Kokkos Kernels 4.3 Release Briefing

Kokkos Kernels team

April 25, 2024

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



4.3 Release Highlights

- ► Block II UK
- Stream RCM re-ordering and ILUK
- ► Implicit time integrators
- SPMVHandle
- Miscellaneous
- Deprecations and other breaking changes

April 25, 2024 2/10

Online Resources:

- ► https://github.com/kokkos:
 - Primary Kokkos GitHub Organization
- ▶ https:
 - //github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
 - Slides, recording and Q&A for the Full Lectures
- ▶ https://github.com/kokkos/kokkos-kernels/wiki:
 - Wiki including API reference
- ► https://kokkosteam.slack.com:
 - Slack channel for Kokkos.
 - Please join: fastest way to get your questions answered.
 - Can whitelist domains, or invite individual people.

April 25, 2024 3/10

Both spiluk_symbolic and spiluk_numeric now support block sparse row data.

- ▶ The block algorithms operate on the block graph of the matrix
- Operations on blocks are performed with dense linear algebra kernels
- ► Increasing level of fill by one adds a new block per row, i.e. block size new entries per row
- The spiluk handle constructor now takes a block_size argument defaulted to 0
- the spiluk handle provides two new methods:
 - get_block_size()
 - set_block_size()

Upcoming:

- new interface that accepts a Crs or Bsr matrix instead of views
- move new Crs interface out of experimental, keep Bsr in experimental at first

April 25, 2024 4/10

Stream RCM re-ordering and ILUK

The utility function kk_extract_diagonal_blocks_crsmatrix_sequential now has an option for reverse Cuthill-McKee (RCM) re-odering

- ► The function is able to
 - apply RCM re-ordering to extracted diagonal sub-matrices as indicated by the Boolean input argument UseRCMReordering
 - return a vector of permutation index views in RCM order corresonding to diagonal blocks if UseRCMReordering is true, or an empty vector if it is false
- Permutation index views have the same memory_space as the input CRS matrix
- Usage example:
 - kk_extract_diagonal_blocks_crsmatrix_sequential(A_in, diagBlk_in_b);(default - no RCM reordering)
 - permute = kk_extract_diagonal_blocks_crsmatrix_sequential(A_in, diagBlk_out, UseRCMReordering);
 - diagBlk_out and permute can typically used as inputs for stream-based processing in Ifpack2::RILUK preconditioner

April 25, 2024 5/10

Kokkos ODE now has implicit time integrators in KokkosODE_BDF.hpp

- backward differentiation formulae order 1 to 5
- automatic order increase/decrease and time step increase/decrease
- automatic selection of the first time step size

Upcoming:

- implementation of Adams-Moulton implicit methods
- more uniform interface for all algorithms

Warning!

This feature is still experimental: please let us know about issues you encounter!

April 25, 2024 6/10



KokkosSparse::spmv now takes an optional handle argument.

- Stores TPL matrix analysis, allowing reuse
 - Especially benefits rocSPARSE (measured 15x speedup vs. setup every call)
- Allows algorithm selection and expert tuning (replaces Controls)
- Setup is performed automatically on the first spmv call
- KokkosSparse::SPMVHandle<ExecSpace, AType, XType, YType> handle;
- KokkosSparse::spmv(space, &handle, "N", alpha, A, ...);

April 25, 2024 7/10

Last BLAS rank update function implemented: SYR2. It performs a symmetric rank-2 update:

$$A = A + \alpha(x * y^T + y * x^T)$$

- ► KokkosBlas::syr2(space, trans, uplo, alpha, x, y, A);
- provides: native, BLAS, cuBLAS and rocBLAS implementations
- it is thread safe and non-blocking

April 25, 2024 8/10

TPL support

 cuSOLVER and rocSOLVER libraries are added and provide vendor optimized implementation for LAPACK algorithms

April 25, 2024 9/10

Only one change this time around:

- ► KokkosSparse::Experimental::spadd_symbolic and spadd_numeric now require two new arguments for number of rows and columns.
- ▶ Before 4.3:
 - spadd_symbolic(&handle, a_rowmap, a_entries, b_rowmap, ...);
 - spadd_numeric(&handle, a_rowmap, a_entries, a_values, ...);
- **4**.3:
 - spadd_symbolic(&handle, m, n, a_rowmap, a_entries, b_rowmap, ...);
 - spadd_numeric(&handle, m, n, a_rowmap, a_entries, a_values, ...);

Upcoming: will have a look at what is in the Experimental and move some kernels out of it and deprecate the experimental version.

April 25, 2024 10/10