LIBRSB: Universal Sparse BLAS Library

A highly interoperable Library for Sparse Basic Linear Algebra Subroutines for Multicore CPUs

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Bruxelles, 05.02.2023

Systems of Linear Equations

$$\begin{cases} a_1 x + b_1 y &= c_1 \\ a_2 x + b_2 y &= c_2 \end{cases}$$

Matrix Representation

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

Exact Solutions

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{c_1 b_2 - b_1 c_2}{a_1 b_2 - b_1 a_2}$$

$$y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{a_1 c_2 - c_1 a_2}{a_1 b_2 - b_1 a_2}$$

Larger systems = ⚠

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
\vdots \qquad\qquad\qquad &\vdots \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n
\end{aligned}
$$

Larger systems = ⚠

$$
\begin{array}{rcl}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n & = & b_1 \\
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\end{array}
$$

Complications

Larger systems = ⚠

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\end{aligned}$$

Complications

- numerical stability

Larger systems = ⚠

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Complications

- numerical stability
- time to solution

What if...

- rows were several thousands

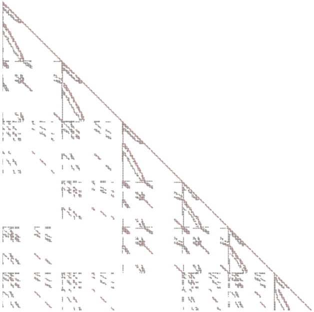
?

What if...

- rows were several thousands
- overwhelmingly populated by *zeros*

?

Is this ...*sparsity*?



12k rows, 300k non-zero elements, symmetric (here only lower triangle)

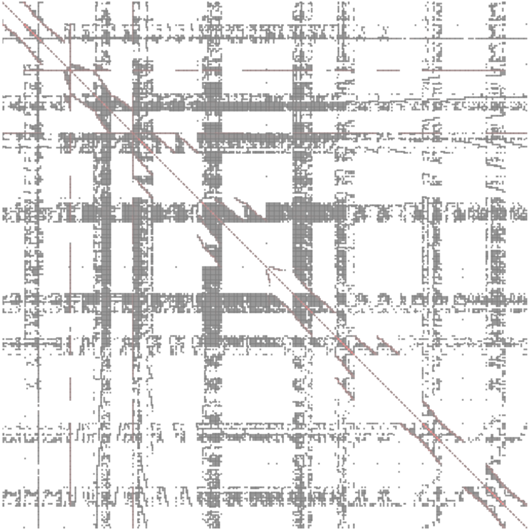
Occupation is ca. 0.4% (triangle only: 0.2%).
Matrix from `https://www.cise.ufl.edu/research/sparse/matrices/Cote/vibrobox`

Sparse Matrices

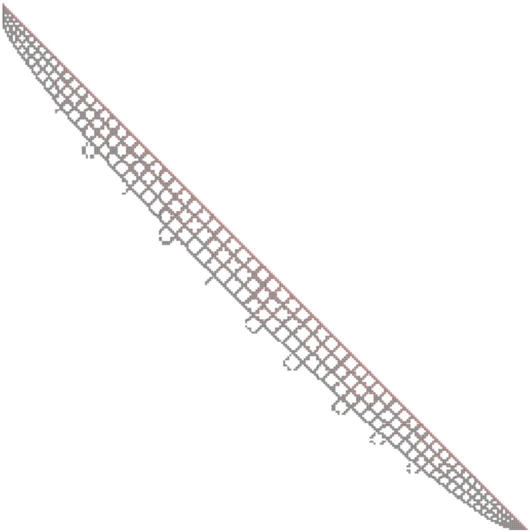
As attributed to James H. Wilkinson:

"any matrix with enough zeros that it pays to take advantage of them";

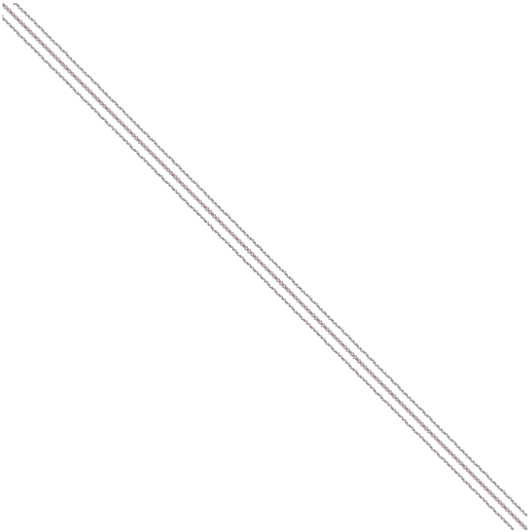
(see Tim Davis' letter http://www.netlib.org/na-digest-html/07/v07n06.html#2)



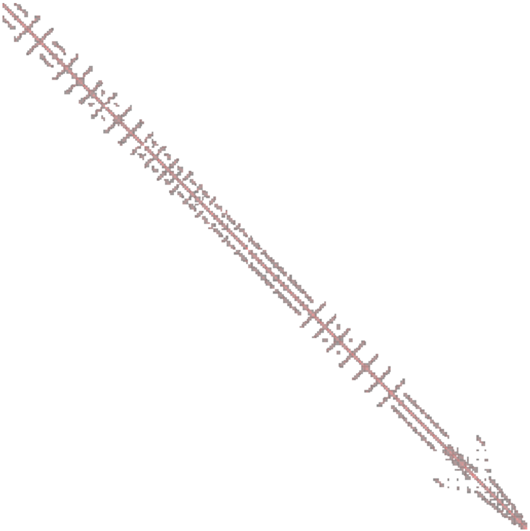
ASIC_320k



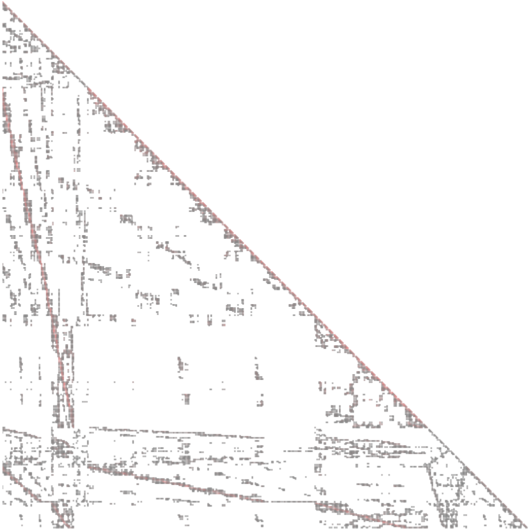
Ga41As41H72



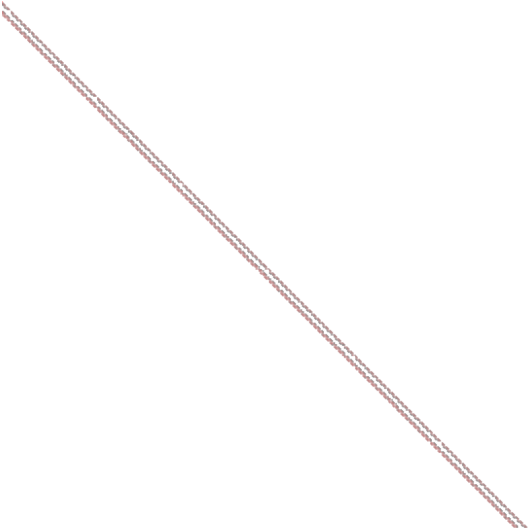
atmosmodl



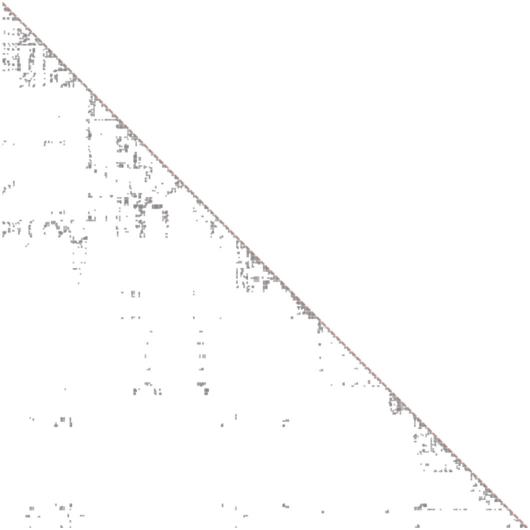
coater2



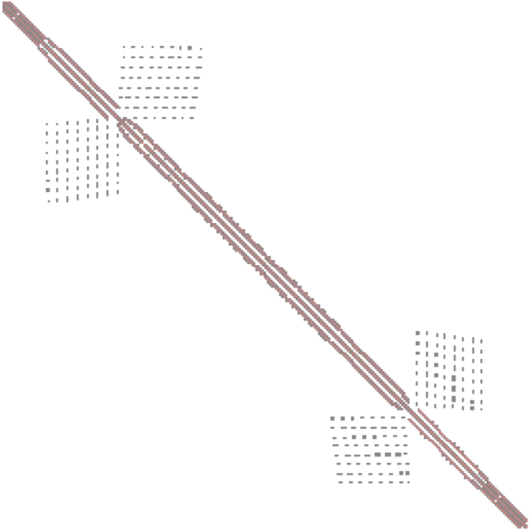
crankseg_1



crystk03



ct20stif



ex11

...Probably!

"Matrix sparsity"...

...depends on the computing techniques we choose.

Sparse Systems and Iterative Methods

```
function [x, flag, relres, iter, resvec] =
        cgs (A, b, tol, maxit, M1, M2, x0)
  ...
    elseif (isnumeric (A) && issquare (A))
      Ax = @(x) A * x;
    elseif (isa (A, "function_handle"))
      Ax = @(x) feval (A, x);
    ...
    for iter = 1:maxit
      ...
      q = Ax (p);
      alpha = ro / (p' * q);
      x = x + alpha * p;
      ...
```

Figure: GNU Octave's Conjugate Gradient Squared

Iterative Methods' frequent Bottlenecks

- SpMM – Sparse Multiply by dense Matrix: $A \cdot B$
- SpSM – Sparse (triangular) Solve by dense Matrix: $T^{-1} \cdot B$

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If operand matrix is wide 1:

- SpMV – Sparse Multiply by dense Vector: $A \cdot x$
- SpSV – Sparse (triangular) Solve by dense Vector: $T^{-1} \cdot x$

SpMM can be defined as...

$$\overbrace{\begin{bmatrix} c_{11} & \dots & c_{1m} \\ \vdots & \ddots & \vdots \\ c_{n1} & \dots & c_{nm} \end{bmatrix}}^{updated\ \ dense\ \ C} \leftarrow \beta \overbrace{\begin{bmatrix} c_{11} & \dots & c_{1m} \\ \vdots & \ddots & \vdots \\ c_{n1} & \dots & c_{nm} \end{bmatrix}}^{dense\ \ C} + \alpha op \left(\overbrace{\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix}}^{sparse\ \ A} \right) \overbrace{\begin{bmatrix} b_{11} & \dots & b_{1m} \\ \vdots & \ddots & \vdots \\ b_{n1} & \dots & b_{nm} \end{bmatrix}}^{dense\ \ B}$$

$op(A)$:

- A, A^T, A'

A:

B, C:

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A:

- general, symmetric, or hermitian

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- optional: non-BLAS types, 64-bit indices

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- by-rows or by-columns representation, custom leading dimension

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B,C:

- by-rows or by-columns representation, custom leading dimension
- unit or non-unit stride

A secondary target problem: SpSM

$$\overbrace{\begin{bmatrix} c_{11} & \dots & c_{1m} \\ \vdots & \ddots & \vdots \\ c_{n1} & \dots & c_{nm} \end{bmatrix}}^{\textit{updated dense } C} \leftarrow \beta \overbrace{\begin{bmatrix} c_{11} & \dots & c_{1m} \\ \vdots & \ddots & \vdots \\ c_{n1} & \dots & c_{nm} \end{bmatrix}}^{\textit{dense } C} + \alpha \overbrace{\begin{bmatrix} t_{11} & \dots & t_{1n} \\ \vdots & \ddots & \vdots \\ t_{n1} & \dots & t_{nn} \end{bmatrix}^{-1}}^{\textit{sparse } \textbf{triangular } T} \overbrace{\begin{bmatrix} b_{11} & \dots & b_{1m} \\ \vdots & \ddots & \vdots \\ b_{n1} & \dots & b_{nm} \end{bmatrix}}^{\textit{dense } B}$$

Options mostly as in SpMM.

Sparse BLAS: an API for iterative methods

- *Sparse BLAS = Sparse Basic Linear Algebra Subroutines*
- consolidated in 2001 by the *BLAS Technical Forum* (`http://www.netlib.org/blas/blast-forum/`)
- built around:
  - create and populate a matrix
  - SpMM, with all the options
  - SpSM, with all the options
  - destroy matrix
- API for C and Fortran (`blas_sparse.h` and `module blas_sparse`)

Merits and Reception

+ quite portable (on the CPU)
+ internal representation or parallelism are internal choices
+ one can imagine extensions...
- though no explicit extension specification
+ namesake and functionality adopted widely...
- but with slightly differing APIs
- no revision over the years (lost the GPU train...)

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Nevertheless

Still useful ☺

Sample SPARSE BLAS program (nothing LIBRSB-specific here)

example: spbusmv_pure.cpp

```
#include <blas_sparse.h>
int main(const int argc, char * const argv[]) {
  blas_sparse_matrix A = blas_invalid_handle;
  const int nnz = 4, nr = 3, nc = 3;
  const int    IA[] = { 0, 1, 2, 2 };
  const int    JA[] = { 0, 1, 0, 2 };
  double VA[] = { 11.0, 22.0, 13.0, 33.0  };
  double X[] = { 0.0, 0.0, 0.0 };
  const double B[] = { -1.0, -2.0, -2.0 };

  A = BLAS_duscr_begin(nr,nc);
  BLAS_ussp(A,blas_lower_symmetric);
  BLAS_duscr_insert_entries(A, nnz, VA, IA, JA);
  BLAS_duscr_end(A);
  BLAS_dusget_element(A, IA[0], JA[0], &VA[0]);
  BLAS_dusmv(blas_no_trans,-1,A,B,1,X,1);
  BLAS_usds(A);

  return 0;
}
```

RSB: Layout and Techniques for Sparse BLAS

- **R**ecursive **S**parse **B**locks
- does not exclude any Sparse BLAS option
- favours cache reuse with **cache blocking**
- **block-level**, coarse-grained threading
- block-level format can vary

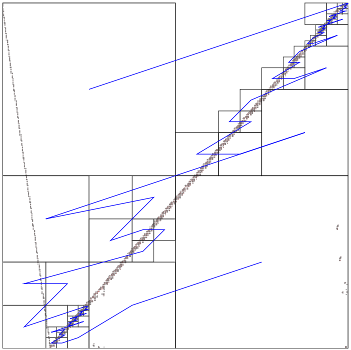
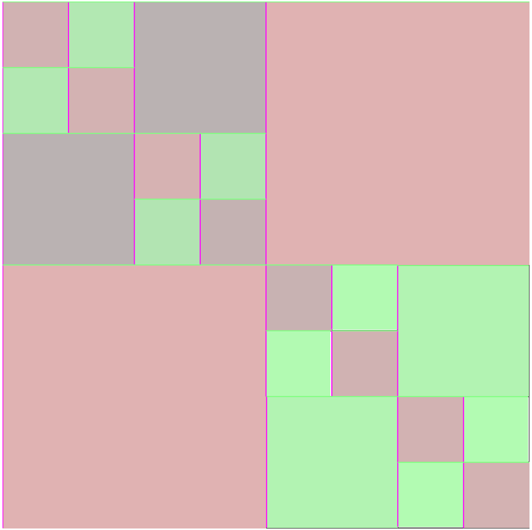
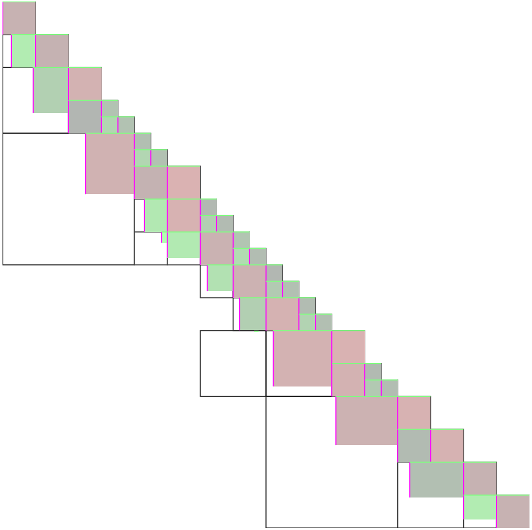


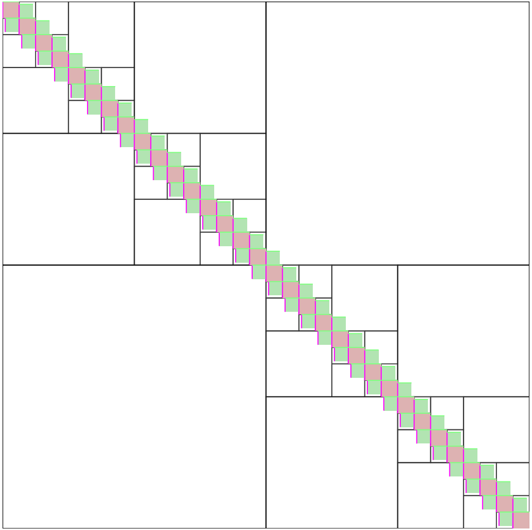
Figure: matrix `bayer02` as RSB



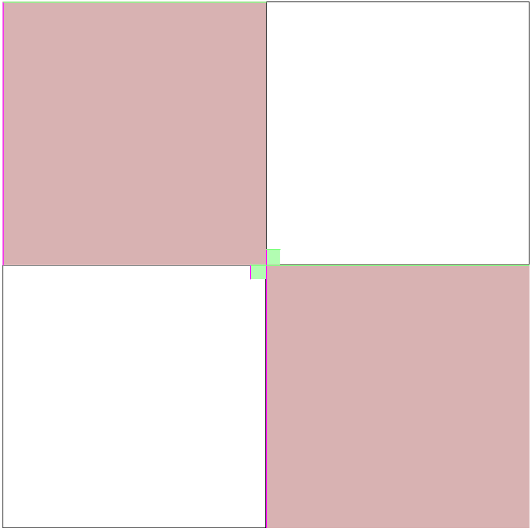
ASIC_320k as RSB



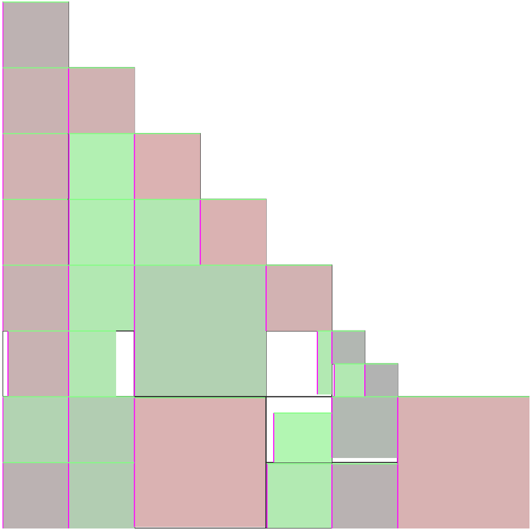
Ga41As41H72 as RSB



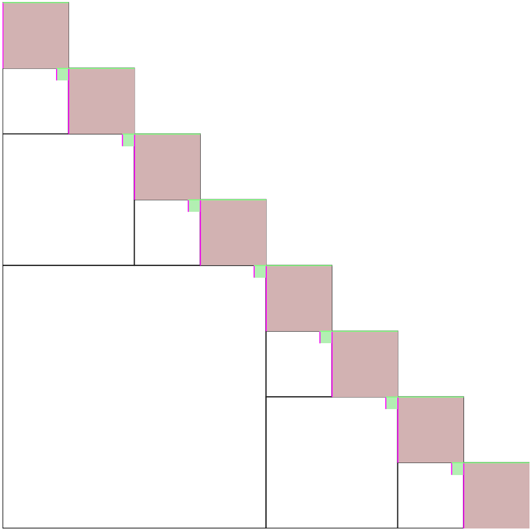
atmosmodl as RSB



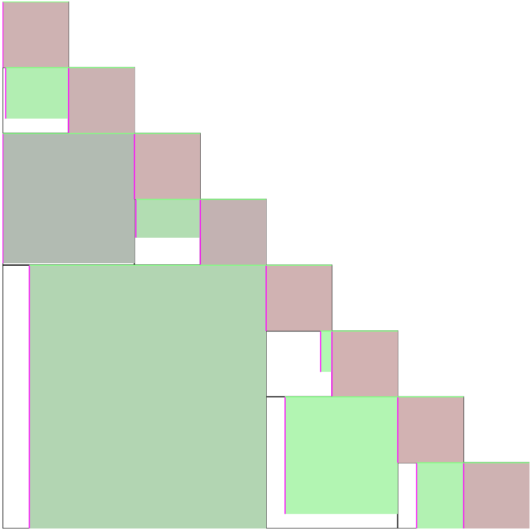
coater2 as RSB



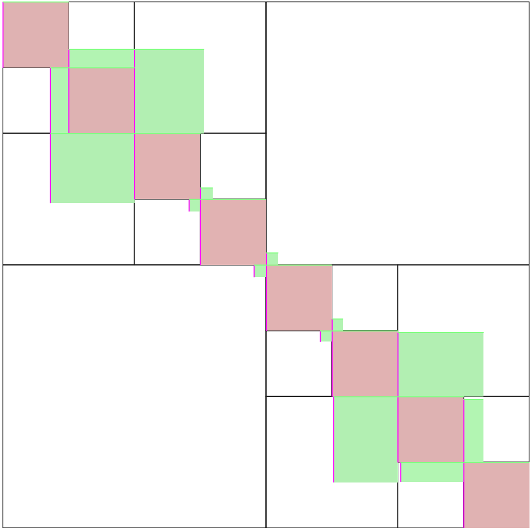
crankseg_1 as RSB



crystk03 as RSB



ct20stif as RSB



ex11 as RSB

LIBRSB: Shared Memory-parallel Sparse BLAS library around RSB

- *building blocks* for iterative solvers
  - interoperability
  - portability
  - compatibility

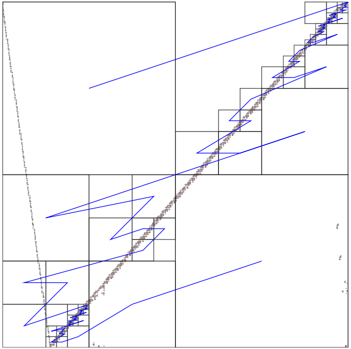


Figure: matrix `bayer02` rendered by LIBRSB

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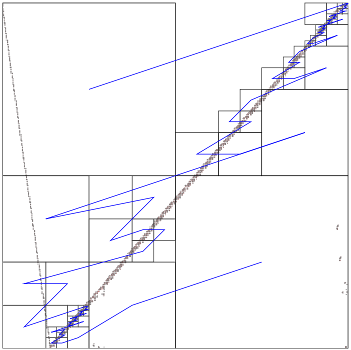

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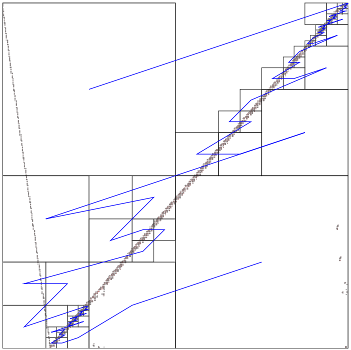

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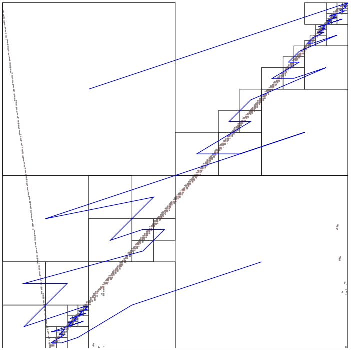
- *building blocks* for iterative solvers
  - interoperability: **C, C++, Fortran, Octave, Python**
  - portability: **no intrinsics, POSIX, C99, OpenMP, C++...**
  - compatibility: **no fill-in, user-provided arrays,...**



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Sample SPARSE BLAS Program with LIBRSB

example: spbusmv.cpp

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  double X[] = { 0.0, 0.0, 0.0 };
  const double B[] = { -1.0, -2.0, -2.0 };
  rsb_lib_init(RSB_NULL_INIT_OPTIONS);
  A = BLAS_duscr_begin(nr,nc);
  BLAS_ussp(A,blas_lower_symmetric);
  BLAS_duscr_insert_entries(A, nnz, VA, IA, JA);
  BLAS_duscr_end(A);
  BLAS_dusget_element(A, IA[0], JA[0], &VA[0]);
  BLAS_dusmv(blas_no_trans,-1,A,B,1,X,1);
  BLAS_usds(A);
  rsb_lib_exit(RSB_NULL_EXIT_OPTIONS);
  return 0;
}
```

Native LIBRSB APIs

Apart from `blas_sparse.h` and `module blas_sparse`...

- C/C++ in `rsb.h`
- C++ in `rsb.hpp`
- Fortran in `rsb.F90` (after `rsb.h`)

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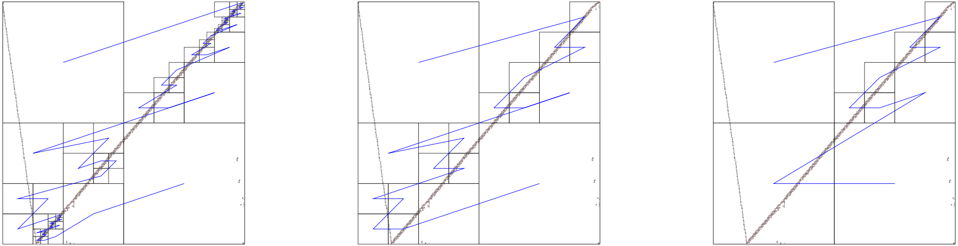
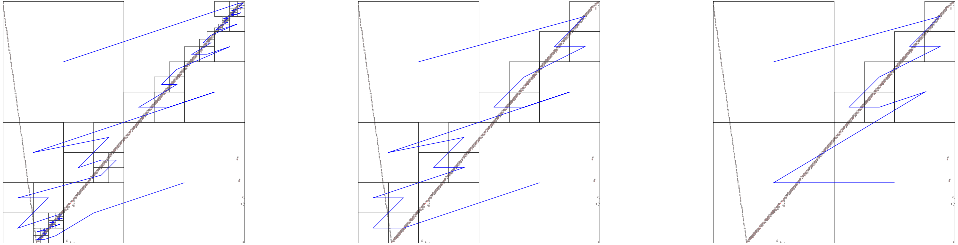
Why another API?

For extras, especially RSB-specific ones; see next slide.



Blocking granularity affects SpMM performance

Automated Empirical Optimization



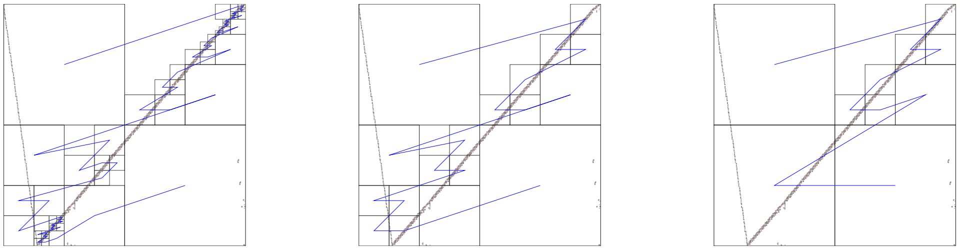
Blocking granularity affects SpMM performance

Automated search of *better* blockings

Essential to utilize LIBRSB at best

Trades off *search time* for savings in SpMM iterations.

Automated Empirical Optimization



Blocking granularity affects SpMM performance

Automated search of *better* blockings

Essential to utilize LIBRSB at best

Trades off *search time* for savings in SpMM iterations.

`rsb_tune_spmm()` in C, ...

C++ example

example: `nozero_span.cpp`

```
#include <array>
#include <vector>
#include <iostream>
#include <rsb.hpp>
int main()
{
  const rsb::RsbLib rsblib;
  const std::vector<rsb_coo_idx_t> IA {0,0,1,1}, JA {0,1,0,1};
  const std::array<double,4> VA {1,0,0,1};
  // square full matrix, no zeroes:
  rsb::RsbMatrix<double> mtx(IA,JA,VA,4,
     RSB_FLAG_DEFAULT_RSB_MATRIX_FLAGS | RSB_FLAG_DISCARD_ZEROS);
  std::cout << mtx.nnz();
}
```

```
2
```

Example: sparsersb in GNU Octave

```
octave:1> R=(rand(3)>.6)
R =

   0   0   0
   0   0   0
   1   0   1

octave:2> A_octave=sparse(R)
A_octave =

Compressed Column Sparse (rows = 3, cols = 3, nnz = 2 [22%])

  (3, 1) ->  1
  (3, 3) ->  1

octave:3> A_librsb=sparsersb(R)
A_librsb =

Recursive Sparse Blocks  (rows = 3, cols = 3, nnz = 2 [22%])

  (3, 1) -> 1
  (3, 3) -> 1
```

https://sourceforge.net/p/octave/sparsersb/ci/default/tree/src/sparsersb.cc

Example: LIBRSB + CYTHON = PYRSB

```
import numpy
import scipy
from scipy.sparse import csr_matrix
from rsb          import rsb_matrix

V = [11.,12.,22.]
I = [  0,  0,  1]
J = [  0,  1,  1]

c = csr_matrix((V,(I,J)))
y = y + c * x;

a = rsb_matrix((V,(I,J)))
y = y + a * x;
```

https://github.com/michelemartone/pyrsb

Default licensing of LIBRSB

Lesser GPLv3, aka LGPLv3

- unmodified, can be combined with proprietary software
- modified, must be released as LGPLv3

Availability

Sources:

http://librsb.sf.net/

Packaged:

- Linux distros: Debian, Ubuntu& derivatives, openSUSE, NixOS, AUR, ...
- Misc: FreeBSD, Cygwin
- Spack, Easybuild

Third party accessors

- Julia, Rust