Sandia National Laboratories

Operated for the U.S. Department of Energy

by

National Technology and Engineering Solutions of Sandia, LLC (NTESS)

Albuquerque, New Mexico 87185

date: March 1, 2019

from: Dr. Michael A. Heroux
Senior Scientist
Center for Computing Research
Sandia National Laboratories

Scientist in Residence
St. John's University

18125 Kreigle Lake Road
Avon, MN USA 56310
Phone: +1 505 379 5518, Fax: +1 320 845 7846
Email: maherou@sandia.gov, mheroux@csbsju.edu
Website: https://maherou.github.io

Report on Xinzhe Wu Doctoral Dissertation entitled "Contribution to the Emergence of New Intelligent Parallel and Distributed Methods Using a Multi-level Programming Paradigm for Extreme Computing"

The dissertation of Xinzhe Wu is focused on two distinct contributions: (1) a software package that generates large non-Hermitian matrices with prescribed eigenvalues and (2) algorithms to solve large non-Hermitian linear systems on advanced parallel computers, including approaches for sequenced and simultaneous collections of multiple right-hand-sides.

After an introduction Mr. Wu provides a discussion of modern high-performance computing (HPC) systems. The discussion includes performance trends, memory system design and a variety of parallel node architectures such as GPUs and Intel PHI. Next, he discusses common on-node parallel programming models and environments including CUDA, OpenMP and distributed models including MPI and UPC++. Finally, he discussed task-based approaches, including YML, which he will use later. To finish out the HPC overview, Mr. Wu discusses modern extreme-scale systems with a particular focus on the coming generation of Exascale (billion-billion operations per second) platforms. In Chapter 3, Mr. Wu provides an overview of Krylov methods, starting with basic methods and ending with an explanation of preconditioned Krylov methods and the challenges of executing them in parallel. This discussion provides the foundation needed for later topics.

Chapter 4 marks the beginning discussion of Mr. Wu's individual contributions. He starts with a discussion of the mathematical theory and algorithms needed for understanding how his software tool SMG2S works. He describes SMG2S, an open source matrix generator with interfaces for C and Python and custom interfaces for PETSc and Trilinos. SMG2S is available on GitHub under the GNU Lesser General Public License.

In Chapter 5, Mr. Wu describes the Unite and Conquer GMRES/LS-ERAM (UCGLE) method. Also, in this chapter, computational results are presented on Tianhe-2, a former number one system, and on a local parallel CPU/GPU system. Results are promising in comparison to standard methods, especially for scalability (including on GPUs), fault tolerance, asynchronous execution and other attractive features at scale.

In Chapter 6, the UCGLE method is extended to cover families of linear systems where the right-hand-sides are available in sequence. Here the ability to re-use spectral information is exploited, so that subsequent solves with different right-hand-sides will be less expensive. Experimental results confirm that the approach has merit.

Chapter 7 provides a discussion of UCGLE applied to systems with multiple simultaneous right-hand-sides. In addition to introducing a variety of other block iterative solvers, this section contains a presentation of a variety of parallel execution strategies, and guidance for checkpointing data and providing fault tolerance. Again, parallel execution results are promising.

In Chapter 8, Mr. Wu presents some approaches to automatically selecting solver parameters to improve performance. This work seems to be preliminary since results are only given for one problem.

In the penultimate Chapter 9, Mr. Wu discusses how the parallel strategies discussed in Chapter 8 for *m*-UCGLE can be implemented in YML. Since the partitioned block solver approach using a manager engine is inherently tasked based, YML is an attractive environment for encoding the parallel algorithm. Complete results were impeded by limitations in the execution environment.

Chapter 10 contains conclusions and future work.

Remarks: Mr. Wu's dissertation represents a large body of work and a clear commitment on his part to contribute to the scientific research community in both mathematical algorithms and software design and development. I find the work on SMG2S to be very good. Visiting the product website and reviewing the GitHub source code repository, I am favorably impressed with the quality of the software design, code, documentation, software release practices, and website design. This is very nice work.

Regarding Mr. Wu's efforts in developing new solvers, the thesis represents a very large volume of work. Some results are quite good, while others may need more exploration or refinement. Regardless, the effort is substantial and impressive. Developing solvers that can scale on modern supercomputers is very challenging, and Mr. Wu has done exceptionally well in his efforts.

Summary: Mr. Wu has completed a large body of work that demonstrates his understanding of parallel iterative linear solvers, high-performance computing systems and high-quality scientific software design, implementation and distribution. His dissertation is well written and organized. English usage is reasonably good. The work he presents is more than adequate to satisfy the requirements for a dissertation.

Without reservation, I believe that Mr. Xinzhe Wu's dissertation is successfully completed.

Sincerely,

Michael A. Heroux

Michael A. Heroux
Senior Scientist, Sandia National Laboratories
Scientist in Residence, St. John's University
Director of Software Technology, US DOE Exascale Computing Project
Distinguished Member, ACM
Senior Member, IEEE