Scientific Report

First name / Family name	Pawan kumar
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Name of the *Host Organisation*	Fraunhofer ITWM
First Name / family name of the *Scientific Coordinator*	Mirko Rahn
Period of the fellowship	01/09/2013 to 31/08/2014

I – SCIENTIFIC ACTIVITY DURING YOUR FELLOWSHIP

In general my work involved research and development of linear algebra and linear solver kernels.

Initially about a month and a half were spent in getting familiarity with GPI programming environment and interoperability with pthreads with simple examples.

During the second phase (3-7 months) I developed a communication optimal block orthogonalization routine namely for tall and skinny matrices TSQR in short, such routines are used in block Krylov subspace methods. The TSQR kernel was later extended to implement a communication optimal least squares solver using GPI and pthread. It is proved that the least squares solver is communication optimal for QR based least squares problem for tall and skinny matrices. Moreover the solver handles multiple right hand sides. In the process, various useful interfaces to existing routines of MKL library (triangular solvers, matrix vector multiply, qr factorization, etc) were written. Such interfaces are often required in linear solvers.

During the final phase (7-11 months), I focussed on sparse linear algebra, in particular on linear solver. The two research exchange programmes provided me with some new directions and a slight deviation from my initial plan. I investigated a frequency filtering and a two grid approach for Schur complement systems for problems with heterogeneous coefficients. A prototype implementation was written in C++. Some parts of the work on parallel implementation will continue as future work. A paper on the original prototype ideas with sequential implementation was written and submitted. The paper on parallel implementation of the method is planned as future work.

II – PUBLICATION(S) DURING YOUR FELLOWSHIP

Published

1. P. Kumar, *Multithreaded direction preserving preconditioners*, ISPDC 2014, Marseille, France, **published**

Abstract: The scalability and robustness of a class of non-overlapping domain decomposition preconditioners using 2-way nested dissection reordering is studied. We consider two different factorizations: nested and block versions. Both these variants have advantages and disadvantages. The nested variants have less than half the memory requirements compared to block variants. On the other hand, the block variants have faster solve phase and converges within similar number of iterations. In particular, four methods are considered: a nested symmetric successive over- relaxation (NSSOR), its block variant block SSOR (BSSOR), nested filtering factorization (NFF), and its block variant block filtering factorization (BFF). The recently introduced filtering preconditioners namely NFF and BFF are two filtering preconditioners that preserve direction on a given filter vector. The scalability and robustness of these methods are discussed on shared memory architecture. We outline the algorithmic differences between NFF and BFF. The implementation is recursive and cache oblivious. The test cases consist of a Poisson problem and convection-diffusion problems with jumping coefficients.

2. P. Kumar, *Communication optimal least squares solvers*, HPCC 2014, Paris, **published**

Abstract: Recently a communication optimal variant of tall skinny QR (TSQR) have been proposed and extensively studied. The TSQR method has found its use in implementing communication avoiding Krylov solvers, and in the panel factorization of the QR method. When the given matrix has full column rank, it is well known that QR algorithm is among the best approaches to solve wider class of least squares problem (LS). Using communication optimal variant of TSQR, we study the scalability of the least squares solver with multiple right hand sides. We show that the communication for TSQR based LS solver for multiple right hand sides is still optimal in the sense that no additional messages are necessary compared to TSQR, thus the least squares solver incurs no additional inter nodal message latencies compared to TSQR. However, LS has additional communication volume, and flops compared to that for TSQR. We derive additional flops and words sent for LS using existing results for TSQR. We use global address space programming framework (GPI) for inter-nodal communication. For shared memory within the NUMA sockets, we use C++-11 threading model. We show the scalability results of the proposed method up to a few several thousand cores.

Submitted/Under Submission

1. P. Kumar, *Spectral two level preconditioning of Schur complement in algebraic domain decomposition framework*, **submitted (Journal)**, 2014

2. P. Kumar, *High performance implementation of Schur complement preconditioner*, under preparation, 2014

3. P. Kumar, Multilevel Communication Optimal Least Squares, **pending (conference)**, 2014

Software

1. P. Kumar, COLS (Communication optimal least squares), **complete** www.kumarslab.com/softwares.php

III – ATTENDED SEMINARS, WORKHOPS, CONFERENCES

1. ISPDC, IEEE 13th international symposium on parallel and distributed computing, 24-27 June 2014, Porquerolles island, France

2. HPCC, IEEE 16th international conference on high performance computing and communications, 20-22 August 2014, Paris, France

3. PMAA, Parallel matrix algorithms and applications, 2-4 July, 2014, Lugano, Switzerland

IV – RESEARCH EXCHANGE PROGRAMME (REP)

1. 7-11 April 2014, Universite Libre de Bruxelles, Brussels

2. 2-6 June 2014, University of Geneva, Geneva