jh190041-NAHI

Kengo Nakajima (Information Technology Center, The University of Tokyo, Japan)

Innovative Multigrid Methods

T. Iwashita[1], K. Nakajima (Leading-PI)[2,4], T. Hanawa[2], A. Ida[2], T. Hoshino[2], N. Nomura[2], A. Fujii[3], R. Yoda[3], M. Kawai[4], S. Ohshima[5], M. Bolten (Co-PI)[6], L. Claus[6], G. Wellein[7], O. Marques[8]
1: Hokkaido U., 2: U. Tokyo, 3: Kogakuin U., 4: RIKEN R-CCS, 5: Kyushu U., 6: U. Wuppertal, Germany, 7: FAU, Germany, 8: LBNL, USA

Background

- Multigrid (MG)
  - ✓ Scalable multilevel method for solving linear equations
  - ✓ GMG (Geometrical Multigrid) and AMG (Algebraic)
  - ✓ Suitable for large-scale problems
  - ✓ Generally, number of iterations until convergence for multigrid method is kept constant as the problem size changes.
  - ✓ The parallel multigrid method is expected to be one of the most powerful tools on exa-scale systems.
  - ✓ Applied to rather well-conditioned problems (e.g. Poisson's equation)
  - ✓ Many sophisticated methods for robustness of MG have been developed for ill-conditioned problems derived from real-world scientific and engineering applications.
- Robust and efficient algorithms for GMG and AMG methods, and PinST towards the Exascale/Post-Moore Era.

Development: 2-Year Project (FY.2018 & 2019)

- Serial Optimization for both of GMG & AMG
  - ✓ Robust & Efficient Smoother (MS-BMC-GS, Multiplicative-Schwartz type Block Multicolor Gauss-Seidel)
  - ✓ Matrix Storage Format by SELL-C-σ [Kreutzer, Wellein et al. 2014]
  - ✓ Extraction of Near-Kernel Vectors
  - ✓ Parallel Optimization for both of GMG & AMG
  - ✓ Parallel Reordering/Aggregation
  - ✓ AM-hCGA (Adaptive Multilevel hCGA)
  - ✓ Fast Parallel Mesh Generation by IME/Burst Buffer
- Parallel in Space/Time (PinST)
  - ✓ PinST-TSC (Time Segment Correction) for Nonlinear Problems
  - ✓ PinST-Explicit (Explicit Time Marching
- Applications
  - ✓ GMG: 3D Groundwater Flow
  - ✓ AMG: 3D Solid Mechanics
  - ✓ PinST-TSC: Nonlinear Heat Transfer
  - ✓ PinST-Explicit: Heat Transfer, Incomp. Navier-Stokes with Pressure Correction
- Target Systems
  - ✓ Oakforest-PACS(OFP) (U.Tokyo) /Polaire(Hokkaido U.): Intel Xeon Phi
  - ✓ ITO-A (Kyushu U.)/Grand Chariot (Hokkaido U.): Intel Xeon (Skylake)
  - ✓ Oakbridge-CX (U.Tokyo): Intel Xeon (Cascade Lake)
- Open-Source Library
  - ✓ Various Types of Applications
  - ✓ One of the First Practical Library of MG including PinST, especially PinST-Exp

PinST-Exp: MGRIT-based Preconditioning (2018)

- We investigated parallelization in time direction especially for explicit methods. We took up the MGRIT method for parallelization of explicit time evolution, and proposed to use MGRIT as a preconditioner of Krylov subspace method.
- Figure 1 shows the residual history of the proposed method, MGRIT, and non-preconditioned GMRES using a single node of OFP.
- MGRIT preconditioned GMRES reached convergence faster than the other 2 methods, and it exemplified that the coarse grid problems' instability can be soothed by using MGRIT as a preconditioner.

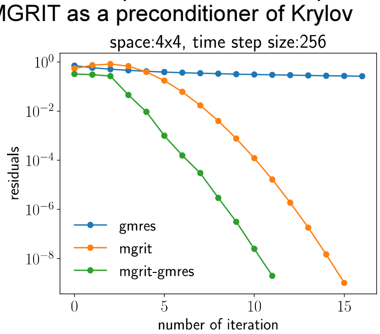

Figure 1. AM-hCGA (Adaptive Multi Level hCGA (Hierarchical Coarse Grid Aggregation)

PinST-Exp/Imp (2018)

- If PinST is applied to applications with explicit time-marching, stability problem occurs at coarser levels in time direction.
- In order to avoid this situation, we proposed a new method PinST-Exp/Imp, where explicit time marching is applied to the finest level in time direction, and implicit ones for other coarser levels.
- Figure 2 shows the results (strong scaling) for 2D heat transfer problem using 4 nodes of OFP.
- The orange line (Exp/Imp) provides the faster computation time than Exp/Exp and Imp/Imp. This is one of the first examples for PinST computations with explicit time-marching

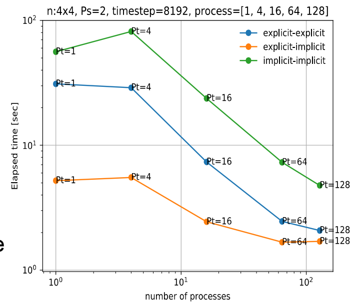

Figure 2. Effect of PinSt-Exp/Imp, Strong Scaling up to 4 Nodes of OFP

Parallel Aggregation (2018)

- We proposed a parallelization method with multi-coloring for parallel aggregation in the AMG
- Figure 3 shows the comparison between the sequential/decoupling aggregation and the proposed method for Parabolic FEM problem.
- If we apply the decoupling aggregation, the convergence varied according to the degree of parallelisms.
- The parallel aggregation with multi-coloring kept almost constant convergence even if the degree of parallelism changed.

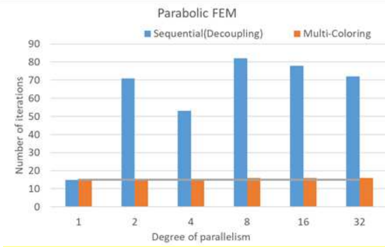

Figure 3. Effect of Parallel Aggregation with Multi-Coloring on Parabolic FEM Problem (Iterations of AMG Solver)

Plan for FY.2019

- GMG
  - ✓ Further Optimization of the pGW3D-FVM on OFP (CM-RCM, SELL-C-σ, MS-BMC-GS)
  - ✓ Improvement of Convergence by Parallel Reordering
  - ✓ Improvement of Convergence by Utilization of Near-Kernel Vectors
  - ✓ Further Optimization of Mesh Generation by IME on OFP
  - ✓ Improvement of Scalability by Adaptive Multilevel hCGA (AM-hCGA)
- AMG
  - ✓ Optimization of GeoFEM SA-AMG on OFP using ELL, SELL-C- σ
  - ✓ Further Improvement of the Algorithm by MS-BMC-GS
  - ✓ Further Improvement of the Convergence by Parallel Reordering/Aggregation
  - ✓ Implementation of hCGA and MA-hCGA for Scalability
- PinST-TSC
  - ✓ Optimization of GeoFEM SA-AMG on OFP using ELL, SELL-C-σ
  - ✓ Further optimization of the pHEAT-3D
  - ✓ Implementation of Multigrid Solver (SA-AMG) in Space Domain for Scalable Computation
- PinST-Exp
  - ✓ Further Optimization of the MGRIT Preconditioner
  - ✓ Further Optimization of pHEAT-3D with PinST Exp/Inp
  - ✓ Development of hybNS for 3D Compressible Navier-Stokes Flow by FVM with PinST-Exp