Speeding up Large Eddy Simulation by Multigrid preconditioned Krylov subspace methods with mixed precision

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§1 Introduction

Background

Large Eddy Simulation (LES)

- LES is a mathematical model for turbulence flow.
- LES is widely used in many scientific applications such as computational climate science, computational fluid dynamics.

Computational climate science

- LES is used for computing the pressure and the velocity.

  → **The 3-dimensional Poisson problems are needed to be solved.**

§1 Introduction

Background

The 3-dimensional Poisson problems arising from LES

- are needed to be solved at the each time step.
- are discretized by the Finite Difference method.

→ **Linear systems with large and sparse matrix.**

- The solution of these linear systems is the time-consuming part.

→ We need to reduce the computation time of this part.

In order to reduce the computation time for solving these linear systems, we apply the preconditioned Krylov subspace methods with mixed precision.

§1 Introduction

Purpose of this study

- We apply the Multigrid preconditioned Krylov subspace methods to the linear systems arising from LES and evaluate their performance.
- Moreover, we also apply the mixed precision approach in order to reduce computation time.

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§2 Linear systems arising from LES

The computation of the velocity and the pressure in LES

The velocity and the pressure are computed by the Simplified Marker and Cell (SMAC) method. In the SMAC method, the velocity $u^{(n+1)}$ and the pressure $p^{(n+1)}$ are computed by the following recursions.

$$
\begin{aligned}
u^{(\mathrm{P})} &= u^{(n)} + \Delta t \left[A^{(n)} + \nabla p^{(n)} + B^{(n)} + F^{(n)} \right], \\
u^{(n+1)} &= u^{(\mathrm{P})} - \Delta t \nabla \phi, \\
p^{(n+1)} &= p^{(n)} + \phi.
\end{aligned}
$$

n : time step number, Δt : time step size, ϕ : pressure correction amount,
$u^{(\mathrm{P})}$: velocity at the intermediate between $u^{(n)}$ and $u^{(n+1)}$,
$A^{(n)}$: advective term, $B^{(n)}$: diffusion term, $F^{(n)}$: external force term.

§2 Linear systems arising from LES

Computation of the pressure correction amount ϕ

Recursion for $u^{(n+1)}$: $u^{(n+1)} = u^{(\mathrm{P})} - \Delta t \nabla \phi$

By taking the divergence of the above recursion and using the equation of continuity $\nabla \cdot u^{(n+1)} = 0$, the following Poisson equation can be obtained.

3-D Poisson equation : $\triangle \phi = \dfrac{1}{\Delta t} \nabla \cdot u^{(\mathrm{P})}$

§2 Linear systems arising from LES

3-dimensional Poisson problem

The Poisson equation

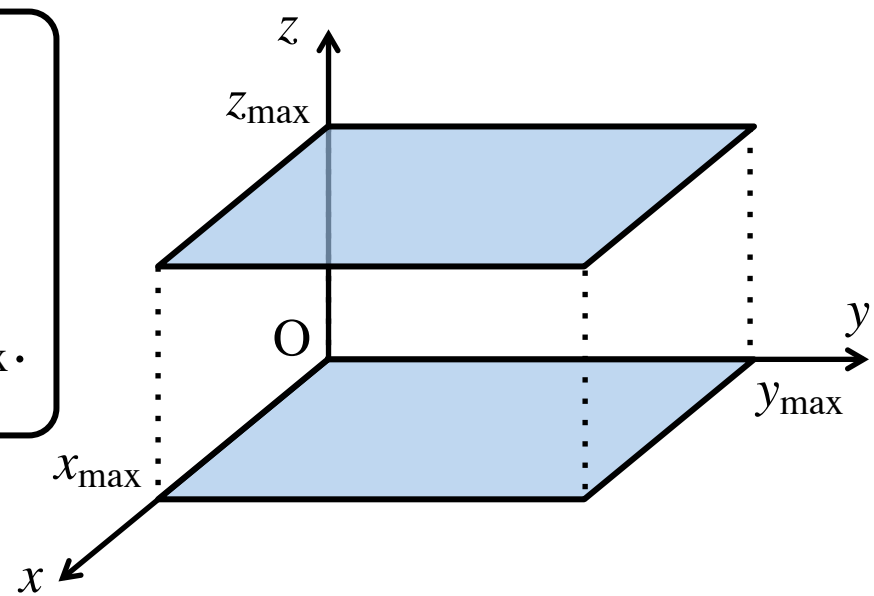
$$\triangle\phi = \frac{1}{\Delta t}\nabla \cdot u^{(\mathrm{P})} \text{ in } (0, x_{\max}) \times (0, y_{\max}) \times (0, z_{\max})$$

The boundary conditions

$$\phi(0, y, z) = \phi(x_{\max}, y, z),$$

$$\phi(x, 0, z) = \phi(x, y_{\max}, z),$$

$$\frac{\partial\phi(x, y, z)}{\partial z} = 0 \text{ at } z = 0 \text{ and } z = z_{\max}.$$



§2 Linear systems arising from LES

3-dimensional Poisson problem

$$\triangle\phi = \frac{1}{\Delta t}\nabla \cdot u^{(\mathrm{P})} \text{ in } (0, x_{\max}) \times (0, y_{\max}) \times (0, z_{\max}),$$

$$\phi(0, y, z) = \phi(x_{\max}, y, z),$$

$$\phi(x, 0, z) = \phi(x, y_{\max}, z),$$

$$\frac{\partial\phi(x, y, z)}{\partial z} = 0 \text{ at } z = 0 \text{ and } z = z_{\max}.$$

Discretization by the Finite Difference method

Linear systems

$$A\boldsymbol{x}^{(n)} = \boldsymbol{b}^{(n)},\ n = 0, 1, \ldots, n_{\max}$$

A is an $N \times N$ real symmetric and singular matrix.
$n_{\max}$ denotes the number of time steps.

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§3 Multigrid preconditioned Krylov subspace methods with mixed precision

Linear systems arising from LES

$$A\boldsymbol{x} = \boldsymbol{b}$$

- The matrix A is a real symmetric and singular.
- The solution $\boldsymbol{x}$ exists since the right-hand side $\boldsymbol{b}$ is in the range of A.

Krylov subspace methods

Krylov subspace methods for symmetric matrix

- Preconditioned Conjugate Gradient (CG) method
- Preconditioned Conjugate Residual (CR) method

➡ The preconditioned CR method cannot minimize the residual of the original linear system $A\boldsymbol{x} = \boldsymbol{b}$.

Krylov subspace method for non-symmetric matrix

- Right preconditioned Orthomin(m) method

➡ The Orthomin(m) method generates the Krylov subspaces from the last m orthonormal vectors. This method can minimize the residual of the original linear system $A\boldsymbol{x} = \boldsymbol{b}$.

§3 Multigrid preconditioned Krylov subspace methods with mixed precision

The Multigrid preconditioner

- The Multigrid method is one of methods for solving linear systems.

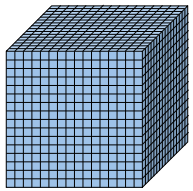
- In the Multigrid method, linear systems are approximately solved by the stationary iterative methods (e.g., Gauss-Seidel method) on the coarse grids and the fine grids.

- By using the coarse grids and the fine grids, the Multigrid method can reduce the low-frequency error components and the high-frequency error components effectively.

In this study, we use the Multigrid method as a preconditioner of the Krylov subspace methods.

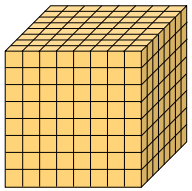
Multigrid preconditioner (V-cycle)

Level 0



Grid width: h

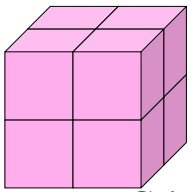
Level 1



Grid width: $2h$

⋮

Level M



Grid width: H

Pre-smoothing: $A^h \boldsymbol{x}^h = \boldsymbol{b}^h$

Compute $\boldsymbol{r}^h = \boldsymbol{b}^h - A^h \boldsymbol{x}^h$

Restriction: $\boldsymbol{r}^{2h} = I_h^{2h} \boldsymbol{r}^h$

$\boldsymbol{b}^{2h} = \boldsymbol{r}^{2h}$

Pre-smoothing: $A^{2h} \boldsymbol{x}^{2h} = \boldsymbol{b}^{2h}$

Compute $\boldsymbol{r}^{2h} = \boldsymbol{b}^{2h} - A^{2h} \boldsymbol{x}^{2h}$

Restriction: $\boldsymbol{r}^{4h} = I_{2h}^{4h} \boldsymbol{r}^{2h}$

$\boldsymbol{b}^{4h} = \boldsymbol{r}^{4h}$

Apply μ steps of the stationary iterative methods to $A^H \boldsymbol{x}^H = \boldsymbol{b}^H$

Prolongation and compute the corrected approximation:

$\boldsymbol{x}^{2h} \leftarrow \boldsymbol{x}^{2h} + I_{4h}^{2h} \boldsymbol{x}^{4h}$

Post-smoothing: $A^{2h} \boldsymbol{x}^{2h} = \boldsymbol{b}^{2h}$

Prolongation and compute the corrected approximation:

$\boldsymbol{x}^h \leftarrow \boldsymbol{x}^h + I_{2h}^h \boldsymbol{x}^{2h}$

Post-smoothing: $A^h \boldsymbol{x}^h = \boldsymbol{b}^h$

In the Pre- and Post-smoothing, ν_1 and ν_2 steps of the stationary iterative methods are executed, respectively.

§3 Multigrid preconditioned Krylov subspace methods with mixed precision

$\boldsymbol{x}_0$ is an initial guess,
Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$,
Roughly solve $Az_0 = \boldsymbol{r}_0$ for z_0 by the Multigrid method (Single precision),
Set $\boldsymbol{p}_0 = \boldsymbol{z}_0$,
For $k = 0, 1, \ldots,$ until $\|\boldsymbol{r}_k\|_2 \le \varepsilon\|\boldsymbol{b}\|_2$ do:

$$\alpha_k = \frac{(\boldsymbol{r}_k, A\boldsymbol{p}_k)}{(A\boldsymbol{p}_k, A\boldsymbol{p}_k)},$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k,$$

$$\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \alpha_k A\boldsymbol{p}_k,$$

Roughly solve $Az_{k+1} = \boldsymbol{r}_{k+1}$ for z_{k+1} by the Multigrid method (Single precision),

$$\beta_{i,k} = -\frac{(A\boldsymbol{z}_{k+1}, A\boldsymbol{p}_i)}{(A\boldsymbol{p}_i, A\boldsymbol{p}_i)} \quad \text{for } i = k-m+1, k-m+2, \ldots, k,$$

$$\boldsymbol{p}_{k+1} = \boldsymbol{z}_{k+1} + \sum_{i=k-m+1}^{k} \beta_{i,k}\boldsymbol{p}_i,$$

$$A\boldsymbol{p}_{k+1} = A\boldsymbol{z}_{k+1} + \sum_{i=k-m+1}^{k} \beta_{i,k}A\boldsymbol{p}_i,$$

End for

Multigrid preconditioned Orthomin(m) method with mixed precision.

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§4 Numerical Experiments

Target problem

$$A\boldsymbol{x}^{(n)} = \boldsymbol{b}^{(n)}, \quad n = 0, 1, \ldots, 100.$$

- The size N of A : 20,709,376,
- The number of nonzero elements of A : 144,441,344.

Numerical experiments

- We apply the Multigrid preconditioned Krylov subspace methods to the linear systems arising from LES, and evaluate the number of iterations and the computation time.

- We also evaluate the performance of the single precision Multigrid preconditioner.

§4 Numerical Experiments

Used iterative methods and preconditioner

- Iterative methods : Conjugate Gradient, Conjugate Residual, Orthomin(1)
- Preconditioner : Multigrid (Single precision, Double precision)

Initial guess $\boldsymbol{x}_0^{(n)}$ of the iterative methods

- Type I : $\boldsymbol{x}_0^{(n)} = \mathbf{0}, \quad n = 0, 1, \ldots, 100$
- Type II : $\boldsymbol{x}_0^{(0)} = \mathbf{0}, \quad \boldsymbol{x}_0^{(n)} = \boldsymbol{x}_*^{(n-1)}, \quad n = 1, 2, \ldots, 100$

  Here, $\boldsymbol{x}_*^{(n-1)}$ is a solution obtained at the n-1 step.

Parameters for the Multigrid preconditioner

- Stationary iterative method: Gauss-Seidel
- The number of iterations of Pre-, and Post-smoothing : $\nu_1 = 2, \nu_2 = 2.$
- The number of iterations at the coarsest level : $\mu = 10.$

§4 Numerical Experiments

Stopping condition of the iterative methods

If the following condition is satisfied, the iteration is stopped.

$$\|\boldsymbol{r}_k^{(n)}\|_2 / \|\boldsymbol{b}^{(n)}\|_2 \leq \sqrt{10^{-5}}$$

Here, $\boldsymbol{r}_k^{(n)}$ denotes the kth residual vector of $A\boldsymbol{x}^{(n)} = \boldsymbol{b}^{(n)}$.

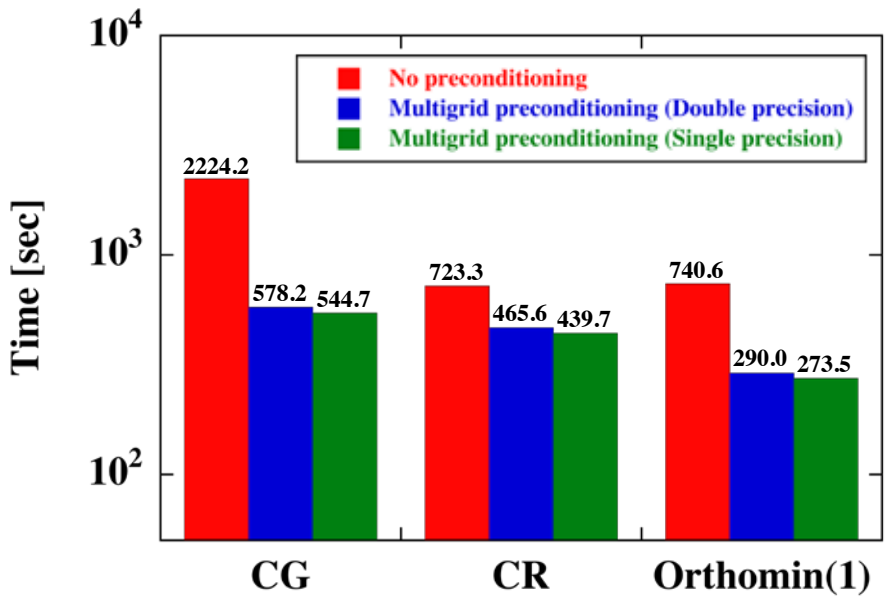
Computational environment

- CPU: Intel Xeon E5-2620 2.4GHz (6 cores) × 2
- Memory: 64GByte
- Compiler: gfortran ver. 5.4.0
- Compile option: `-O3`

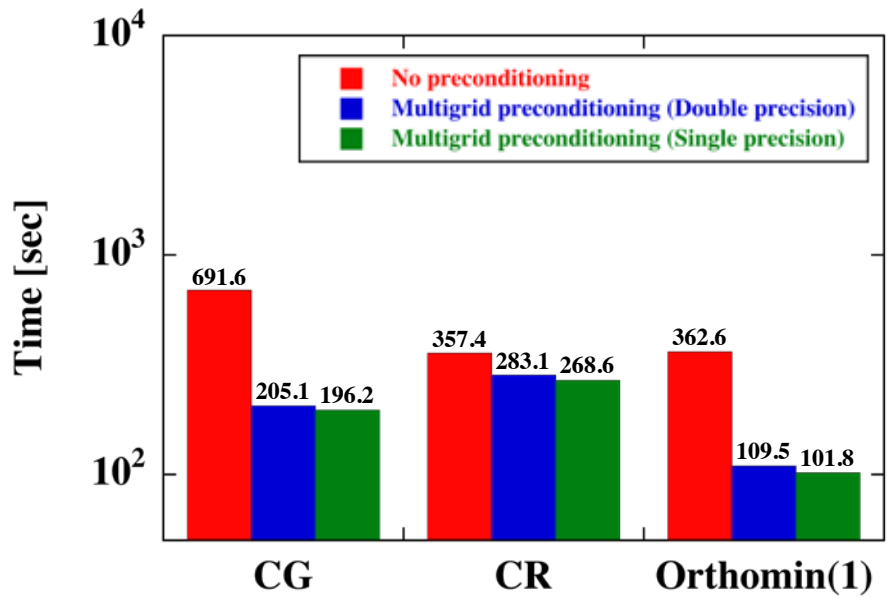
In this example, only a single core is used.

§4 Numerical Experiments

- **Single precision Multigrid + Orthomin(1) is the fastest.**
- **The use of the solution at the previous time step is effective.**



(a) Type I.

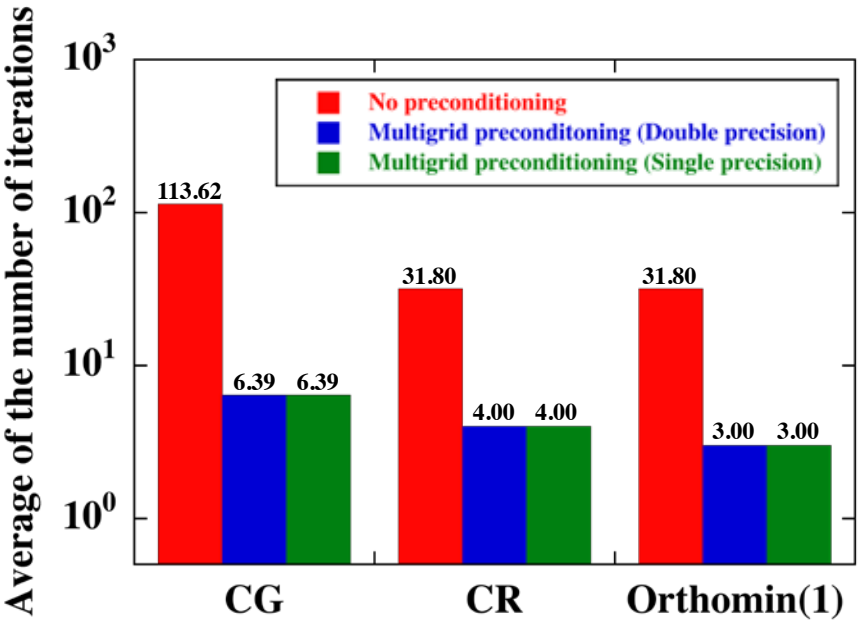


(b) Type II.

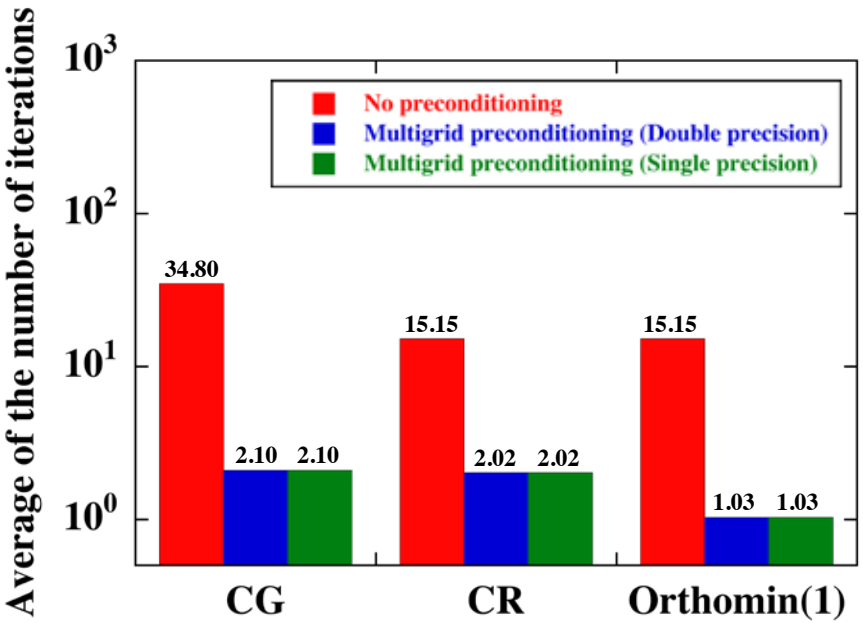
Total computation time (sec) for solving 101 linear systems.

§4 Numerical Experiments

- The #iterations can be reduced by using the MG preconditioner.
- The #iterations of the single precision MG preconditioned iterative methods is the same as the double precision ones.



(a) Type I.



(b) Type II.

The average of the number of iterations for solving each linear system.

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§5 Summary and Future work

Summary

- In order to reduce the computation time of LES, we applied the Multigrid preconditioned Krylov subspace methods with mixed precision.

- In our experiments, the combination of the Orthomin(1) method and the Multigrid method with single precision arithmetic is the fastest. Moreover, the use of the solution at the previous time step was also effective.

Future work

- Reducing the computational cost of the Multigrid preconditioner.
- The use of the more low precision arithmetic (e.g., half precision).

§4 Numerical Experiments

Target problem

Linear systems arising from LES :

$$A\boldsymbol{x}^{(n)} = \boldsymbol{b}^{(n)}, \quad n = 0, 1, \ldots, n_{\max}$$

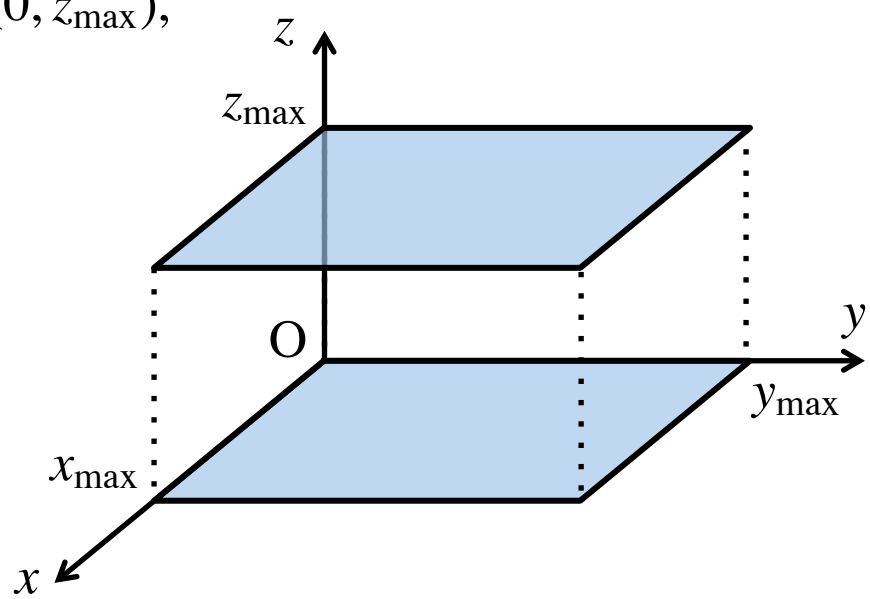
Poisson problem

$$\triangle\phi = \frac{1}{\Delta t}\nabla \cdot u^{(\mathrm{P})} \text{ in } (0, x_{\max}) \times (0, y_{\max}) \times (0, z_{\max}),$$

$$\phi(0, y, z) = \phi(x_{\max}, y, z),$$

$$\phi(x, 0, z) = \phi(x, y_{\max}, z),$$

$$\frac{\partial\phi(x, y, z)}{\partial z} = 0 \text{ at } z = 0 \text{ and } z = z_{\max}.$$



Parameters

- $x_{\max} = y_{\max} = 25,600, z_{\max} = 4,000.$
- The mesh size: 50.
- The time step size: $\Delta t = 1$, the number of time steps: $n_{\max} = 100$.

§4 Numerical Experiments

The problem size and the number of nonzero elements of the linear systems which appear in the Multigrid preconditioner.

Level	Problem size	#Nonzero elements
0	20,709,376	144,441,344
1	2,555,904	17,760,256
2	311,296	2,146,304
3	36,864	249,856
4	4,096	26,624

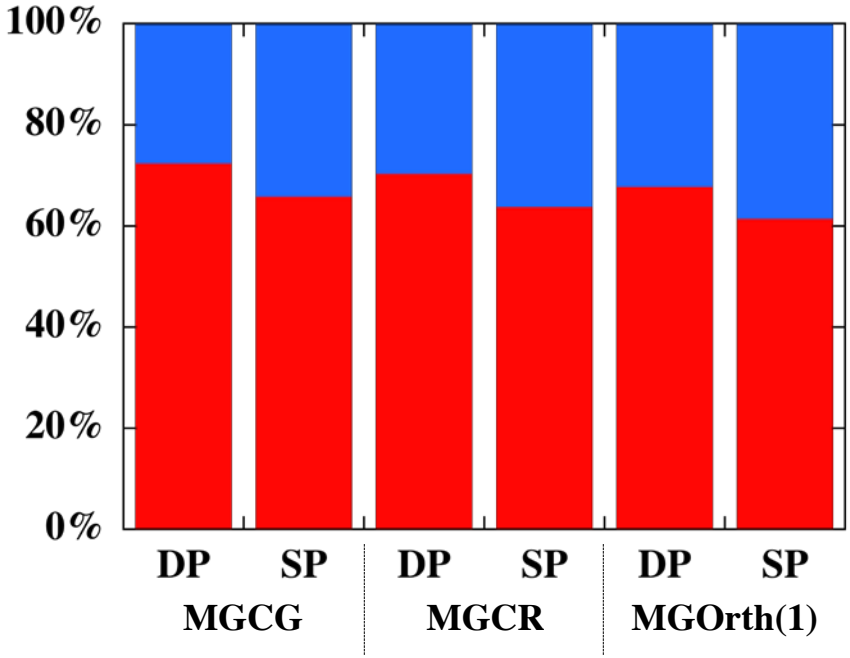
Level 0 ～ Level 3 ： Pre-, Post-smoothing

→ The two iterations of Gauss-Seidel is performed.

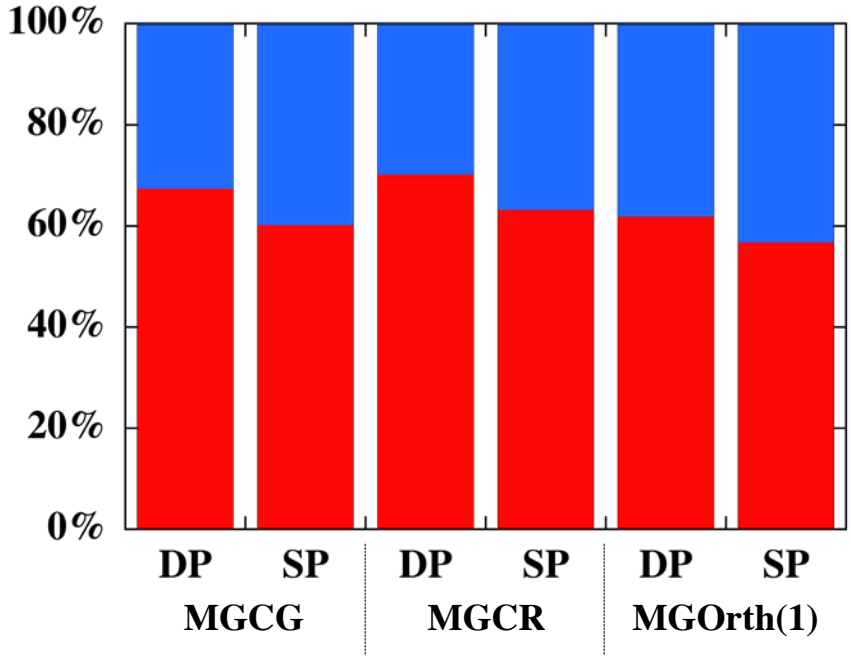
Level 4 ： The ten iterations of Gauss-Seidel is performed.

§4 Numerical Experiments

The computation time of the preconditioning part can be reduced by using single precision arithmetic.



(a) Type I.



(b) Type II.

The ratio of the computational time.

■ : Preconditioning part, ■ : Other part.