A Hybrid Factorzation Solver with Mixed Precision Arithmetic for Sparse Matrices

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1 INTRODUCTION

A linear system with sparse matrix needs to be solved for numerical simulation of partial differential equations that are discretized by a finite element method or a finite volume method. The condition number of the coefficient matrix A of the linear system sometimes becomes very high due to the jump of physical parameter, multiple constraints in a monolithic form of the system, and/or large variety of the discretization parameter introduced by adaptive mesh refinement. For the problem of elasticity with composite material, due to different material parameters, the condition number $\kappa(A)$ will exceed 10^9. For the incompressible flow, the condition number will take 10^6 because the linear system consists of both kinematic state and divergence free constraint. Extremely large condition number like 10^{14} appears in the system for semi-conductor problem where the diffusion coefficient for hole or electron distribution depends on the electrostatic field with exponential weight due to modeling of the drift term. For free boundary problem solved by the level set approach, the condition number is rather moderate around 10^3 due to adaptive mesh refinement for locally higher resolution with reasonable number of unknowns in global. Furthermore, the coefficient matrix could be singular due to setting of the boundary conditions, which may naturally happen by modelization or by algorithm for parallelization by domain decomposition methods. Hence, floating point operation at least with double precision are mandatory for such simulations.

The direct solver based on the LDU-factorization with proper pivoting strategy [1, 2] can solve such sparse matrices with very high condition number. However computational complexity of the factorization algorithm is very high as $O(N^{2.5})$ with degrees of freedom N for sparse matrix obtained from finite element approximation by P1 or P2 element. This complexity cannot be reduced, but by using lower precision arithmetic, we could expect faster computation with smaller memory footprint.

The computation by lower precision arithmetic or mixed precision arithmetic is one of most hot topics for the latest or the next generation computing system in HPC environment. It is obvious that lower precision arithmetic can reduce computational time thanks to large amount of arithmetic units than higher precision units, and smaller amount of memory accessing, but it looses accuracy due to less mantissa of the floating point format. Nowadays, it is thought that mixed precision arithmetic can provide a remedy for solution in lower accuracy by using a technique to recover the accuracy, for example the iterative refinement method.

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2 ALGORITHM

We propose an improved method with mixed precision arithmetic in a hybrid factorization algorithm [4]. The hybrid algorithm consists of decomposition of the sparse matrix into a union of moderate and hard parts during factorization procedure with symmetric pivoting strategy. Here solution of the moderate part by an iterative method in higher precision with preconditioner consisting of lower precision arithmetic generates the Schur complement matrix, whereas the standard factorization method generates the Schur complement matrix by recursive factorizing process. In precise, the Schur complement matrix $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$ is computed by the block GCR solver for $A_{11}X_{12} = A_{12}$ with multiple right hand side (RHS) A_{12}, whose entries consist of the postponed pivots during factorization process for A_{11}. The block GCR solver utilizes solution of the sparse matrix A_{11} in lower precision as a preconditioner and process of multiplication of A_{11} to search vectors in higher precision can be easily implemented of SpMM (Sparse Matrix multiplication to dense Matrix) of the global sparse matrix A, thanks to the restriction by symmetric pivoting [4]. During the first factorization process A_{11} is decomposed into the LDU-form and the solution $A_{11}^{-1}A_{12}$ is obtained by forward and backward substitutions following multi-frontal algorithm with symmetric pivoting and also blocking strategy for parallelization of the factorization of dense sub-matrices in higher levels of the bisection tree [2]

In final, performing forward and backward substations for multiple RHS solution in higher precision with factorized matrices in lower precision is the essential part of the preconditioning procedure, where actual mixed precision arithmetic is necessary without type conversion of RHS data from higher to lower precision. Here, TRSM of BLAS level 3 is used for diagonal blocks and GEMM for off-diagonal blocks for updating.

3 IMPLEMENTATION AND NUMERICAL RESULTS

In R-CCS RIKEN, Japan, we have developed tmBLAS library for mixed precision arithmetic using C++ template which can handle different data types in operands and operator in all BLAS routines [3]. Thanks to mixed precision TRSM and GEMM in tmBLAS library, we can avoid down-cast from higher precision to lower precision, which will truncate the mantissa of the given RHS data before calling TRSM in lower precision. The new implementation can keep the mantissa of RHS data against factorized matrix in lower precision. This strategy results in more accurate computation for preconditioner of the iterative method in higher precision.

This poster will report numerical efficiency of the proposed algorithm and implementation by using mixed precision BLAS in three different sparse matrices, an invertible symmetric matrix taken from the matrix market, with few very small eigenvalues, which results in large condition number, and finite element matrices for simulation of incompressible flow problem and semi-conductor problem, where the coefficient matrices are both singular. The first two examples are compared between double arithmetic and float-double mixed precision arithmetic and the third in quadruple and double-quadruple, where quadruple operation is realized by Double-double. Substantial speedup of mixed-precision computation by double-quadruple arithmetic has been verified.

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