Cache and Energy Efficiency of Sparse Matrix-Vector Multiplication for different BLAS Numerical Types with the RSB Format

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Presentation outline

Goal of this Study

- quantify and relate energy, cache usage and time savings of `librsb`'s RSB over Intel's MKL[1] CSR for SParse Matrix-Vector multiply (*SpMV*) for matrices of an example application
- ... for different numerical types

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[1] Math Kernel Library

Context: Sparse Matrix Computations

- numerical matrices which are *large* and populated mostly by zeros
- ubiquitous in scientific/engineering computations (e.g.: PDE)
- the *performance* of sparse matrix codes computation on modern CPUs can be problematic (a fraction of peak)!

Context: The four *Basic Linear Algebra Subroutines* (BLAS) numerical types

For each, its occupation (`sizeof()`) S in bytes:

- D: *double precision real*
  $S_D = 8$
- Z: *double precision complex*
  $S_Z = 16$
- S: *single precision real*
  $S_S = 4$
- C: *single precision complex*
  $S_C = 8$

Matrix representations that matter to us

- *coordinate* (COO): used mostly in matrix specification
- *compressed sparse rows* (CSR): used often in computations

In most common implementations (e.g.: Intel's MKL), 4 byte integers are used for COO/CSR indices types.

Basic representation: Coordinate (COO)

$$A = \begin{vmatrix} a_{1,1} & a_{1,2} & a_{1,3} & 0 \\ 0 & a_{2,2} & a_{2,3} & 0 \\ 0 & 0 & a_{3,3} & 0 \\ 0 & 0 & 0 & a_{4,4} \end{vmatrix}$$

- $VA = [a_{1,1}, a_{1,2}, a_{1,3}, a_{2,2}, a_{2,3}, a_{3,3}, a_{4,4}]$ (*nonzeroes*)
- $IA = [1, 1, 1, 2, 2, 3, 4]$ (*nonzeroes row indices*)
- $JA = [1, 2, 3, 2, 3, 3, 4]$ (*nonzeroes column indices*)
- so, $a_{i,j} = VA(n) \;\; iff \;\; IA(n) = i, JA(n) = j$
- occupation for type T: $nnz \cdot (S_T + 4 + 4)$

Standard representation: Compressed Sparse Rows (CSR)

$$A = \begin{vmatrix} a_{1,1} & a_{1,2} & a_{1,3} & 0 \\ 0 & a_{2,2} & a_{2,3} & 0 \\ 0 & 0 & a_{3,3} & 0 \\ 0 & 0 & 0 & a_{4,4} \end{vmatrix}$$

- $VA = [a_{1,1}, a_{1,2}, a_{1,3}, a_{2,2}, a_{2,3}, a_{3,3}, a_{4,4}]$ (*nonzeroes*)
- $JA = [1, 2, 3, 2, 3, 3, 4]$ (*nonzeroes column indices*)
- $RP = [1, 4, 6, 7, 8]$ (*row pointers, for each row*)
- so, elements on line i are in positions $VA(RP(i))$ *to* $VA(RP(i+1)) - 1$
- so, $a_{i,j} = VA(n)$ *iff* $JA(n) = j$
- occupation for type T: $nnz \cdot (S_T + 4) + 4 \cdot nrows$

Pros and Cons of CSR in a nutshell

- + common, easy to work with
- + parallel *SpMV* is feasible
- - parallel *SpMV-T* is feasible ...but poor performance
- - the above are relatively inefficient with *large*[2] matrices
- - impractical for parallel sparse *triangular solve*

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[2] Matrices that don't fit in the cache memory.

A recursive matrix storage: *Recursive Sparse Blocks* (RSB)

we propose:

- a *quad-tree* of sparse *leaf* submatrices
- outcome of recursive *partitioning* in *quadrants*
- leaf submatrices are stored by either *row oriented Compressed Sparse Rows* (CSR) or *Coordinates* (COO)
- an *unified* format for Sparse **BLAS**[3] operations and variations (e.g.: diagonal implicit, one or zero based indices, transposition, complex types, stride, ...)
- partitioning with regards to both the underlying cache size **and** available threads
- leaf submatrices are *cache blocks*

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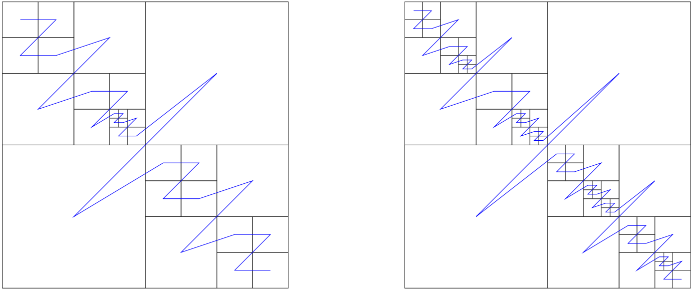
[3] Sparse Basic Linear Algebra Subprograms standard, as in TOMS Algorithm 818 (Duff and Vömel, 2002).

Design goals of `librsb` and the RSB format

- parallel, efficient *SpMV*/triangular solve/*COO* → *RSB*
- in-place *COO* ↔ *RSB* conversions
- no oversized COO arrays / no *fill-in* (e.g.: in contrast to BCSR)
- no need to pad x, y vectors arrays with extra elements
- developed on/for shared memory cache based CPUs:
  - *locality of memory references*
  - coarse-grained *workload partitioning*
- architecture independent (C'99, POSIX, OpenMP)
- `librsb` is available as *free software* on SourceForge

Adaptivity to Cache Size

Sample matrix from our application (a *small* one). Each block should occupy approximately the same amount of memory.



On the left, blocking for S type; on the right, for Z.

Adaptivity to threads count

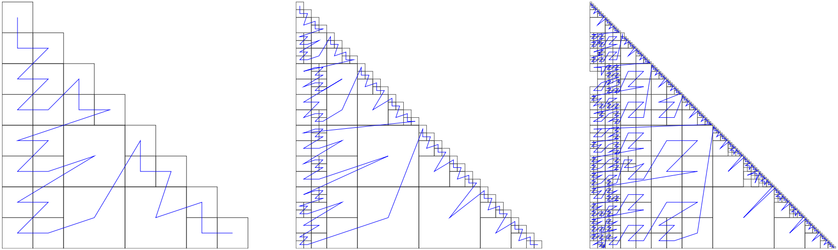


Figure: Matrix *audikw_1* (symmetric, 943695 rows, $3.9 \cdot 10^7$ nonzeroes) for 1, 4 and 16 threads on a Sandy Bridge.

Memory Occupation of CSR and RSB

- CSR's is fixed:

  $$nnz \cdot (S+4) + nrows \cdot \; 4$$

- `librsb` RSB's varies between:

  $$nnz \cdot (S+2) + nrows \cdot \; 4$$

  and

  $$nnz \cdot (S+8)$$

Occupation of RSB w.r.t CSR

For the different types:

Δ / type	S	D/C	Z
min	-25%	-16%	-10%
max	+50%	+33%	+20%

(approximately)

Impact of Matrix Memory Occupation

- it can influence run-time (*SpMV*) accessed memory
- run-time accessed memory is what matters
- it's better if the access pattern leads to less cache traffic

Experimental Setup (1)

- Matrices resulting from the description of global, resistive, linear MHD (Magnetohydrodynamics) studied in toroidal geometry (see Bondeson and Vlad, 1992).
  We concentrate on the largest: $9.62 \cdot 10^7$ nonzeroes, $1.99 \cdot 10^5$ equations (with an average of 484 nonzeroes per row).[4]
- On a 2 x "Sandy Bridge E5-2670"; L3: 20MB, L2: 256KB, L1:32KB
- We instrument the code with the LIKWID *performance tool* (Treibig, Hager, Wellein'2011) to collect "`ENERGY`" and "`L2 data volume`" metrics
- We report:
  - performance in canonical GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$)
  - spent energy in kJ/GFlop
  - L2 traffic in bytes/nonzero

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[4] Results are similar for smaller matrices, as long as outermost cache size is exceeded.

Experimental Setup (2)

- Intel C Compiler
- `CFLAGS=-O3 -fPIC -restrict -openmp`
- `mkl_dcsrmv`, `mkl_zcsrmv`, `mkl_ccsrmv`, `mkl_scsrmv` from *"MKL 11.0-1, Product, 20121009 ..."*
- no memory placement tool, no clock control

Serial Results: S

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
CSR/S/1	2.31	-7.95	28.08	+6.71	8.55	+2.65
MKL/S/1	2.51	0.00	26.31	0.00	8.33	0.00
RSB/S/1	2.33	-7.03	27.11	+3.01	6.19	-25.71

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Serial Results: *D*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
CSR/D/1	1.81	-5.25	36.40	+2.94	12.20	-0.10
MKL/D/1	1.91	0.00	35.36	0.00	12.21	0.00
RSB/D/1	1.84	-3.73	35.10	-0.74	10.20	-16.50

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Serial Results: *C*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
CSR/C/1	3.55	-50.54	17.66	+87.77	13.87	+0.70
MKL/C/1	7.19	0.00	9.40	0.00	13.78	0.00
RSB/C/1	3.53	-50.89	17.52	+86.32	11.44	-16.98

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Serial Results: Z

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
CSR/Z/1	2.68	-30.29	23.83	+37.23	49.43	-4.19
MKL/Z/1	3.85	0.00	17.37	0.00	51.59	0.00
RSB/Z/1	2.69	-30.12	23.69	+36.39	34.41	-33.29

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Parallel Results: *S*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
MKL/S/12	10.13	0.00	25.47	0.00	8.26	0.00
MKL/S/16	8.26	0.00	35.39	0.00	8.25	0.00
RSB/S/12	14.48	+43.01	17.98	-29.43	6.18	-25.15
RSB/S/16	13.15	+59.07	24.34	-31.21	6.30	-23.66

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Parallel Results: *D*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
MKL/D/12	7.18	0.00	35.15	0.00	12.22	0.00
MKL/D/16	5.50	0.00	51.99	0.00	12.22	0.00
RSB/D/12	8.61	+19.95	29.58	-15.83	10.33	-15.43
RSB/D/16	8.50	+54.61	35.79	-31.16	10.35	-15.31

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Parallel Results: *C*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
MKL/C/12	28.79	0.00	9.03	0.00	13.80	0.00
MKL/C/16	21.62	0.00	13.52	0.00	13.81	0.00
RSB/C/12	32.27	+12.08	8.40	-6.92	10.43	-24.43
RSB/C/16	31.77	+46.93	9.94	-26.53	10.44	-24.44

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Parallel Results: *Z*

Implem.	Speed	%Δ to MKL	Energy	%Δ to MKL	L2 Traffic	%Δ to MKL
MKL/Z/12	17.21	0.00	15.20	0.00	49.61	0.00
MKL/Z/16	13.09	0.00	22.45	0.00	49.62	0.00
RSB/Z/12	19.36	+12.50	13.59	-10.64	19.30	-61.08
RSB/Z/16	18.25	+39.44	17.07	-23.96	19.38	-60.94

Table: Metrics: execution Speed in (canonical) GFlops ($2 \cdot 10^{-9} \cdot nnz \cdot elapsed\_seconds^{-1}$; 3 times that for complex); Energy in kJ/GFlop; L2 Traffic in bytes/nnz.

Conclusions, serial runs

- serially, RSB is slower than MKL by respectively:

  3.73% (D), 30.12% (Z), 7.03% (S), 50.89% (C)
- with no bandwith limitations, MKL's optimized serial kernels are better!

Conclusions, parallel runs

- RSB results were better than MKL's by respectively:

  19.95% (D), 12.50% (Z), 43.01% (S), 12.08% (C)
- the *energy-cheapest Flops* were associated to the fastest executions, confirming e.g.: (Hager et al., 2012)
- 12-threaded performed better than 16-threaded!
- energy savings over MKL were roughly half the savings in speed

Further Work

extend study to...

- *auto-tuning*: locating *best core count* and *best subdivision*
- other operations (symmetric multiply, transposed multiply, conversion, ...)
- other matrices
- compilers impact on *bandwidth limited* RSB kernels

References

- Sparse BLAS: Iain S. Duff and Christof Vömel. *Algorithm 818: A reference model implementation of the Sparse BLAS in Fortran 95* In ACM Trans. on Math. Softw., n. 2, vol. 28, pages 268–283, ACM, 2002

- `librsb`: `http://sourceforge.net/projects/librsb`
- RSB: Michele Martone, Salvatore Filippone, Salvatore Tucci, Marcin Paprzycki, and Maria Ganzha. *Utilizing recursive storage in sparse matrix-vector multiplication - preliminary considerations.* In Thomas Philips, editor, CATA, pages 300-305. ISCA, 2010.
- Our sample application: A. Bondeson, G. Vlad, et al.. *Resistive toroidal stability of internal kink modes in circular and shaped tokamaks.* In Physics of Fluids B: Plasma Physics, 4(7):1889–1900, 1992.

Acknowledgements

I wish to thank my colleagues at HLST for providing me with criticism with this presentation.

Questions / discussion welcome!

Thanks for your attention.

Please consider using `librsb`:
`http://sourceforge.net/projects/librsb`

Extra: Minimal Memory Occupation of RSB

at most, RSB saves:
$\frac{4\ nnz+4\ nrows-2\ nnz-4\ nrows}{4\ nnz+4\ nrows+nnzS} = \frac{2\ nnz}{4\ nnz+4\ nrows+nnzS} \approx \frac{2\ nnz}{4\ nnz+nnzS} = \frac{2}{4+S}$
over CSR:
this is $1/4$ for$S = S_S$, $1/6$ for S_D/S_C, $1/10$ for S_Z.

Extra: Maximal Memory Occupation of RSB

at most, RSB uses:

$$\frac{8\ nnz - 4\ nnz - 4\ nrows}{4\ nnz + 4\ nrows + nnz S} = \frac{4\ nnz - 4\ nrows}{4\ nnz + 4\ nrows + nnz S} \approx \frac{4\ nnz}{4\ nnz + nnz S} = \frac{4}{4+S}$$

more than CSR:

this is $1/2$ for S_S, $1/3$ for S_D/S_C, $1/5$ for S_Z.