Interfacing Epetra to the RSB sparse matrix format for shared-memory performance

Michele Martone

High Level Support Team
Max Planck Institute for Plasma Physics
Garching bei München, Germany

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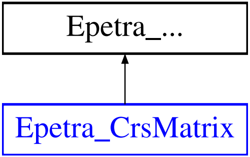
Background: sparse kernels can be performance critical

Sparse kernel	Operation definition[1]
SpMV: Matrix-Vector Multiply	"$y \leftarrow \ \beta\ y\ +\ \alpha\ A\ x$"
SpMV-T: (Transposed)	"$y \leftarrow \ \beta\ y\ +\ \alpha\ A^T\ x$"
SpSV : Triangular Solve	"$x \leftarrow \ \alpha\ L^{-1}\ x$"
SpSV-T : (Transposed)	"$x \leftarrow \ \alpha\ L^{-T}\ x$"



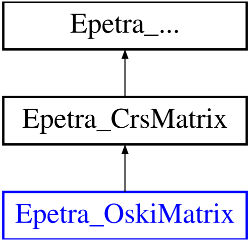
Epetra_...

Epetra_CrsMatrix

- CRS (Compressed Row Storage) versatile and straightforward
- `class Epetra_CrsMatrix` can rely on Intel MKL

[1] A is a sparse matrix, L sparse triangular, x, y vectors or multi-vectors, α, β scalars.

Background: optimized sparse matrix classes



- OSKI (Optimized Sparse Kernels Interface) library, by R.Vuduc
  - kernels for iterative methods, e.g. *SpMV*, *SpSV*
  - autotuning framework
- OSKI + `Epetra` = `class Epetra_OskiMatrix`, by I.Karlin

Background: librsb

- a stable "Sparse BLAS"-like kernels library:
    - Sparse BLAS API (blas_sparse.h)
    - own API (rsb.h)
- LGPLv3 licensed
- librsb-1.2 at http://librsb.sourceforge.net/
- OpenMP threaded
- C/C++/FORTRAN[2] interface

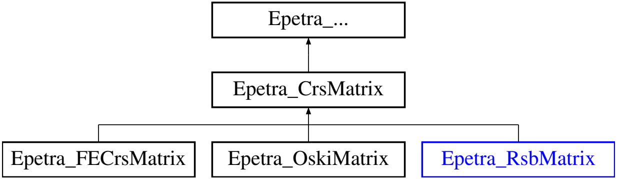
[2] ISO-C-BINDING for own and F90 for Sparse BLAS

What can librsb do

- can be multiple times faster than Intel MKL's CRS in[3]
  - symmetric/transposed sparse matrix multiply (SpMV)
  - multi-RHS (SpMM)
  - large matrices
- threaded SpSV/SpSM (sparse triangular solve)
- iterative methods ops: scaling, extraction, update, ...
- usable from GNU Octave (sparsersb plugin+keyword)

[3] Please see:
Auto-tuning shared memory parallel Sparse BLAS operations in librsb-1.2
Poster presented at Sparse Solvers for Exascale: From Building Blocks to Applications, Greifswald, Germany
http://hdl.handle.net/11858/00-001M-0000-0029-A8D3-E

Focus of this talk: `class Epetra_RsbMatrix`



- `librsb + Epetra` =
  `class Epetra_RsbMatrix: public Epetra_CrsMatrix`
- analog to `class Epetra_OskiMatrix`

RSB sparse matrix format: Recursive Sparse Blocks

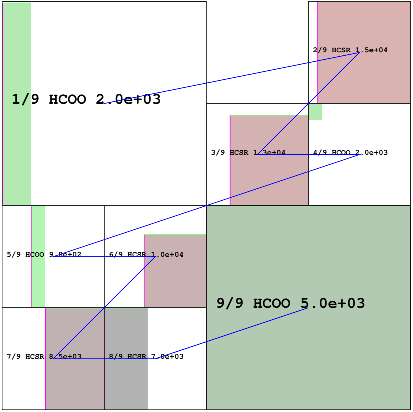
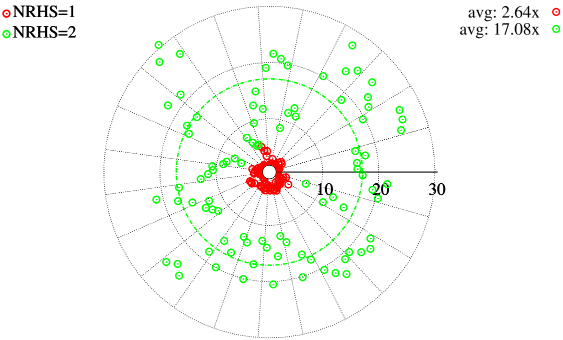


Figure: RSB instance of *bayer02*

- `CSR` (=`CRS`) and `COO` blocks
- 32 or 16 (sHort) bit indices
- with fewer, or more than average nonzeroes
- inter-block Z-Morton order
- **adaptive** (cache blocking) to cache size + threads count

Example results[4]: RSB vs MKL *CRS* Speedup, *SymSpMV*



A matrix per sector, four BLAS types on 2x8 threaded Sandy Bridge

[4] From poster *Auto-tuning shared memory parallel Sparse BLAS operations in librsb-1.2*, `http://hdl.handle.net/11858/00-001M-0000-0029-A8D3-E`

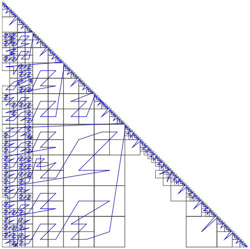
RSB and autotuning

- similar concept as in `Epetra_OskiMatrix`
- empirical autotuning:

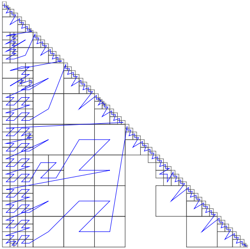
```
  A_Rsb.tune_spmm(... transA, alpha, nrhs,
                 order, B, ldB, beta, C, ldC);
```

- adapts data structure to operation
- tuning can cost e.g. $10^2 \approx 10^3$ operations
- iterated faster operations shall amortize tuning cost

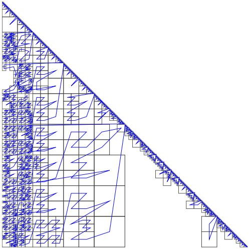
Example of autotuning[5]



Untuned.



Tuned for NRHS=1.



Tuned for NRHS=3.

Sample instances of symmetric *audikw_1* (ca. 1M × 1M, 39M nonzeroes), node with 256 KB sized L2 cache, 16 threads.

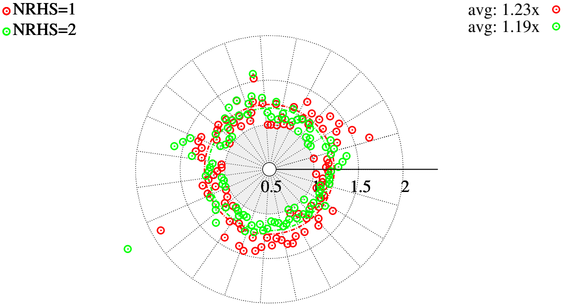
Left (625 blocks, avg 491 KB) before tuning.

Middle tuning merged blocks (271, avg 1133 KB).

Right tuning subdivided blocks (1319, avg 233 KB).

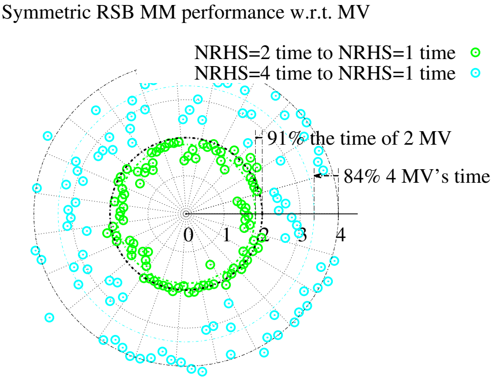
[5] From poster *Auto-tuning shared memory parallel Sparse BLAS operations in librsb-1.2*, `http://hdl.handle.net/11858/00-001M-0000-0029-A8D3-E`

Example results[6]:*SymSpMV* autotuning speedup:19 ≈ 23%



[6] From poster *Auto-tuning shared memory parallel Sparse BLAS operations in librsb-1.2*, `http://hdl.handle.net/11858/00-001M-0000-0029-A8D3-E`

Example results[7]: Blocking operations favours multi-RHS



Currently: reuse of sparse blocks in *SpMM* (and can be improved)

[7] From poster *Auto-tuning shared memory parallel Sparse BLAS operations in librsb-1.2*, `http://hdl.handle.net/11858/00-001M-0000-0029-A8D3-E`

What is librsb being used for ?

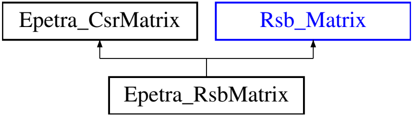
- Plasma Physics
  A.K.Stegmeir
  GRILLIX: A 3D turbulence code for magnetic fusion devices based on Field line map
  PhD Thesis, July 2015
  Max-Planck-Institut fuer Plasmaphysik, Garching, Germany
  `http://dx.doi.org/10.17617/2.2085490`
- Environmental Modelling
  P.A. Browne, S. Wilson
  A simple method for integrating a complex model into an ensemble data assimilation system using MPI
  Environmental Modelling & Software, Volume 68, June 2015, Pages 122-128
  `http://dx.doi.org/10.1016/j.envsoft.2015.02.003`
- Machine Learning
  Fast Matrix-vector Multiplications for Large-scale Logistic Regression on Shared-memory Systems
  M-C. Lee, W-L. Chiang, C-J. Lin; National Taiwan University
  15th IEEE International Conference on Data Mining (ICDM 2015), Atlantic City, NJ, U.S.A., November 14-17, 2015
  `https://www.csie.ntu.edu.tw/~cjlin/papers/multicore_liblinear_icdm.pdf`
- Singular Value Decomposition, Big Data
  High-Performance Algorithms for Large-Scale Singular Value Problems and Big Data Applications
  L. Wu, A. Stathopoulos, College of William and Mary, Williamsburg, Virginia, USA
  `http://sc15.supercomputing.org/sites/all/themes/SC15images/doctoral_showcase/doc_files/drs110s2-file7.pdf`

Prototype class Epetra_RsbMatrix

```
Epetra_CsrMatrix A_Csr(...);
...
/* Populate, set options. */
...
Epetra_RsbMatrix A_Rsb(A_Csr);
/* just as Epetra_CsrMatrix: */
A_Rsb.Multiply(...);
A_Rsb.Solve(...);
A_Rsb.ReplaceMyValues(...);
A_Rsb.ExtractDiagonalCopy(...);
/* ...and so on. */

/* But additionally: */
A_Rsb.tune_spmm(... transA, alpha, nrhs,
          order, B, ldB, beta, C, ldC);
A_Rsb.tune_spsm(... transA, alpha, nrhs,
          order, B, ldB, beta, C, ldC);
```

Backbone of class Epetra_RsbMatrix



- class Rsb_Matrix: a proper C++ interface to librsb
- soon part of librsb
- base class providing many internals to class Epetra_RsbMatrix

Differences with OSKI/Epetra_OskiMatrix

Epetra_RsbMatrix

- needs no install time tuning
- memory occupation:
  the three arrays of COO for i, j, val (so, no fill-in)
  and the quad-tree structure, $O(nonzeroes)$
- works with Epetra_Vector and Epetra_MultiVector
  (faster if ConstantStride() == true in multi-RHS)
- offers nearly all operations of what class Epetra_CrsMatrix does

Differences with `Epetra_CrsMatrix`

- construction can cost time of a dozen of *SpMV*
- access / modify functions: `ReplaceMyValues()`, `SumIntoMyValues()`, `ExtractDiagonalCopy()`, `ReplaceDiagonalValues()...` cost a little more (need tree traversal)

`class Epetra_RsbMatrix`: Conclusions and outlook

- transparent access to OpenMP parallel kernels of `librsb`
- best for symmetric large matrices, multi-RHS
- not really reliant on `class Epetra_CrsMatrix`
  (so far, a transitory solution)
- potential for:
  - **distributed matrices**
  - **Tpetra**,
    64 bit indices,
    further numerical types (e.g. `long long double, ...`)
- expertise of Trilinos developers beneficial here!