XAMG: A library for solving linear systems with multiple right-hand side vectors

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Abstract

This paper presents the XAMG library for solving large sparse systems of linear algebraic equations with multiple right-hand side vectors. The library specializes but is not limited to the solution of linear systems obtained from the discretization of elliptic differential equations. A corresponding set of numerical methods includes Krylov subspace, algebraic multigrid, Jacobi, Gauss-Seidel, and Chebyshev iterative methods. The parallelization is implemented with MPI+POSIX shared memory hybrid programming model, which introduces a three-level hierarchical decomposition using the corresponding per-level synchronization and communication primitives. The code contains a number of optimizations, including the multilevel data segmentation, compression of indices, mixed-precision floating-point calculations, vector status flags, and others. The XAMG library uses the program code of the well-known hypre library to construct the multigrid matrix hierarchy. The XAMG’s own implementation for the solve phase of the iterative methods provides up to a twofold speedup compared to hypre for the tests

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performed. Additionally, XAMG provides extended functionality to solve systems with multiple right-hand side vectors.

*Keywords:* systems of linear algebraic equations, Krylov subspace iterative methods, algebraic multigrid method, multiple right-hand sides, hybrid programming model, MPI+POSIX shared memory

| Nr. | Code metadata                          |
|-----|----------------------------------------|
| C1  | Current code version                   | Version 1.0                           |
| C2  | Permanent link to code/repository used for this code version | https://gitlab.com/xamg/xamg         |
| C3  | Code Ocean compute capsule             | N/A                                    |
| C4  | Legal Code License                     | GPLv3                                 |
| C5  | Code versioning system used            | git                                    |
| C6  | Software code languages, tools, and services used | C++, MPI                             |
| C7  | Compilation requirements, operating environments & dependencies | C++11 compiler, POSIX, MPI, hypre. The build instructions: https://gitlab.com/xamg/xamg/wiki/docs/XAMG_build_guideline |
| C8  | If available Link to developer document/manual |                                           |
| C9  | Support email for questions            | Gitlab issue tracker section           |

Table 1: Code metadata

1. **Motivation and significance**

Despite the wide use of open-source libraries for solving systems of linear algebraic equations in computational software, in some cases there is still the need for developing novel libraries, which can extend the functionality of well-known ones or add some features, allowing to improve performance of the
calculations. The hypre library [1] is an example of an outstanding piece of software containing powerful and highly scalable algorithms for solving large sparse systems of linear algebraic equations (SLAEs). The classical algebraic multigrid method [2] implemented in hypre is a robust method widely applied for solving SLAEs derived from elliptic or parabolic differential equations. However, the implementation of the methods in hypre, as well as many other libraries containing various modifications of multigrid methods, is limited by algorithms performing calculations with a single right-hand side vector (RHS). Meanwhile, the solution of systems with multiple RHSs,

\[ AX = B, \]

where \( A \in \mathbb{R}^{n \times n} \), and \( X, B \in \mathbb{R}^{n \times m} \), \( m \ll n \), in terms of computational efficiency can be preferable compared to multiple solutions of systems with single RHS. The reasons to this include: (i) increasing the arithmetic intensity, (ii) regularization of the memory access pattern, (iii) vectorization of calculations, and others.

The SLAEs with multiple RHSs occur in a variety of mathematical physics applications. For example, the need for solving the corresponding systems of linear algebraic equations appears in structural analysis applications [3], in uncertainty quantification problems [4], in Brownian dynamics simulations [5], quantum chromodynamics [6], computational fluid dynamics [7], and others.

Despite the variety of applications and several advantages mentioned above, implementations of iterative methods for solving SLAEs with sparse matrices and multiple RHSs can rarely be found in publicly available li-
braries of numerical methods. Among the only few exceptions is the Trilinos library [8] containing the implementation of several Krylov subspace and aggregation-based algebraic multigrid methods. These, however, do not fully cover the entire set of the methods used in numerical modeling, e.g. the classical algebraic multigrid methods, provided by the hypre library. This issue complicates the development of the computational algorithms performing calculations with multiple RHSs.

The XAMG library focuses on the solution of a series of systems of linear algebraic equations with multiple RHSs (that, e.g. occur in incompressible turbulent flow simulations [7]). The code extends the functionality of the classical algebraic multigrid method, implemented in hypre, and provides implementations of both classical and merged formulations of the Krylov subspace iterative methods [9] to solve systems with multiple RHSs. The XAMG library aims to develop an optimized implementation for the solve phase of the methods, while the hypre library can be reused “as is” to construct a multigrid matrix hierarchy.

The library provides additional optimization features, including the hierarchical multilevel parallelization, low-level intra-node shared memory communications featuring synchronization primitives based on POSIX shared memory and atomics, multi-block data segmentation in accordance with hierarchical parallelization, mixed-precision floating-point calculations, compression of indices, vector status flags, and others, which allow to outperform the hypre library calculation times.
2. Software description

2.1. Mathematical methods

The XAMG library contains a set of numerical methods typically used for solving systems of linear algebraic equations coming from the discretization of elliptic partial differential equations. These include several Krylov subspace iterative methods (CG [10] and BiCGStab [11]), classical algebraic multigrid method [2], block Jacobi and symmetric Gauss-Seidel methods, Chebyshev iterative method, and a direct solver. All these methods are adopted to solve SLAEs with multiple RHSs. In addition to the classical BiCGStab method, the library also contains several modified methods, including the Reordered BiCGStab [12], Pipelined BiCGStab [13] and merged formulations of these methods [9], which combine vector updates and dot products to minimize the overall amount of vector read/write operations. The possible combinations of the methods, which can be used as a standalone solver, preconditioner, or smoother with the multigrid method, are summarized in Tab. 2. The full list of the methods and corresponding method parameters is presented in [14].

| Method       | Solver | Preconditioner | Pre-/post-smoother |
|--------------|--------|----------------|--------------------|
| CG           | +      | -              | -                  |
| BiCGStab     | +      | +              | +                  |
| MultiGrid    | +      | +              | -                  |
| Jacobi       | +      | +              | +                  |
| Gauss-Seidel | +      | +              | +                  |
| Chebyshev    | -      | +              | +                  |
| Direct       | +      | -              | -                  |

Table 2: Combinations of the methods and solver types implemented in the XAMG library.
2.2. Advantages of calculations with multiple RHSs

The solution of SLAEs with multiple RHSs opens up opportunities for several optimizations. The main advantage of using iterative methods with performing simultaneous independent solutions for multiple RHSs is an increasing arithmetic intensity of calculations. The flop per byte ratio is a measure of floating-point operations relative to the amount of memory accesses. Basic linear algebra operations like vector updates, dot products, and sparse matrix-vector multiplications (SpMV) are characterized by flop per byte ratio of only about 0.1. This means that the corresponding operations are memory bound \cite{15,9}, and its performance mostly depends on the amount of memory traffic and memory bandwidth. The solution of SLAEs with multiple RHSs allows to load a matrix for SpMV operations with \( m \) right-hand sides only once, compared to \( m \) loads when performing \( m \) SLAE solutions with a single RHS. This typically leads to about a twofold reduction in the total amount of memory traffic for SLAE solver per each RHS, an increase of the flop per byte ratio, and, subsequently, to a significant calculation speedup.

The use of specialized data storage formats for sparse matrices is necessary for performing the operations with large matrices arising in numerical simulations. The compressed sparse row (CSR) format \cite{16} is the universal one, which is widely used for the matrices of general form. However, the implementation of SpMV operation for CSR format requires indirect memory accesses, which reduces cache efficiency and gives no chance for loop vectorization. The generalized SpMV operation performed for multiple RHSs allows to partially regularize an access to the memory and vectorize the computations over the right-hand sides.
2.3. Software architecture

The XAMG library is designed as a header-only template C++ library. The template polymorphism is used to implement variability of all basic data types for matrices and vectors, both interface-level and internal ones. The number of RHSs is also given as a template parameter.

The specialization of the number of RHSs at compile time is a key design point. This approach allows to vectorize all the relevant subroutines with respect to a constant range of loops iterating over the RHSs. Keeping in mind the appropriate vectors’ data placement and some pragma directives code instrumentation, such a design allows a regular C++ compiler to vectorize subroutines to the greatest extent possible.

One can highlight the following XAMG program code elements:

- matrix and vector data structures;
- basic sparse linear algebra subroutines gathered in “blas” and “blas2” groups;
- solver classes inherited from an abstract interface, which exposes the main library functions: setup() and solve();
- solver parameter classes.

The matrix and vector data structures are used to store the corresponding data objects. The "blas" group of subroutines consists of a collection of primitives operating with vectors (linear updates, dot products, etc.) The "blas2" group of subroutines includes several SpMV-like matrix-vector operations. Solver classes implement various iterative methods used to solve systems of linear algebraic equations. Finally, the solver parameter classes are used to store the lists of numerical method parameters, specifying each numerical method's configuration.

The `setup()` virtual function of the MultiGrid solver class implements the classical algebraic multigrid "setup" phase. This is done by wrapping up the `hypre` functions to construct the multigrid matrix hierarchy. This is the only place where the `hypre` library codebase is used inside the XAMG library program code.

An important design feature of the XAMG library is the hierarchical hybrid parallel programming model. This model combines the Message Passing Interface (MPI) standard \[17\] for cross-node communication and a special kind of shared memory parallel programming model on the intra-node level, based on POSIX shared memory (ShM) functionality. The MPI+ShM model implies that MPI ranks, which reside on the same compute node, allocate and use the common POSIX shared memory regions to store data objects. Unlike many other MPI+X programming models, MPI+ShM does not use threading within a node. The MPI rank to CPU core mapping is one-to-one.

To benefit from better data locality, most well-known distributed linear algebra algorithms implement a data decomposition that splits the calcula-
tions into fully local and fully non-local parts [18]. The MPI+ShM programming model also implements a specific data decomposition for matrix and vector data structures. The idea behind this decomposition is the hierarchical segmentation of the data into: (i) those with only local algorithmic dependencies, and (ii) those requiring some parallel communication to work with. In Figure 1, the blue-colored boxes represent the “local dependency” blocks, whereas the white-colored ones are for “remote dependency”. The local dependency blocks can also be called “diagonal blocks” since they contain matrix diagonal elements for square matrices. The Figure 1 also illustrates why the data decomposition is called hierarchical. In fact, the recursive data decomposition introduces three logical layers: the node layer, the numa layer, and the core layer. They are meant to reflect the natural hierarchy of a modern CPU-based high performance computing system hardware, consisting of the compute nodes, the NUMA blocks inside each node, and the CPU cores.

The hierarchical decomposition principle makes it possible to split the local and non-local data dependencies. As a practical result of this, the number of non-local MPI communications (on a cross-node layer) as well as non-local data accesses (for a cross-NUMA layer) is reduced significantly.

To summarize, the hybrid MPI+ShM parallel programming model implies: (i) the direct shared memory data access instead of MPI communications on an intra-node scope, and (ii) a specific hierarchical data and algorithms decomposition. Both features combined significantly improve the single-node parallel performance and the multi-node scalability compared to the pure MPI model.

The data compression features of the XAMG library try to benefit from
reducing the number of data transfers in the main library algorithms and communication procedures. These features include the turnover to the reduced precision for floating-point numbers and using lesser bits for integer indices for the matrices stored in the CSR format. The reduced precision floating-point numbers typically cannot be used for the whole solver without losing the solution accuracy. However, it is known that switching to the reduced precision when performing preconditioner calculations \cite{19, 20} may be a compromise variant, preserving the basic precision of the resulting vector and having only a minor or no reduction of the convergence rate. Depending on the fraction of the calculations with the reduced precision in the overall SLAE solver calculations, the 5-30\% cut on the full amount of data to transfer allows to obtain the proportional calculations speedup. Since the reduced precision feature is only applied to a part of the multigrid matrices hierarchy, this data compression model is called “mixed-precision”.

The second type of optimizations related to compression of indices for the CSR matrix storage format is applicable to all matrices. The hierarchical data decomposition leads to a multiblock matrices representation, and for the small blocks CSR indices data types can be changed to the smaller ones like uint16\_t or uint8\_t. This modification also results in reducing the amount of memory accesses.

2.4. Software usage examples

The main API of the XAMG library has a header-only C++11 template-based interface, but the C language binding also exists. The below overview shows an example of using the main C++ library interface.

The solver code is configured at compile-time depending on the classes’
Figure 2: The XAMG library general usage example, C++ API.

and functions’ concrete template parameters. The C++ template instantiation is a mechanism behind this. A basic matrix type is instantiated with integer types (uint8_t, uint16_t, and uint32_t are allowed) and floating-point type (float or double). The integer template types specify the storage types for nonzero matrix elements indices. The floating-point template type defines
the storage type for the values of these elements. The same floating-point
type is also used to instantiate the functions operating with input and output
vectors. The majority of the XAMG data structures and library functions
have an additional template parameter $NV$, the number of RHSs within a
single SLAE solution operation.

The code listing in Figure 2 presents a basic working code portion that
uses the XAMG library to solve a linear system with a sparse matrix stored
in the CSR format. Lines 9-12 set up the compile time definitions for the
above mentioned basic data types and the number of RHSs for a solution.
The library initialization call in line 14 passes an optional colon-separated
configuration string. This string can be used to specify the parameters of
the hybrid three-level parallel programming model. The details on these
parameters are given in the program documentation.

Lines 16-19 represent a basic code to read a matrix from a binary file.
The file is supposed to hold a CSR format matrix, an RHS, and an initial
guess vector (as an option). Lines 21-27 fill in the distributed versions of
the matrix and the vectors with a correct decomposition, and map the data
structures to the MPI+ShM data hierarchy. The desired solver parameters
are set in lines 29-32. A preconditioned BiCGStab method is set for usage
in this example, with the Jacobi method serving as a preconditioner. All
the default parameters for the solver/preconditioner pair are set up in line
32. Lines 34-35 create a C++ object representing a solution plan based on
the solver and preconditioner parameters, and this plan becomes connected
to the distributed matrix and the vectors $A$, $x$, and $b$. The SLAE solution

\[1\text{The number of RHSs, } m, \text{ is denoted in the source code as a template parameter } NV.\]
process for $NV$ RHSs is done in line 37. The solution result is stored in $x$ vector, and some solution statistics are held in the $stats$ variable of the $solver$ object.

The example set of parameters for a simple algebraic multigrid configuration of a solver is shown in Figure 3. In lines 4-8, the multigrid method is set as a preconditioner for a preconditioned BiCGStab solver. A few parameters which tune the multigrid hierarchy setup process are set explicitly. In lines 9-12, we take care of an explicit smoothers set up for the multigrid method. Specifically, the Chebyshev method with a polynomial order of 2 is set. The $set_defaults()$ function call in line 13 ensures that all the solver parameters, as well as preconditioner and smoother methods, which are not set explicitly in previous lines, are correctly initialized with the default values.

### 3. Example case: performance evaluation

The example case presents the study on the efficiency of the XAMG library and the impact of implemented optimization features on the overall code performance. It demonstrates (i) the XAMG library performance com-
pared to hypre, (ii) the effect of data compression optimizations on the calculation time reduction, (iii) the performance gain due to calculations with multiple RHSs, and (iv) the parallel efficiency results for various numbers of RHSs. The Lomonosov-2 supercomputer is used for the performance evaluation to demonstrate the potential of the developed library. It consists of compute nodes with a single Intel Xeon Gold 6126 processor and InfiniBand FDR interconnect. In all the cases all available 12 physical CPU cores per node are utilized during the calculations. The XAMG library is compiled with the Intel C/C++ compiler 2019 Update 9. The internal integration test application `xamg_test` is used for the tests; the YAML configuration files are provided within the XAMG source code repository [21] in examples/test/yaml/ directory.

The test runs are performed for several test SLAEs. They correspond to the systems obtained as a result of spatial discretization of the 3D Poisson’s equation

\[ \Delta u = f \]

with the 7-point stencil in various computational domains, including the regular grid in the cube (grids with 150\(^3\) and 250\(^3\) cells), and the computational grid, corresponding to the direct numerical simulation of the incompressible turbulent flow in a channel with a matrix of wall-mounted cubes (matrix of 9.7 mln. unknowns [7]). The corresponding matrix generators are embedded into the `xamg_test` integration test application.

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\(^2\)The compilation options are: `-ip -03 -no-prec-div -static -fp-model fast=2 -xCORE-AVX512`
3.1. Calculations with single RHS

The first set of experiments is performed with two test SLAEs corresponding to cubic computational domain with the grids of $150^3$ and $250^3$ unknowns. The numerical method configuration, identical for both XAMG and hypre, comprises the BiCGStab method supplemented with an algebraic multigrid preconditioner and hybrid symmetric Gauss-Seidel smoother. The runs performed include five different test series: the hypre library tests in pure MPI and hybrid MPI+OpenMP execution modes, the XAMG library tests in pure MPI and MPI+ShM execution modes, and the XAMG library tests in hybrid MPI+ShM mode with data compression optimizations.

The obtained performance evaluation results are shown in Figure 4. The data is presented in terms of the relative speedup, which is defined as a ratio of the single node calculation time for the hypre library in a pure MPI mode, to the calculation time with the specific number of compute nodes and execution mode:

$$S_p^i = \frac{T_{hypre, MPI}^1}{T_p^i}.$$ 

Results presented in Figure 4 show similar scalability for the pure MPI implementations of XAMG and hypre. However, the MPI+ShM hybrid programming model of the XAMG library provides a big scalability improvement: with MPI+ShM programming model enabled, XAMG outperforms hypre, employing the MPI+OpenMP model, more than twice. Additionally, the data compression optimization of XAMG adds an extra 10% speedup.

The difference in the hybrid programming model benefits, observed when

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3 The most recent hypre library version 2.20.0 available to date is used in the performance comparison tests.
Figure 4: Relative calculation speedup for the XAMG and hypre libraries in various execution modes, test matrices with 150³ (left) and 250³ (right) unknowns.

comparing XAMG and hypre libraries, is related to different hybridization principles for these codes. The MPI+OpenMP hybrid programming model is known to suffer from fundamental multithreading issues within the MPI parallel paradigm [22]. The MPI+ShM programming model avoids these pitfalls with the single-threaded design. Among the other reasons can be the difference in data decomposition principles, solver implementation aspects, implementation of inter-node communications, or some other algorithmic or programming aspects. However, this topic cannot be elaborated in detail within the scope of this article.

3.2. Calculations with multiple RHSs

3.2.1. Single-node performance

The performance gain parameter is a key characteristic indicating the benefit of solving the SLAE with multiple RHSs over multiple solutions with a single RHS. This parameter is defined as:

$$P_m = \frac{mT_1}{T_m},$$
Figure 5: Performance gain for the calculations with multiple RHSs.

where $m$ is the number of RHSs, $T_1$ is the calculation time for a single RHS, and $T_m$ is the calculation time for $m$ RHSs. The number of RHSs in the tests varied in the range 1–64 for the smaller test matrix, and in the range 1–16 for the bigger ones (due to the single node memory capacity limitations). The corresponding results are presented in Figure 5. The plot shows at least twofold performance gain when performing calculations with multiple RHSs, which is in agreement with the theoretical estimates [7]. The peak values vary in the range 2–2.5, depending on the fraction of SpMV-like operations in the overall SLAE solver calculation loop.

3.2.2. Parallel efficiency

The XAMG library performance is also evaluated by the multiple RHS calculations parallel efficiency. The corresponding tests are performed with the test matrix of 9.7 mln. unknowns with 1, 4, and 16 RHS vectors. The parallel efficiency results,

$$E_p = \frac{T_1}{p T_p},$$

are obtained for the hybrid execution mode. The corresponding results are presented in Figure 6. These results show that the parallel efficiency for
Figure 6: The parallel efficiency for the multiple RHSs calculations with the XAMG library, 9.7 mln. unknowns test matrix.

multiple RHSs is, at least, not worse compared to the one for the single RHS calculations.

4. Impact and conclusions

The new linear solver code XAMG is a modern C++ project which adds a rare feature for the libraries of iterative methods, as it solves systems with multiple right-hand side vectors. The key advantage of the solver with multiple RHSs is a potential speedup over multiple solutions with single RHS, and this feature can be effectively used in some well-known mathematical methods for structural analysis, uncertainty quantification, Brownian dynamics simulations, quantum chromodynamics, modeling of incompressible turbulent flows, and others. However, despite evident advantage in time to solution, this functionality is not implemented in most libraries containing robust and scalable iterative methods, like algebraic multigrid.

Among the real applications already taking up this advantage, we highlight an in-house code for incompressible turbulent flow simulations [7], since the XAMG library is already successfully integrated with it. The integration
can be done as well for any other project written in C/C++ that is able to exploit the multiple RHS feature of a linear solver because the initial release of the XAMG library has been recently published as an open repository on gitlab.com [21].

The XAMG project also features a number of leading source code and computational method optimizations which impact the generic problem of a linear solver speedup on modern multicore and manycore HPC systems. This problem stays aside from the multiple RHS feature. These optimizations like a novel hybrid parallel programming model (MPI+ShM), mixed-precision calculations, matrix indices compression, and others make it possible to improve the productivity of a linear solver compared to other well-known libraries containing robust and scalable iterative methods (e.g. hypre). The modern C++11 codebase allows for broad future research prospects in this direction.

The experimental performance evaluation shows the XAMG library speedup against hypre by a factor of 2 for the multi-node runs performed. The comparison of calculations with multiple RHSs against multiple runs with single RHS shows 2-2.5 times speedup for single-node runs. Additionally, the multi-node parallel efficiency of the multiple RHSs calculations is, at least, not worse compared to the one for the single RHS.

**Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
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