Numerical Computation

Automatic Tuning of Computation-Communication Overlap for Parallel 1-D FFT

Background

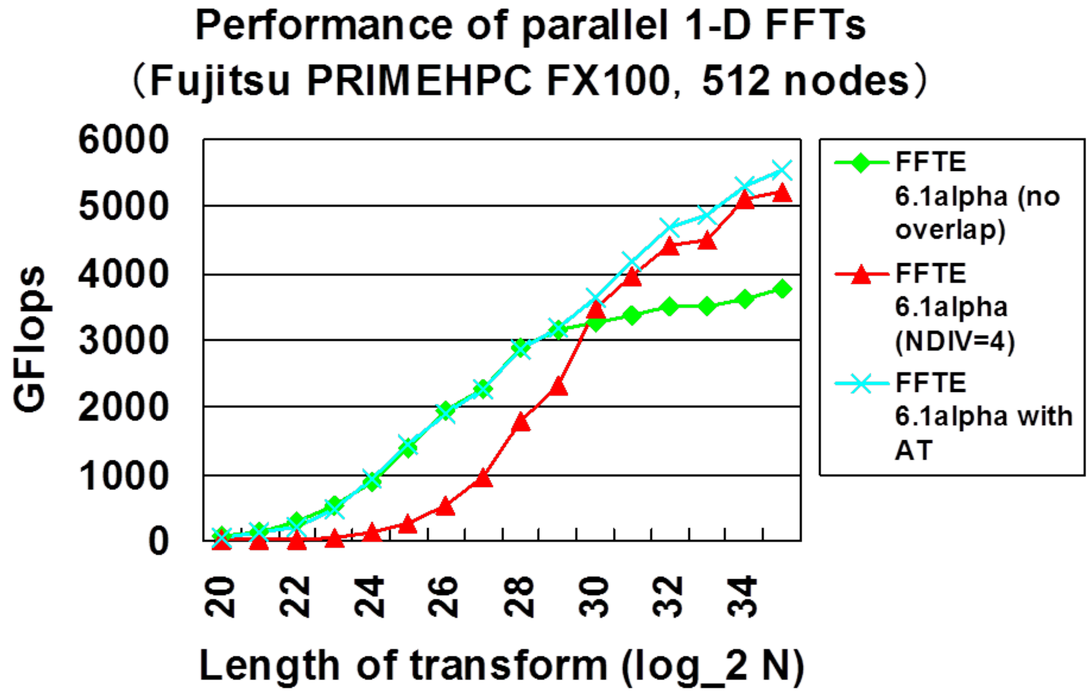
The fast Fourier transform (FFT) is widely used in science and engineering. Parallel FFTs on distributed-memory parallel computers require intensive all-to-all communication, which affects their performance. How to overlap the computation and the all-to-all communication is an issue that needs to be addressed for parallel FFTs.

Overview

We proposed an automatic tuning of computation-communication overlap for parallel 1-D FFT. We used a computation-communication overlap method that introduces a communication thread with OpenMP. An automatic tuning facility for selecting the optimal parameters of the computation-communication overlap, the radices, and the block size was implemented.

Performance

To evaluate the parallel 1-D FFT with automatic tuning, we compared its performance against that of FFTE 6.1alpha (http://www.ffte.jp/) and that of FFTE 6.1alpha with automatic tuning (AT). The performance results demonstrate that the proposed implementation of a parallel 1-D FFT with automatic tuning is efficient for improving the performance on Fujitsu PRIMEHPC FX100.

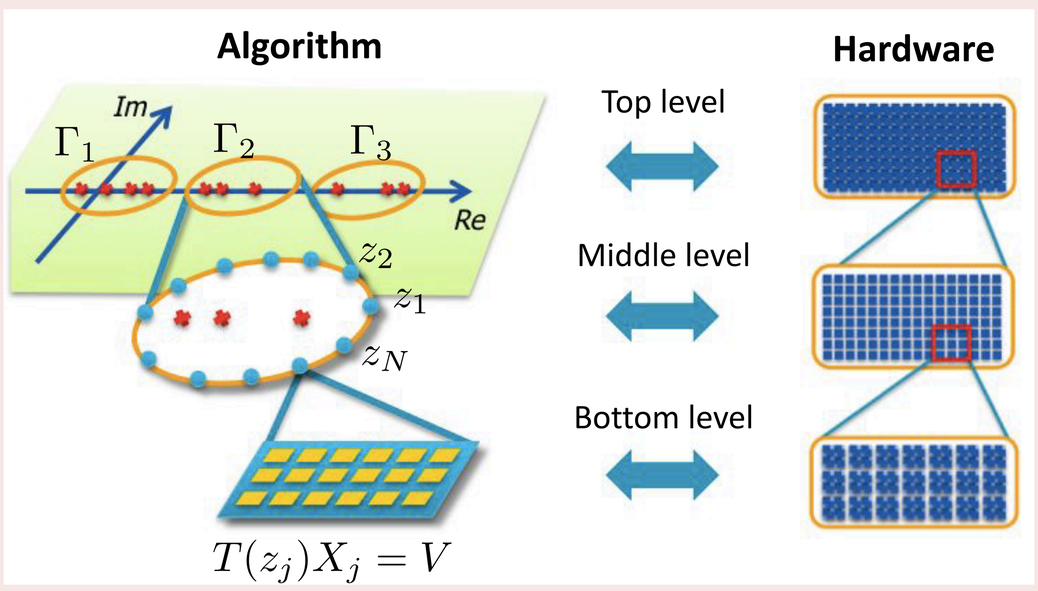


Development of Parallel Sparse Eigensolver Package: z-Pares

The aim of this research project is to develop numerical software for large- scale eigenvalue problems for post-petascale computing environment. An eigensolver based on contour integral (the SS method) has been proposed by Sakurai and Sugiura [3]. This method has a hierarchical structure and is suitable for massively parallel supercomputers [2]. Moreover, the SS method can be applicable for nonlinear eigenvalue problem [1]. Block Krylov method [4] improves the performance of the method. Based on these newly designed algorithms, we have developed a massively parallel software z-Pares freely-available from http://zpares.cs.tsukuba.ac.jp/. MATLAB version is also available in our webpage. We have also developed CISS eigensolver in SLEPc.

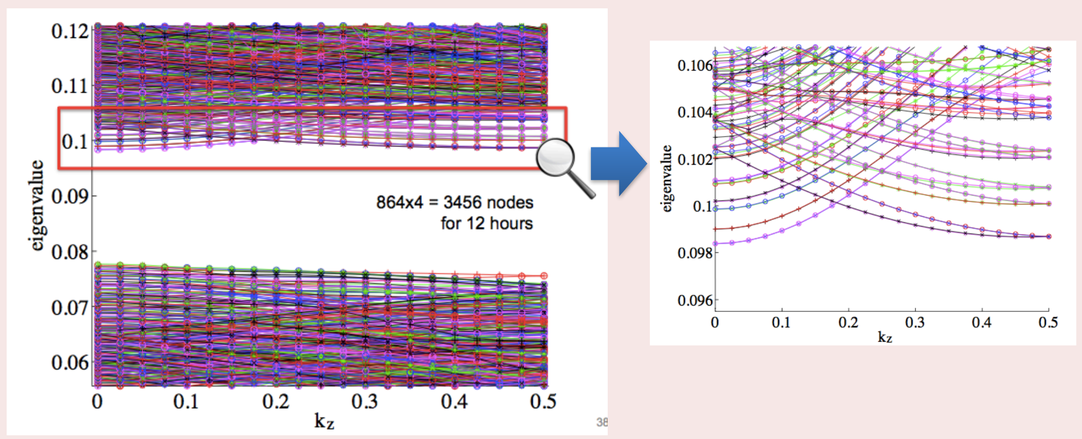
Hierarchical Parallel Structure

Hardware is grouped according to a hierarchical structure of the algorithm.



Numerical Example on the K Computer

Application for band calculation with real space density functional theory (RSDFT) [2].



Band structure of silicon nanowire of 9,924 atoms.
(matrix size = 8,719,488, Number of cores = 6,144)

*The results are tentative since they are obtained by early access to the K computer.

Reference

[1] J. Asakura, T. Sakurai, H. Tadano, T. Ikegami and K. Kimura, A numerical method for nonlinear eigenvalue problems using contour integrals, JSIAM Letters, 1 (2009) 52-55.

[2] Y. Futamura, T. Sakurai, S. Furuya and J.-I. Iwata, Efficient algorithm for linear systems arising in solutions of eigenproblems and its application to electronic-structure calculations, Proc. 10th International Meeting on High-Performance Computing for Computational Science (VECPAR 2012), 7851 (2013), 226-235..

[3] T. Sakurai and H. Sugiura, A projection method for generalized eigenvalue problems, J. Comput. Appl. Math., 159 (2003) 119-128.

[4] H. Tadano, T. Sakurai and Y. Kuramashi, Block BiCGGR: A new block Krylov subspace method for computing high accuracy solutions, JSIAM Letters, 1 (2009) 44-47.

Acknowledgment

This research was partially supported by the Core Research for Evolutional Science and Technology (CREST) Project of JST and the Grant-in-Aid for Scientific Research of Ministry of Education, Culture, Sports, Science and Technology, Japan, Grant number: 23105702.