrix} 0 & \cdot \\ \cdot & \cdot \end{pmatrix} \\ \cdot & \begin{pmatrix} 0 & \cdot \\ \cdot & \cdot \end{pmatrix} \\ \cdot & \begin{pmatrix} 0 & \cdot \\ \cdot & \cdot \end{pmatrix} \end{bmatrix} \cdot B$$

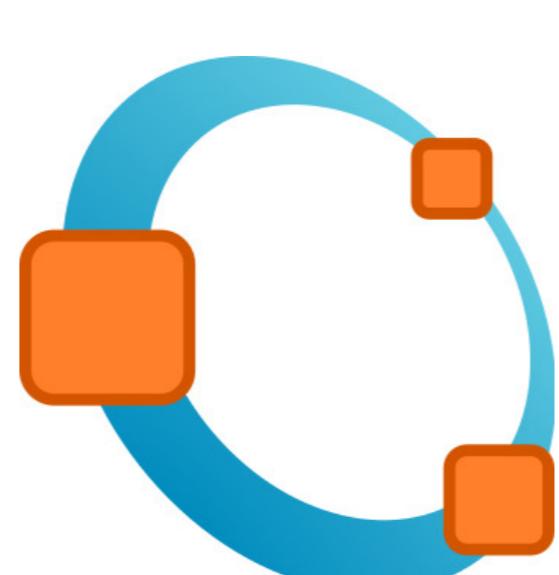
LIBRSB: Universal *Sparse BLAS* Library

<https://librsb.sf.net>

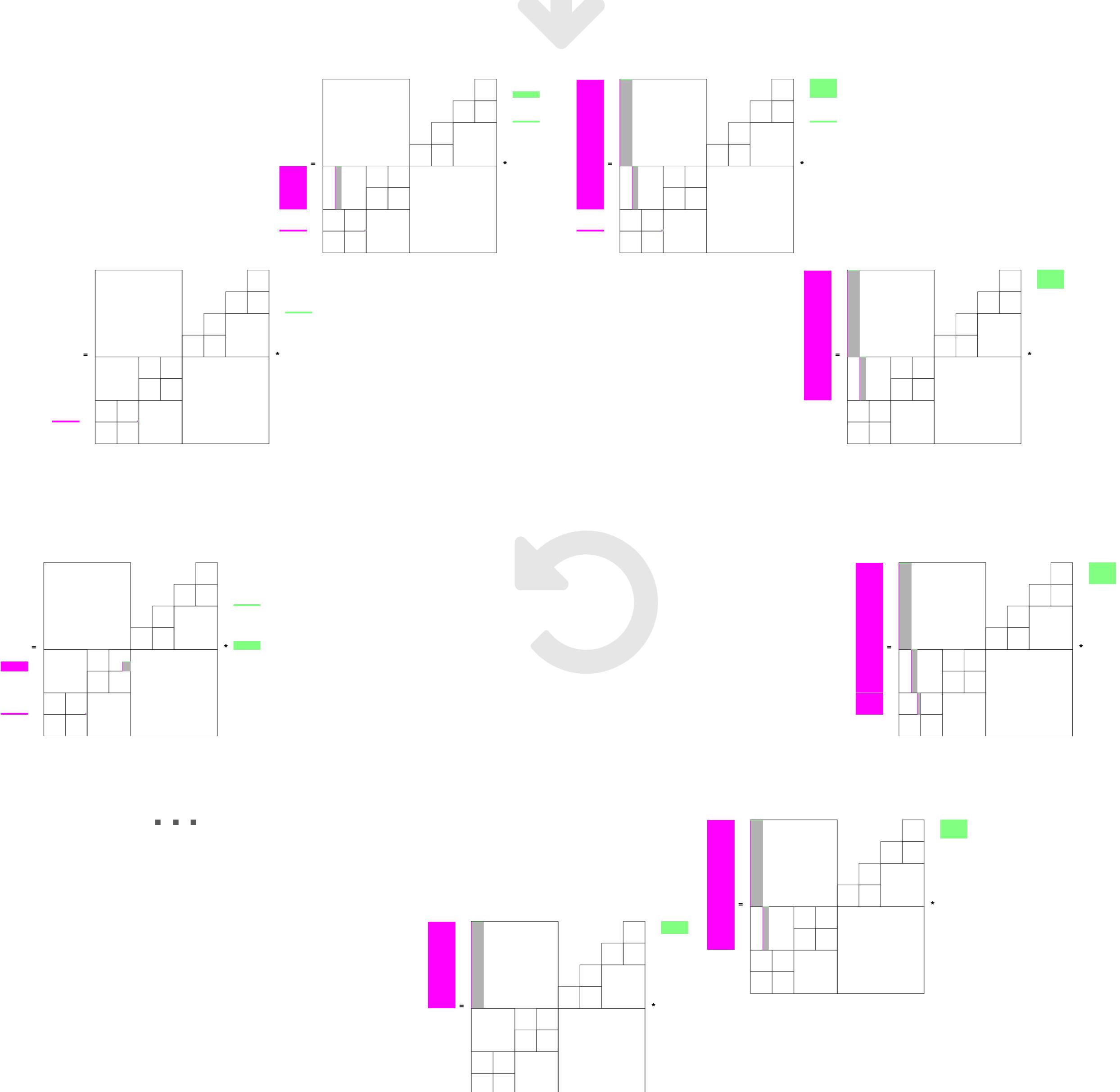
THE
C
PROGRAMMING
LANGUAGE



SciPy.org



GNU OCTAVE



apt install librsb-dev # spack install librsb # guix install librsb # eb search librsb #
Programming languages-related images with permission from www.octave.org, scipy.org, cplusplus.org, fortran-lang.org, wikipedia.org

A portable Sparse BLAS

“Sparse Basic Linear Algebra Subroutines”

for multicore CPUs (node-level)

one library, multiple APIs

this poster: LIBRSB overview and ongoing work

Numerical Techniques of Interest

iterative methods: *block Krylov*

require efficient Sparse Matrix-Matrix multiplication aka SpMM

SpMM in matrix form (*m* aka *NRHS* aka *number of right hand sides*):

$$\begin{bmatrix} \text{updated dense } C \\ \vdots \\ c_{n1} \dots c_{nm} \end{bmatrix} \leftarrow \beta \begin{bmatrix} \text{dense } C \\ \vdots \\ c_{n1} \dots c_{nm} \end{bmatrix} + \alpha \begin{bmatrix} \text{sparse } A \\ \vdots \\ a_{n1} \dots a_{nm} \end{bmatrix} \begin{bmatrix} \text{dense } B \\ \vdots \\ b_{n1} \dots b_{nm} \end{bmatrix}$$

Modern C++ interface (rsb.hpp)

```
1 #include <rsb.hpp>
2 #include <vector>
3 #include <array>
4 using namespace ::rsb;
5
6 int main() {
7     RsbLib rsllib;
8     const int nnzA { 7 }, nrhs { 2 };
9     const int nrA { 6 }, ncA { 6 };
10    const std::vector<int> IA { 0,1,2,3,4,5,1 };
11    const int JA [] = { 0,1,2,3,4,5,0 };
12    const std::vector<double> VA { 1,1,1,1,1,1,2 }, B(nrhs * ncA, 1);
13    std::array<double, nrhs * nrA> C;
14    const double alpha { 2 }, beta { 1 };
15
16    RsbMatrix<double> mtx(IA,JA,VA,nnzA); // Notice above declarations of IA,JA,VA
17
18    mtx.spmm(RSB_TRANSPOSITION_N, alpha, nrhs, RSB_FLAG_WANT_ROW_MAJOR_ORDER, B,
19    beta, C); // ditto for B and C
```

Figure 2: RsbMatrix's `spmm()` and others use C++20's `std::span`. Gives freedom in vectors' type choice. Wraps rsb.h.

New: ongoing work

Improve performance of SpMM CSR kernels:

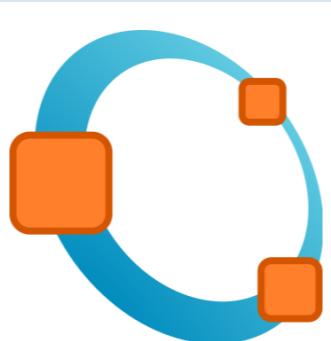
- AVX512 intrinsics (*by-rows*, unsymmetric, untransposed)
- more specializations
- autotuning challenges: e.g. use CSR if more performant than RSB

LIBRSB

project page: <http://librsb.sf.net>

- >100KLOC of C99, OPENMP, and modern templated C++
- node-level **shared-memory**-parallel operations, for:
 - Sparse BLAS: matrix assembly/destroy, **SpMM**, triangular solve
 - *interactive* applications (update, sparse-sparse ops, conversions)
 - *distributed-memory* applications (block extract, update, etc.)
- with own interface in **C/C++** and **FORTRAN**
- with **Sparse BLAS** interface (BLAS Technical Forum Standard)
- with interfaces for **GNU OCTAVE** and **PYTHON** interpreters
- **LGPLv3-licensed** free software, available via SPACK, GUIX-HPC, EasyBuild, and on Debian, Ubuntu, OpenSUSE, Windows,...

GNU Octave + liboctave + LIBRSB = SparseRSB



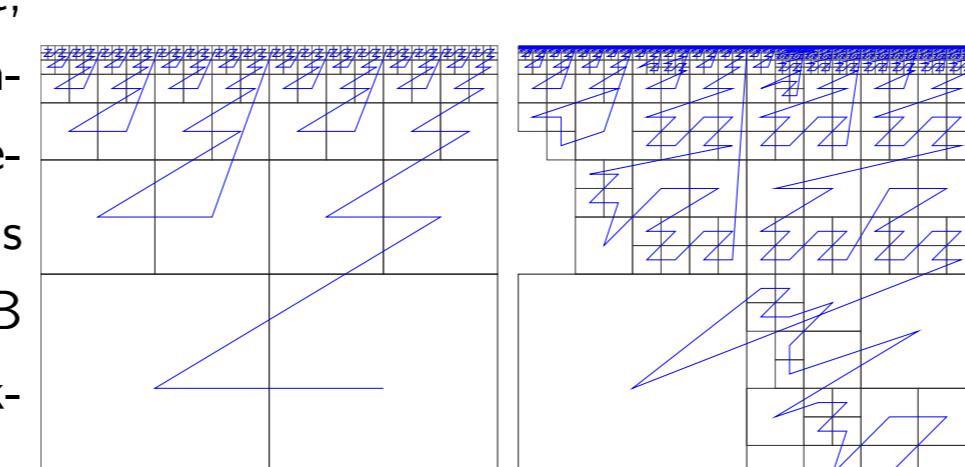
- GNU OCTAVE: a MATLAB-like interactive numerical language
- liboctave: access OCTAVE via C++

```
1 octave:1> A = sparsersb ( sparse ( rand ( 3 ) > .6 ) )
2 A =
3
4 Recursive Sparse Blocks (rows = 3, cols = 3, nnz = 2 [22%])
5
6 (3, 1) -> 1
7 (3, 3) -> 1
```

Figure 3: The sparsersb usage is styled after the sparse built-in. So most of operators (*,*,=,(:,...)) work the same way.

Remarks

Two RSB block layouts (a *coarser* left, a *finer* right) of a Machine Learning matrix sized 57k × 230k and 41M nonzeros (courtesy Dr. Diego De Cao). This matrix is particularly favourable to RSB over CSR. Determining optimal blocking and threads is eased by the autotuning functionality.



Recursive Sparse Blocks (RSB) Layout

- for *large* matrices (uses *cache locality*, *coarse thread parallelism*)
- supports *autotuning* (layout adjusted to maximize performance)

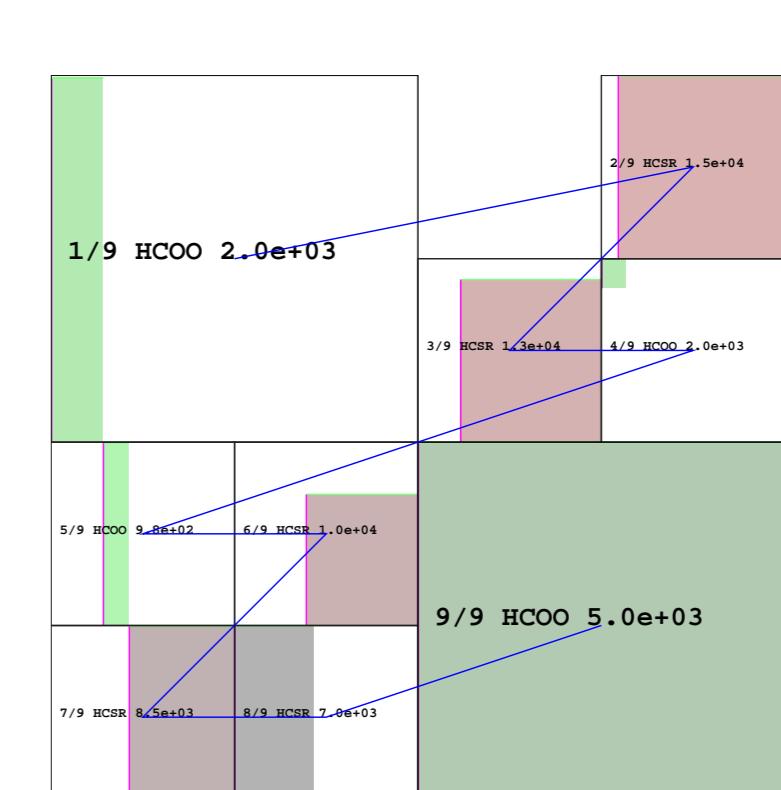


Figure 1: Instance of classical test matrix *bayer02* (14k × 14k, 64k nonzeros). Black-bordered boxes are *sparse blocks*, and are *Z-ordered*. Greenish have fewer nnz than average, redder have more. Either in “Coordinate” format (COO) or “Compressed Sparse Rows” (CSR). Blocks rows (LHS) and columns (RHS) ranges evidenced (left and top side).

Python + Cython + LIBRSB = PyRSB

SciPy.org

Cython

- SCIPY: popular PYTHON scientific computing API
- CYTHON: *optimising static compiler* for C extensions to PYTHON

```
1 import numpy
2 import scipy
3 from rsb import rsb_matrix
4 V=[ 11.,12.,22.]
5 I=[ 0, 0, 1]
6 J=[ 0, 1, 1]
7 a = rsb_matrix((V, (I, J)), [3,3])
8 ...
9 y = y + a * x;
```

Figure 4: API styled after SCIPY's widely known `csr_matrix`. Additionally, it offers RSB-specific functionality, e.g. blocks autotuning.

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