Towards Fast, Accurate and Reproducible LU Factorization

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The process of finding the solution of a linear system of equations is often the core of many scientific applications. Usually, this process relies upon the LU factorization, which is also the most compute-intensive part of it. Although current implementations of the LU factorization may reach 70% of the peak performance, their accuracy and, even more, reproducibility cannot be guaranteed, mainly, due to the non-associativity of floating-point operations and dynamic thread scheduling.

In this work, we address the problem of reproducibility of the LU factorization due to cancelations and rounding errors, resulting from floating-point arithmetic. Instead of developing a completely independent version of the LU factorization, we benefit from the hierarchical structure of linear algebra libraries and start from developing/enhancing reproducible algorithmic variants for the kernel operations – like the ones included in the BLAS library – that serve as building blocks in the LU factorization. In addition, we aim at ensuring the accuracy of these underlying BLAS routines.

We consider an unblocked algorithmic variant of the LU factorization that can be expressed in terms of BLAS level 1 and 2 routines: triangular solver (TRSV), dot product (DOT) and matrix-vector product (GEMV). We prevent cancellations and rounding errors during the accumulation stage thanks to a long accumulator and error-free transformations [1]. Consequently, we tackle the problem of accuracy in the reproducible triangular solver (ExTRSV) [2] through iterative refinement. Moreover, we provide an accurate and reproducible algorithmic variant as well as an implementation of the matrix-vector product. Thus, following the bottom-up approach, we construct the reproducible algorithmic variant of the LU factorization. Up to our knowledge, this is the first implementation of a reproducible LU factorization. Finally, we present initial evidence that both accurate and reproducible higher-level linear algebra routines can be constructed following our hierarchical bottom-up approach.

References:

[1] S. Collange, D. Defour, S. Graillat, R. Iakymchuk, Numerical Reproducibility for the Parallel Reduction on Multi- and Many-Core Architectures, *Parallel Computing*, 49 (2015), pp. 83–97.

[2] R. Iakymchuk, S. Collange, D. Defour, S. Graillat, *Reproducible Triangular Solvers for High-Performance Computing*, In the Proceedings of the 12th International Conference on Information Technology: New Generations (ITNG 2015), Special track on: Wavelets and Validated Numerics, April 13-15, 2015, Las Vegas, Nevada, USA, pp. 353-358.