A Fast Parameter-Free Preconditioner for Structured Grid Problems

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Introduction

We consider the problem of solving large sparse linear systems of the form

$$Ax = b, \quad A \in \mathbb{R}^{m\times m}, \quad b \in \mathbb{R}^m, \tag{1}$$

which arises, for example, during the numerical solution of the following diffusion equation

$$\begin{aligned} -\mathrm{div}(\kappa(x)\nabla u) &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega_D, \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \partial\Omega_N. \end{aligned} \tag{2}$$

Here Ω is the interior of the domain, and $\partial\Omega_D$ and $\partial\Omega_N$ are the Dirichlet and Neumann boundaries respectively. Such problems appear as sub-problems to wide variety of numerical simulations in fluid dynamics, material science, etc. On a structured grid, the discretization schemes such as finite difference, finite element, and finite volume methods lead to a "nested" block tridiagonal matrix. Exploiting this structure is essential to obtaining a scalable and memory efficient solver. To know more about other solvers for this problem, see [1].

Objectives

To design fast and memory efficient linear solver for structured linear system.

Proposed Method

A matrix arising from a finite difference of finite element discretization on a structure 3D grid leads to a nested tridiagonal structure. Let the plane block be denoted by $\hat{D}_i$, the line blocks by $\overline{D}_i$, and the cell blocks by $\tilde{D}_i$. Similarly, let us denote the interface unknowns for plane blocks be denoted by $\hat{L}_i, \hat{U}_i$, line blocks by $\overline{L}_i, \overline{U}_i$, and so on. The blocks are twisted around middle block row, see [1]. We next define the preconditioner that exploits this nested tridiagonal structure.
To expose parallelism in the proposed Filtering Decomposition (called NTD), In actual implementation, we only need to store the bands of A.
To create the preconditioner, we first consider the block LU factorization $A = (P + L_3)(I + P^{-1}U_3)$. The A in this equation is already known to us, and on simplifying the right hand side, and solving for diagonal blocks P_i of P, we get the following recurrence solution for P_i

$$P_i = \begin{cases} \widehat{D}_1, \quad i \;=\; 1, \\ \widehat{D}_i - \widehat{L}_3^{i-1}(P_{i-1}^{-1})\widehat{U}_3^{i-1}, \quad i = 2,\cdots,j-1, \\ \widehat{D}_{nz}, \quad i \;=\; nz, \\ \widehat{D}_i - \widehat{L}_3^{i}(P_{i+1}^{-1})\widehat{U}_3^{i}, \quad i = nz-1,\cdots,j+1, \\ \widehat{D}_i - \widehat{L}_3^{i-1}(P_{i-1}^{-1})\widehat{U}_3^{i-1} - \widehat{L}_3^{i}(P_{i+1}^{-1})\widehat{U}_3^{i}, \quad i = j. \end{cases} \tag{4}$$

In the above iteration, as i increases, P_i tends to become denser, hence, it is costly to compute terms such as $\widehat{L}_3^{i-1}(P_{i-1}^{-1})\widehat{U}_3^{i-1}$. Moreover, storing P_i is costly, hence, we will replace P_i^{-1} by its sparse approximation. Reusing the notation P_i for approximated P_i, we define the following approximation to P_i

$$P_i = \begin{cases} \widehat{D}_1, \quad i \;=\; 1, \\ \widehat{D}_i - \widehat{L}_3^{i-1}(2\beta_{i-1} - \beta_{i-1}P_{i-1}\beta_{i-1})\widehat{U}_3^{i-1}, \\ \quad i = 2,\cdots,j-1, \\ \widehat{D}_{nz}, \quad i \;=\; nz, \\ \widehat{D}_i - \widehat{L}_3^{i}(2\beta_{i+1} - \beta_{i+1}P_{i+1}\beta_{i+1})\widehat{U}_3^{i}, \\ \quad i = nz-1,\cdots,j+1, \\ \widehat{D}_i - \widehat{L}_3^{i-1}(2\beta_{i-1} - \beta_{i-1}P_{i-1}\beta_{i-1})\widehat{U}_3^{i-1} \\ \qquad -\widehat{L}_3^{i}(2\beta_{i+1} - \beta_{i+1}P_{i+1}\beta_{i+1})\widehat{U}_3^{i}, \quad i = j. \end{cases} \tag{5}$$

The Proposed Method Continued

Here j is the block row index where the twist happens, β_i are diagonal matrices defined as

$$\beta_i = \mathrm{diag}((P_{i-1}^{-1}\hat{U}^{i-1})./(\hat{U}^{i-1}\hat{t}_i)),$$

where $\hat{t}_i$ is a vector of all ones, and $2\beta_{i-1} - \beta_{i-1}P_{i-1}\beta_{i-1}$, or $2\beta_{i+1} - \beta_{i+1}P_{i+1}\beta_{i+1}$ for the lower half is claimed to be a better approximation to $(P_i)^{-1}$. Note that the product on the rhs no longer equals A after substituting P^{-1} with it's β approximated form. After approximation, we define the NTD preconditiner B_{NTD} as follows

$$B_{\mathrm{NTD}} = (P + L_3)(I + P^{-1}U_3). \tag{6}$$

Since $\beta_i's$ are diagonals, the sparsity pattern of P_i is same as that of $\widehat{D}_i$. Hence, like $\hat{D}_i$ blocks, the individual P_i blocks are themselves nested block tridiagonal, we can obtain a further factorization as follows

$$P = (T + L_2)(I + T^{-1}U_2). \tag{7}$$

As for P_i blocks before, we have the following recurrence solution for T_i blocks

$$T_i = \begin{cases} \overline{D}_1, \quad i \;=\; 1, \\ \overline{D}_i - \overline{L}_2^{i-1}(2\beta_{i-1} - \beta_{i-1}T_{i-1}\beta_{i-1})\overline{U}_2^{i-1}, \\ \quad i = 2,\cdots,j-1, \\ \overline{D}_{nz}, \quad i \;=\; nz, \\ \overline{D}_i - \overline{L}_2^{i}(2\beta_{i+1} - \beta_{i+1}T_{i+1}\beta_{i+1})\overline{U}_2^{i}, \\ \quad i = nz-1,\cdots,j+1, \\ \overline{D}_i - \overline{L}_2^{i-1}(2\beta_{i-1} - \beta_{i-1}T_{i-1}\beta_{i-1})\overline{U}_2^{i-1} \\ \qquad -\overline{L}_2^{i}(2\beta_{i+1} - \beta_{i+1}T_{i+1}\beta_{i+1})\overline{U}_2^{i}, \quad i = j, \end{cases} \tag{8}$$

where j is the block row index, $\beta_i's$ are diagonal matrices defined as $\beta_i = \mathrm{diag}((T_{i-1}^{-1}\overline{U}^{i-1})./(\overline{U}^{i-1}\bar{t}_i))$, where $\bar{t}_i$ is vector of all ones, and as shown above, we consider the approximation $2\beta_{i-1} - \beta_{i-1}T_{i-1}\beta_{i-1}$ for upper half, and similarly the approximation $2\beta_{i+1} - \beta_{i+1}T_{i+1}\beta_{i+1}$ for the lower half is claimed to be a better approximation to $(T_i)^{-1}$.
Again sparsity pattern of T_i is same as $\bar{D}_i$, i.e., the T_i blocks are themselves pointwise tridiagonal matrices, and can be approximated similarly as follows:

$$T = (M + L_1)(I + M^{-1}U_1). \tag{9}$$

Since T is block diagonal with tridiagonal blocks, the above factorization is exact. We obtain the recurrence for M_i as follows:

$$M_i = \begin{cases} \tilde{D}_1, \quad i \;=\; 1, \\ \tilde{D}_i - \tilde{L}_1^{i-1}M_{i-1}^{-1}\tilde{U}_1^{i-1}, \; i = 2,\cdots,j-1, \\ \tilde{D}_{nz}, \quad i \;=\; nz, \\ \tilde{D}_i - \tilde{L}_1^{i}M_{i+1}^{-1}\tilde{U}_1^{i}, \quad i = nz-1,\cdots,j+1, \\ \tilde{D}_i - \tilde{L}_1^{i-1}M_{i-1}^{-1}\tilde{U}_1^{i-1} - \tilde{L}_1^{i}M_{i+1}^{-1}\tilde{U}_1^{i}, \quad i = j, \end{cases} \tag{10}$$

where j is the row index, and M_{i-1}^{-1} (or M_{i+1}^{-1}) is reciprocal of M_{i-1} (or M_{i+1}). Note that during construction of the preconditioner, we only need to store the bands as vectors with proper padding by zeros.
Also, note that to extract these bands, we do not construct the matrices T, P, and B. We only extract these bands during the recurrence for T_i and P_i. Also, the outermost bands ℓ_3 and u_3 are same as the outermost bands of A. We note that due to twists, there is two way parallelism in computing P_i, T_i, and M_i, hence a total of 8-way parallelism. We found it more efficient to use SIMD operations for recurrence for M_i, see [1] for details. Due to the twists, solves and setup can now be done in parallel. For more parallelism, the solver can be used as a subdomain solver inside additive Schwarz, or other structured domain decomposition solver. See [1] for details.

Graphical Results

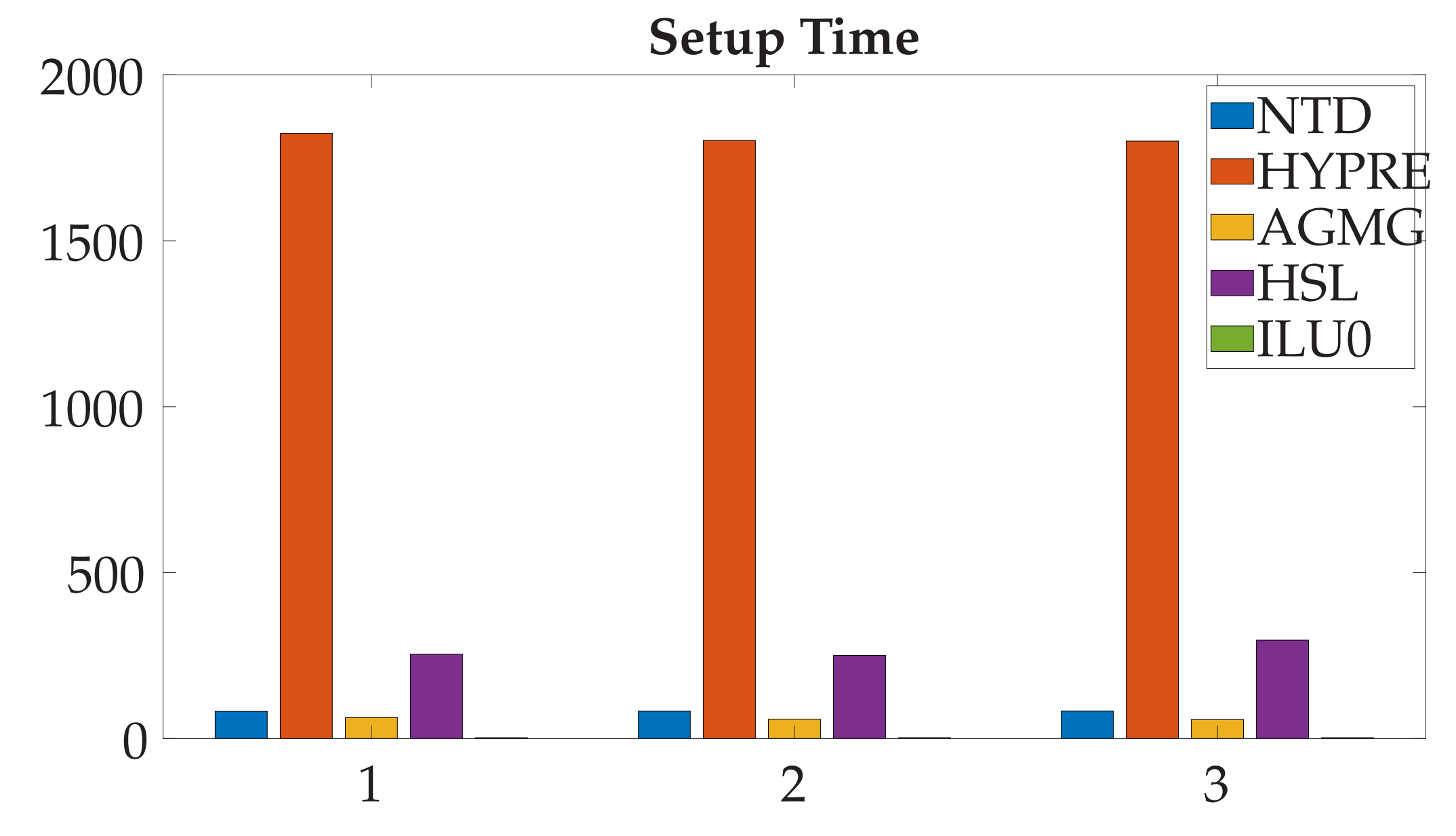

Figure 1: Comparison of setup times for various solvers.

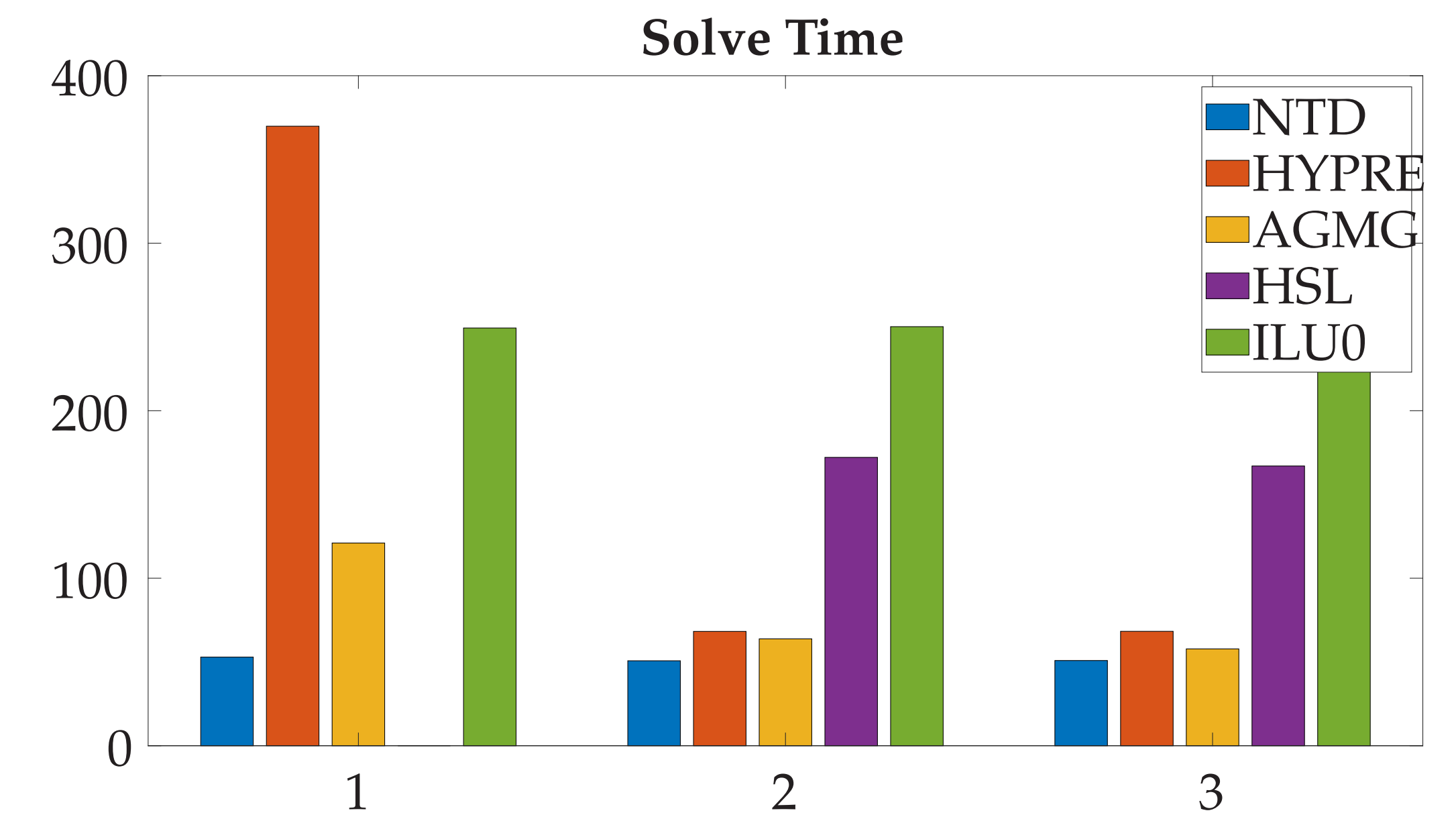

Figure 2: Comparison of solve times for various solvers..

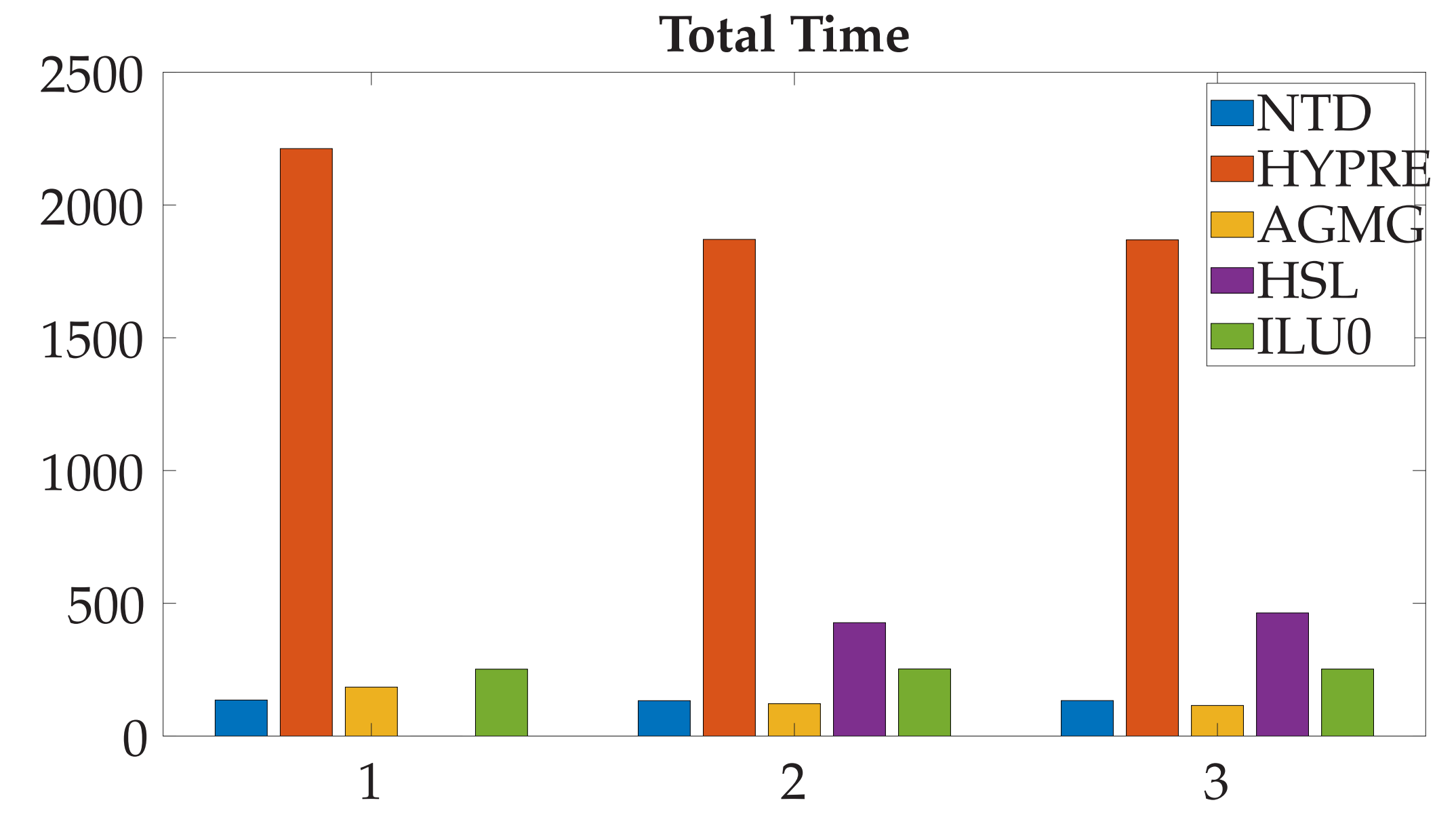

Figure 3: Comparison of total time (setup+solve) for various solvers.

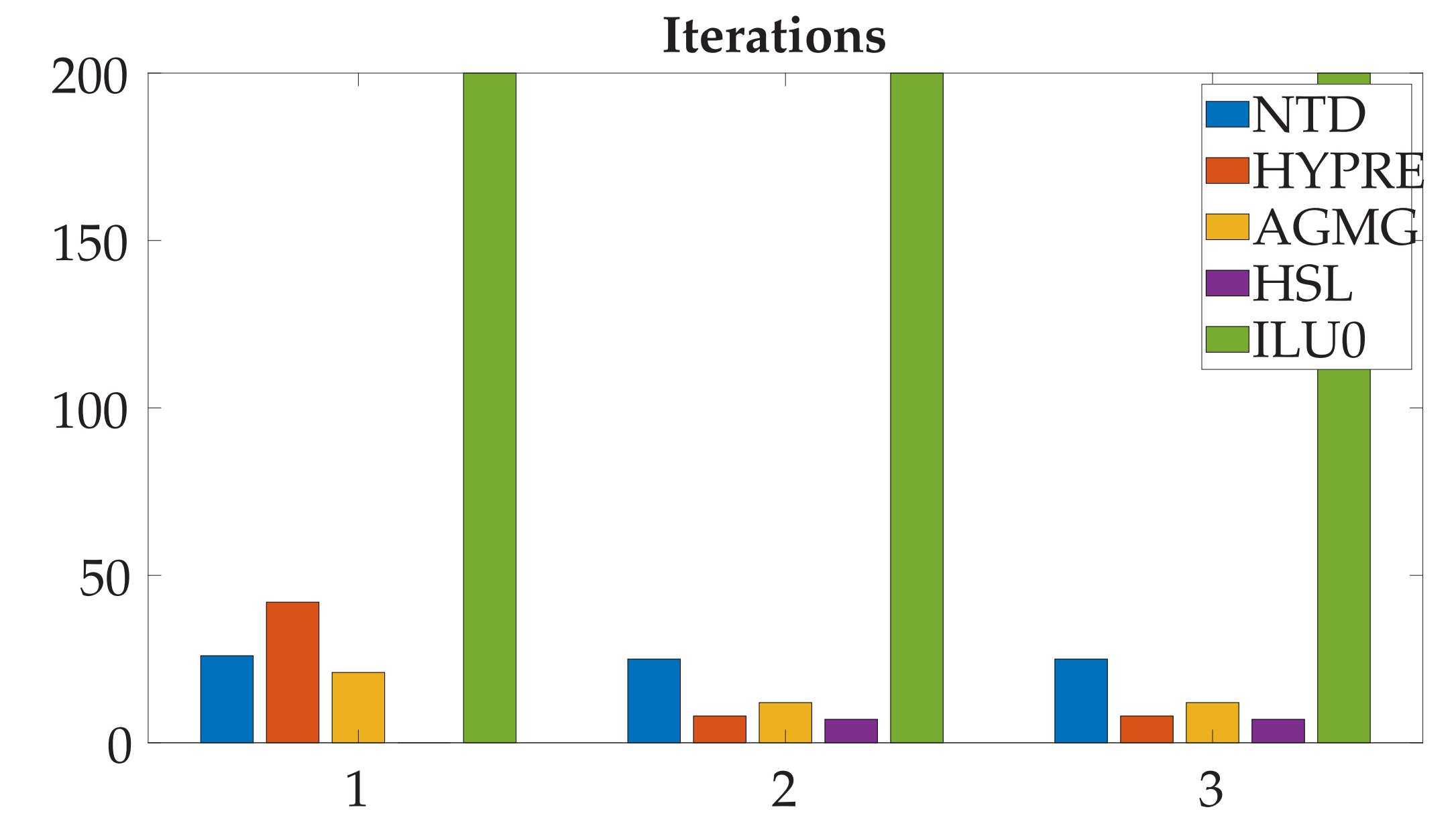

Figure 4: Comparison of iterations for various solvers.

Numerical Experiments

All the results shown have been obtained by running the experiments on intel i7-7700K CPU with 4 physical cores, 64 GB DDR4 RAM. The compiler version used is `gcc 7.3` with `-march=native` and `-O3` flags.
We consider Type-1, Type-2, and Type-3 matrices. Details can be found in [1].
As in multigrid, we use incomplete LU factorization of given matrix A with no fill-in as a smoother and combine it with NTD preconditioner described previously. The combination preconditioner denoted by B_c can be defined as follows:

$$B_c^{-1} = B_{\mathrm{NTD}}^{-1} + B_{\mathrm{ILU0}}^{-1} - B_{\mathrm{NTD}}^{-1}AB_{\mathrm{ILU0}}^{-1}, \tag{3}$$

where B_{ILU0} denotes the ILU preconditioner [2].
From the equation (3) above, we notice that solving with the preconditioner B_c requires solving with B_{NTD} and B_{ILU0}, and a matrix vector multiplication with the given coefficient matrix A. We have showed how to solve with B_{NTD} on a quad core in previous sections. The solve with B_{ILU0} requires triangular solves, i.e. forward sweep followed by a backward sweep, which are inherently sequential in nature.
To address this bottleneck, instead of doing ILU0 for full matrix A, we do an ILU0 of a block diagonal approximation $\tilde{A}$ of matrix A.
Such an approximation does not lead to any degradation in the performance of the combination preconditioner, and allowed us to engage two threads during the construction and solve phase of B
ILU0.
For the matrix times vector operation, we have implemented a parallel banded matrix vector multiply routine engaging 4 threads, further leveraging SIMD operations inside each thread. Please refer to [1].
Parameters for conjugate gradient: For detail on parameters used for solvers, please refer to [1].
The number of unknowns of the linear system is 43 Million.
The figures 1 and 2 show clearly that the proposed solver NTD is fastest solve times for all types of the problems. In setup times, it is as fast as AGMG. In total time, it is fastest on type-1, and comparable to AGMG for type-2 and type-3 problems. Also, the iterations are plotted in Fig 4. Note that bar corresponding to HSL for type-1 matrix is missing, because the code error for this method for this type. Also, compared to the methods, our method does not require parameter tuning. For other methods, we choose best parameters.
For detailed analysis of experimental results and the state-of-the-art solvers, see the detailed report [1].

References

[1] A. Aggarwal, S. Kakkar, P. Kumar, Multithreaded Filtering Preconditioner for Diffusion Equation on Structured Grid, arXiv 1909.09771v1, 2020
[2] Saad, Y.: Iterative Methods for Sparse Linear Systems. PWS publishing company, Boston, MA, 1996.

Ongoing Research

The ongoing research is on testing the proposed solver as subdomain solver in structured domain decomposition methods.