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Innovative Multigrid Methods III

Akihiro Fujii(Kogakuin University)

Abstract

Multigrid methods are important for large-scale simulation and supercomputers. We started this ‘Innovative Multigrid Methods III’ as 3-year project from FY2023. As a first year, we have studied Communication Computation overlapping with IC(0) smoother, scalable AMG implementation research, new algorithms related with PinT, PinST researches targeted for realistic simulations such as shallow water simulation and magnetic field problems.

1 Basic information

1.1 Collaborating JHPCN centers

- Hokkaido University
- The University of Tokyo
- Nagoya University
- Kyushu University

1.2 Theme area

- Large-scale computational science

1.3 Research area

- Very large-scale numerical computation

1.4 Project members and their roles

Research items (1), (2) and (3) are described in section 2.

Akihiro Fujii³ : (1)

Kengo Nakajima^{2,4} :(CoPI) (3),(1)

Matthias Bolten⁸ :(CoPI) (1),(2)

Takeshi Iwashita¹ : (1),(2)

Akihiro Ida¹³ : (2)

Masatoshi Kawai⁶ : (2)

Satoshi Ohshima⁵ : (1),(3)

Tetsuya Hoshino⁶ : (2),(3)

Toshihiro Hanawa² : (2),(3)

Gerhard Wellein⁹ : (3)

Osni Marques¹⁰ : (1),(3)

Kenji Ono⁵ : (1)

Ryo Yoda⁸ : (1),(3)

Yasuhito Takahashi⁷ : (1)

Yen-Chen Chen¹⁴ : (1)

Martin Schreiber¹⁵ : (3)

Christie Alappat⁹ : (3)

Teruo Tanaka³ : (1)

Hiromichi Sakuta³ : (1)

Kota Yoshimoto³ : (1)

Georg Hager⁹ : (3)

Ayesha Afzal⁹ : (3)

Bole Ma⁹ : (3)

1: Kyoto U., 2: U. Tokyo, 3: Kogakuin U., 4: RIKEN R-CCS, 5: Kyushu U., 6: Nagoya U., 7: Doshisha U. 8: U. Wuppertal*, 9: FAU*, 10: LBNL, USA, 11: Technical U. of Munich*, 12: Juelich Supercomputing Centre*, 13: JAMSTEC, 14: KIT* 15: Univer-

sité Grenoble Alpes in France, *:Germany

2 Purpose and Significance of the Research

We are planning to conduct research and development on the following three items:

- (1) Research and development of fundamental algorithms in multigrid methods
- (2) Parallel reordering methods
- (3) Performance evaluation models for parallel multigrid procedures

(1) includes researches focusing on scalable performance and fundamental algorithms such as parallel in time (PinT). In (2), we study parallel reordering technique on the unstructured problem domain. (3) deals with performance evaluation models for multigrid solvers on supercomputers.

The purpose of the first year of the 3-year project is to check and update the original researches.

3 Significance as JHPCN Joint Research Project

Multigrid method is scalable and used in many fields. It is known as one of the most efficient linear solvers. It can also be applied to parallel time integration problems, which exploits parallelism in time dimension. Our research project has original codes and algorithms. Therefore, research papers and codes from the project will enhance the efficiency of the multigrid solver, and will help many researchers exploit parallelism in time direction.

Our research focuses on hierarchical al-

gorithms and their performance on supercomputers. Thus, availability of supercomputers with different kinds of architectures helps us verify the codes we are developing. In addition, a JHPCN joint research project offers collaborative research opportunity with JHPCN members who have expertise knowledge in various application fields. Our project members include international experts in Germany, U.S., France and Japan on multigrid methods and PinT. We are sure that this JHPCN joint research project promotes the international collaborative activity with JHPCN members.

4 Outline of Research Achievements up to FY2022 (Only for continuous projects)

We did our research project ‘Innovative Multigrid II’ from FY2020 to FY2022. Although researches progressed, there were research items to be done. Thus, We organized three research areas as written in Sec.2, and started new three-year project ‘Innovative Multigrid III’ from FY2023.

5 Details of FY2023 Research Achievements

We are researching in the 3 areas, (1) fundamental algorithm and PinT, (2) multicoloring technique, and (3) performance models, as written in Sec. 2.

At first, we picked up parallel in time researches. Takahashi and Iwashita investigated effectiveness of the parallel-in-space-and-time finite-element method (Pin-STFEM) in a more practical electromag-

netic field analysis. PinSTFEM was applied to a time-periodic magnetic field analysis that took magnetic hysteresis into account. The developed PinSTFEM program uses both the domain decomposition method (DDM) and parallel time-periodic explicit-error-correction (PTP-EEC) method. The magnetization history of each finite element is corrected appropriately based on time-series data of flux density vectors. The parallel performance of the developed analysis program is verified by analyses for a ring core specimen and a practical interior permanent magnet synchronous motor (IPMSM) fed by a pulsewidth modulation (PWM) inverter.

Yoda and Bolten investigated the enhancement of coarse level time integration of MGRIT by using parameterized Runge-Kutta integrators. For PinT applications, coarse level time integrators become the key element that determines the convergence behavior and the parallel performance. They also study block epsilon-circulant preconditioner for time-dependent PDEs. By approximating the time-dependent governing equation by the circulant matrix, they try to create a good preconditioner that can be calculated efficiently with circulant property.

Schreiber investigated the effectiveness of parareal and MGRIT for shallow water equations on the rotating sphere. Chen and Nakajima proposed multi-level cascadic parareal method especially for explicit time integration. Its convergence was evaluated for compressible supersonic flow problems.

Secondly, Fujii, Tanaka and Nakajima investigated the scalable implementation for

AMG solvers with so many processes like 500,000 processes. When the number of processes is large, it needs to be adjusted efficiently on the coarse levels. We proposed a method which creates the parallelism adjusted coarse level matrix at one time. By utilizing the proposed method, our solver shows the performance improvement and reaches the same or better level performance with the state-of-the-art AMG library.

Thirdly, in our research on multi-coloring, Kawai et al. are developing methods that can satisfy multiple requirements, such as degree of parallelism, data locality, and load balancing, in order to achieve high-performance parallel computing. In this research, a new coloring method using a pseudo-quantum annealer is investigated to achieve the objectives. Quantum annealing computes approximate solutions that satisfy multiple requirements that can be obtained in a short time. However, there is no pseudo-quantum annealing that can handle problems that have a large degree of freedom that can be solved by the multigrid method. Therefore, we are considering applying a hierarchical multi-coloring method and a method that can dissolve the coloring in a subregion with a pseudo-quantum annealer.

Finally, Nakajima investigated halo communication and computation overlapping (CC-overlapping). In parallel finite element methods (FEM) and finite volume methods (FVM), CC-Overlappings are commonly employed, often in conjunction with the dynamic loop scheduling feature of OpenMP. This approach has been primarily applied to

sparse matrix-vector products (SpMV) and explicit solvers. Previous studies by the author have proposed reordering techniques for applying CC-Overlapping to processes involving global data dependencies, such as the Conjugate Gradient method preconditioned by Incomplete Cholesky Factorization (ICCG). Successful implementations on massively parallel supercomputers demonstrated high parallel performance, but the application of CC-Overlapping was limited to SpMV. Nakajima proposed a method to apply CC-Overlapping to the forward and backward substitutions of the IC(0) smoother of the parallel Conjugate Gradient method preconditioned by Multigrid (MGCG).

6 Self-review of Current Progress and Future Prospects

This year is the first year of this multigrid project. As a first year, we were able to advance individual researches. Next year, we would like to increase collaborative activity including parallel multi-coloring technique, performance models and CC-overlapping.

7 List of publications and presentations

Journal Papers (Refereed)

- Yasuhito Takahashi, Koji Fujiwara and Takeshi Iwashita, “Parallel-in-Space-and-Time Finite-Element Method for Time-Periodic Magnetic Field Problems with Hysteresis”, IEEE Transactions on Magnetics, doi: 10.1109/TMAG.2023.3307498
- João Guilherme Caldas Steinstraesser

a, Pedro da Silva Peixoto a, Martin Schreiber(+), “Parallel-in-time integration of the shallow water equations on the rotating sphere using Parareal and MGRIT”, Journal of Computational Physics, Vol.496, Jan. 2024.

- Yen-Chen Chen(+), Kengo Nakajima, A Cascadic Parareal Method for Parallel-in-Time Simulation of Compressible Supersonic Flow, IPSJ Transaction on Advanced Computing Systems (in press), 2024
- Akihiro Fujii, Teruo Tanaka and Kengo Nakajima, “Light Weight Coarse Grid Aggregation for Smoothed Aggregation Algebraic Multigrid Solver”, IEEE ACCESS, 12 pp.57345-57355, 2024 年

Proceedings of International Conference Papers (Refereed)

- Kengo Nakajima, Communication-Computation Overlapping for Parallel Multigrid Methods, IEEE Proceedings of iWAPT 2024 in conjunction with IPDPS 2024 (in press), 2024

Presentations at International conference (Non-refereed)

- Ryo Yoda(+) and Matthias Bolten(+), “Parallel Performance of Block Epsilon-circulant Preconditioner for Time-dependent PDEs”, SIAM Conference on Parallel Processing for Scientific Computing (PP24), Baltimore, Maryland, U.S., March 5-8, 2024
- Ryo Yoda(+) and Matthias Bolten(+), “An investigation of parallel perfor-

mance of block epsilon-circulant preconditioner for time-dependent PDEs”, HP-CAAsia 2024: International Conference on High Performance Computing in Asia-Pacific Region (Poster), Nagoya, Japan, January 25-27, 2024

- Ryo Yoda(+), Matthias Bolten(+), “Multilevel extension of parameterized Runge-Kutta methods for Multigrid Reduction in Time” , The 12th Workshop on Parallel-in-time Integration, July 17-21, 2023
- Kengo Nakajima, “Communication-Computation Overlapping in Parallel Multigrid Methods” , 21st Copper Mountain Multigrid Conference, Copper Mountain, Colorado, April 19, 2023

Presentations at domestic conference (Non-refereed)

- 中島研吾, 「並列多重格子法における通信・計算オーバーラップの最適化」, 2023年並列／分散／協調処理に関する『函館』サマー・ワークショップ, 日本応用数理学会「行列・固有値問題の解法とその応用」研究部会 (MEPA) 2023年8月3日, 北海道函館市

Published open software library and so on

Other (patents, press releases, books and so on)