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Innovative Multigrid Methods II

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Abstract

Multigrid method is known as one of the most efficient and scalable methods on the supercomputers. It is applicable to partial differential equations with fine and coarse grids, linear matrix problems, and parallel time integration. Our project studies multigrid related themes in 3-year plan. This report is for the final year. Although we continue studying the area, we've conducted researches in 2022, including the topics of computation and communication overlapping for a multigrid solver, new "near kernel" setting approach of AMG solver, PinST researches for FEM application and coarse grid optimization using Runge-Kutta method in PinT.

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

Akihiro Fujii[3] :AMG, PinST
Kengo Nakajima[2,4] : (Co-PI) Application, GMG, PinST, AMG
Matthias Bolten[8] : (Co-PI) GMG, PinST, AMG
Masatoshi Kawai[2] : GMG, AMG
Akihiro Ida[13] : GMG, AMG
Gerhard Wellein[9] : GMG, AMG
Christie Alappat[9] : GMG, AMG
Martin Schreiber[11] : GMG, AMG
Tetsuya Hoshino[2] : GMG, AMG
Satoshi Ohshima[6] : GMG, AMG
Toshihiro Hanawa[2] : GMG, AMG
Osni Marques[10] : GMG, AMG
Kenji Ono[5] : PinST
Takeshi Iwashita[1] : AMG, PinST
Yasuhito Takahashi[7] : PinST
Robert Speck[12] : PinST
Atsuhiro Miyagi[14]: PinST
Teruo Tanaka[3] :AMG, PinST
Alexander T.Magro[2] : GMG
Ryo Yoda[2] : PinST, AMG
Yen-Chen Chen[2] : PinST
Gayatri Caklovic[12]:PinST
Ryo Sagayama[3] : PinST
Hiromichi Sakuta[3] : AMG
Kota Yoshimoto[3] : AMG

1: Hokkaido 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: Taisei Corp. *:Germany

2 Purpose and Significance of the Research

Multigrid method is a promising approach for large-scale computing in exa-scale era. We develop robust and efficient parallel multigrid methods for both of geometric multigrid (GMG) and algebraic multigrid(AMG), focusing on robust and efficient smoothers, and hierarchical methods which are proposed and developed by ourselves. We have original PinST methods. Developed methods will be implemented as a numerical library and it will be applied to various types of applications. These researches are expected to help achieve high performance for large-scale real-world applications.

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 as written in Research purpose. 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 algorithms 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, US, and Japan on multigrid methods and PinST. We are sure that this JHPCN joint research project promotes the international collaborative activity with JHPCN members.

4 Outline of Research Achievements up to FY2021 (Only for continuous projects)

Research results have been presented in fields GMG, AMG, and PinST. The main research items of last year are as follows.

GMG	Communication and computation overlapping technique
AMG	Weak scaling performance enhancement
PinST	Coarse level redistribution for scalability

A part of the research items were continued to be researched in 2022.

5 Details of FY2022 Research Achievements

This project started as a research activity in 3 fields: GMG, AMG, PinST. It was set as a 3-year project, and this report is for the final year. Main research presentation and publication of the final year is listed in section 7. Here, 3 research items are picked up for introduction.

5.1 PinST method for an electromagnetic field analysis

We enhanced the parallel performance of a parallel-in-space-and-time (PinST) finite-element method (FEM) using time step overlapping. The developed PinST FEM is based on a combination of the domain decomposition method (DDM) as a parallel-in-space (PinS) method and a parallel time-periodic explicit error correction (PTP-EEC) method, which is one of the parallel-in-time (PinT) approaches. The parallel performance of the PinST FEM was further improved by overlapping the time steps with different processes in the PTP-EEC method. By applying the overlapping PTP-EEC method, the convergence of the transient solution to its steady state was accelerated drastically. Consequently, the good parallel performance of the PinST FEM was achieved in magnetic field analyses of the practical IPMSM using a massively parallel computing environment, in which over 10 000 processes were used.

5.2 MGRIT method for hyperbolic PDEs

MGRIT is one of the multigrid-based parallel-in-time methods and still faces convergence challenges for time-dependent problems of hyperbolic PDEs. These difficulties and failures are due to the coarse-grid operator constructed by the simple rediscretization approach. Therefore, in this work, we tested a new construction approach for coarse-grid operators of MGRIT. This method assumes time integration of Runge-Kutta methods on the coarse level and regards the coefficients of the Butcher tableau as parameters. The coefficients are then determined to reduce the convergence rates based on MGRIT's convergence analysis. The obtained Butcher tableau is dedicated to the MGRIT convergence and is a multistage zeroth order scheme, which is not widely used as an ODE solver.

Preliminary numerical experiments confirm that our approach yields convergence for one-dimensional linear advection problems with explicit time discretization and upwind difference schemes that diverges in MGRIT with a simple rediscretization approach. Even for particularly challenging high-order discretization schemes, our approach achieves convergence at about half the cost of ideal coarse-grid operators, confirming that it is particularly effective for problems discretized with high-order schemes.

In future work, we plan to investigate the robustness of obtained schemes by our approach. Our approach does not require additional assumptions about the fine-level discretized time-stepping method. However, the cost of searching and determining coefficients is relatively high, and it is necessary to verify how well coefficients obtained for one particular problem are valid for other problems.

5.3 Near-kernel components setting for SA-AMG

It is known that the SA-AMG method can improve the convergence by specifying the "near kernel" component according to the problem. Although the cost of finding the near-kernel component of the problem matrix is high, the hard-to-converge component of the iterative solution method corresponds to finding the large eigenvalue component of the iteration matrix that updates the error components, and may be found at low cost.

Therefore, in this study, we focused on the Gauss-Seidel method, which is used as a smoother for the SA-AMG method, and investigated whether the convergence of the SA-AMG method could be improved when using the hard-to-converge component of the Gauss-Seidel method. Those components were calculated by Gauss-Seidel iteration matrix with eigenvalue calculation library. In numerical experiments, it was found that in many cases the convergence was improved more than when specifying the near-kernel component of the problem matrix.

Fig.1 shows the residual history of SA-AMG solver with near kernel components. The left figure shows the case with near kernel components of the problem matrix. The right figure shows the case with the hard-to-converge components of Gauss-Seidel method. There are 7 lines correspond to the number of components. For this problem, hard-to-converge components of Gauss-Seidel work better than near kernel components of the problem matrix.

We have to study the method to balance the calculation cost of the hard-to-converge components of Gauss-Seidel and convergence improvements, in near future.

6 Self-review of Current Progress and Future Prospects

Our project made research presentations and publications successfully every year in 3 years. The major challenges we faced were performance issues that depended on supercomputer types and the time required for basic researches. They are taken over to JHPCN project in 2023. In the next JHPCN project, we will continue multigrid related researches, specifically focusing on basic research issues, parallel reordering methods, and performance modeling for parallel multigrid methods.

7 List of publications and presentations

Journal Papers (Refereed)

1. Yasuhito Takahashi, Koji Fujiwara and Takeshi Iwashita, Parallel-in-space-and-time finite-element analysis of electric machines using time step overlapping in a massively parallel computing environment, COMPEL-The international journal for computation and mathematics in electrical and electronic engineering, Vol. 42 No. 2, pp. 449-462, (2023).

Proceedings of International Conference Papers (Refereed)

1. R. Yoda, M. Bolten(+), K. Nakajima, A. Fujii, Acceleration of Optimized Coarse-Grid Operators by Spatial Re-

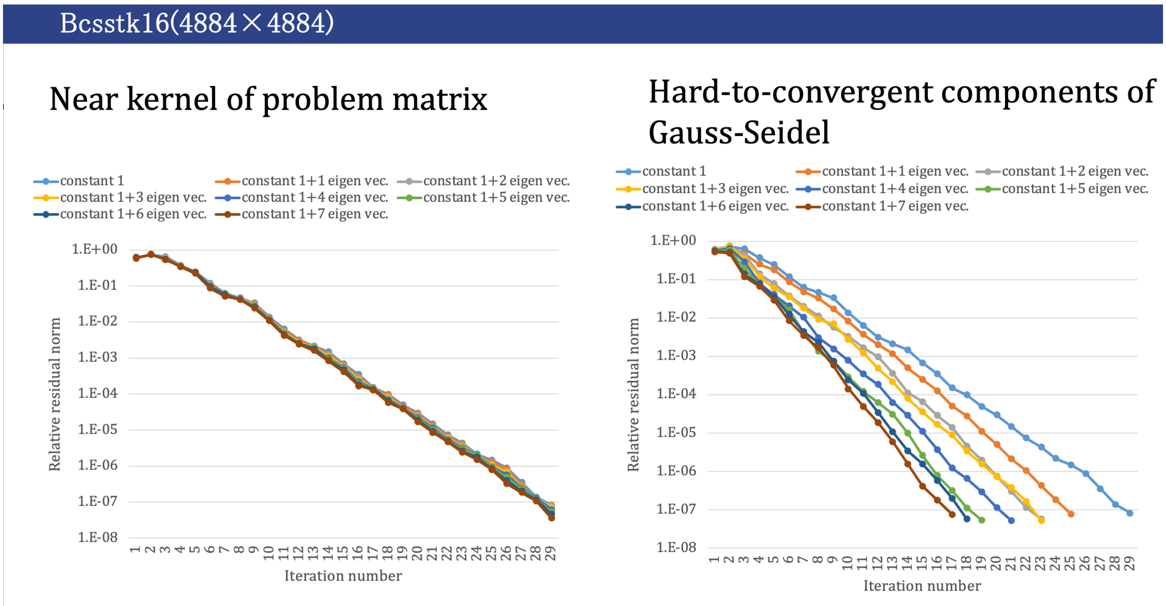

Fig. 1 Residual history of SA-AMG solver with near kernel components. Left graph shows the result of setting near kernel components of the problem matrix, and right graph shows the result with hard-to-converge component of Gauss-Seidel method

distribution for Multigrid Reduction in Time. In: D. Groen, C. de Mulatier, M. Paszynski, V.V. Krzhizhanovskaya, J.J. Dongarra, P.M.A. Sloot(eds), Computational Science – ICCS 2022. ICCS 2022. Lecture Notes in Computer Science, vol 13351. Springer, Cham. https://doi.org/10.1007/978-3-031-08754-7_29

Presentations at International conference (Non-refereed)

1. K. Nakajima, Innovative Scientific Computing by Integration of (Simulation + Data + Learning) in Information Technology Center, The University of Tokyo, NHR PerfLab Seminar, 2022 (Invited Talk)
2. K. Nakajima, T. Iwashita, H. Yashiro, H. Nagao, T. Shimokawabe, H. Matsuba, T. Ogita, T. Katagiri, h3-Open-BDEC: Innovative Software Infrastructure for Scientific Computing in the Exascale Era by Integrations of (Simulation + Data + Learning), The 31st International Toki Conference on Plasma and Fusion Research (ITC31), 2022 (Invited Talk)
3. Ryo Yoda, Matthias Bolten(+), Kengo Nakajima and Akihiro Fujii, “Parameterized Runge-Kutta Integrators on Coarse Levels in Multigrid Reduction in Time”, 21st Copper Mountain Conference on Multigrid Methods, April 16–20, 2023, Denver, CO, U.S.
4. Ryo Sagayama, Akihiro Fujii, Teruo Tanaka, Takumi Washio, Takeshi Iwashita, TSC Method using Semi-Implicit Method for Spring Mass

Simulation, HPCAsia2023 (poster), March 1, 2023.

Presentations at domestic conference (Non-refereed)

1. 中島研吾，通信と計算のオーバーラップによる前処理付き並列反復法，第 27 回計算工学会講演会，2022 年 6 月
2. 中島研吾，Wisteria/BDEC-01（Odyssey）における前処理付き反復法の高速化，2022 年並列／分散／協調処理に関する『下関』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），2022 年 7 月
3. 中島研吾，通信・計算オーバーラップによる並列多重格子法，日本応用数理学会年会 2022，2022 年 9 月
4. 中島研吾, 住元真司, 八代尚, 荒川隆, 松葉浩也, h3-Open-BDEC：「計算・データ・学習」融合による革新的スーパーコンピューティング，RIMS 共同研究：数値解析が拓く次世代情報社会～エッジから富岳まで～，2022 年 10 月 14 日 (金)、京都大学 益川ホール
5. 中島研吾，通信・計算オーバーラップによる並列多重格子法，情報処理学会第 187 回 HPC 研究会，2022 年 12 月（in press）
6. 岩下武史、池原紘太、多森浩俊、深谷猛、誤差ベクトルのサンプリングによるクリロフ分空間反復法の収束性改善、RIMS 共同研究 (公開型)、数値解析が拓く次世代情報社会～エッジから富岳まで～、2022 年 10 月 14 日 (金)、京都大学 益川ホール
7. 依田凌, Bolten Matthias(+), 中島研吾, 藤井昭宏, MGRIT の粗格子演算子に対する Runge-Kutta 法の係数最適化とその高速化, 第 185 回 HPC 研究会 (SWoPP2022)
8. Y.C. Chen, K. Nakajima, A Parallel-in-Time Method for Compressible Fluid Explicit Simulation, IPSJ SIG Technical Report, 2022-HPC-185-27, 2022
9. 高橋康人, 藤原耕二, 岩下武史;「空間分割・時間分割併用型並列有限要素法を用いた電気機器のヒステリシス磁界解析に関する検討」, 電気学会静止器・回転機合同研究会資料, SA-23-019/RM-23-019, 於 東海大学＆オンライン, 2023 年 3 月.
10. 作田啓倫, 藤井昭宏, 田中輝雄, 岩下武史, SA-AMG 法における反復行列を用いたニアカーネル成分の設定手法の評価, 第 188 回 HPC 研究会, 2023 年 3 月

Published open software library and so on

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