Efficient solution of 3D elasticity problems with smoothed aggregation algebraic multigrid and block arithmetics

D. E. Demidov¹,*

(Submitted by A. M. Elizarov)

¹ Kazan Branch of Joint Supercomputer Center, Scientific Research Institute of System Analysis, the Russian Academy of Sciences; 2/31, Lobachevskii str., Kazan 420111 Russia

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Abstract—Efficient solution of 3D elasticity problems is an important part of many industrial and scientific applications. Smoothed aggregation algebraic multigrid using rigid body modes for the tentative prolongation operator construction is an efficient and robust choice for the solution of linear systems arising from discretization of elasticity equations. The system matrices on every level of the multigrid hierarchy have block structure, so using block representation and block arithmetics should significantly improve the solver efficiency. However, the tentative prolongation operator construction may only be done using scalar representation. The paper proposes a couple of practical approaches for enabling the use of block arithmetics with smoothed aggregation algebraic multigrid based on the open-source AMGCL library. It is shown on the example of two real-world model problems that the suggested improvements may speed up the solution by 50% and reduce the memory requirements for the preconditioner by 30%. The implementation is straightforward and only requires a minimal amount of code.

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1. INTRODUCTION

Solution of large sparse linear systems obtained by discretization of 3D elasticity equations is an important part in many industrial and scientific simulation applications. Iterative solvers from Krylov subspace preconditioned with smoothed aggregation algebraic multigrid (AMG) are considered to be an efficient and robust choice for solving such systems [2, 14, 15]. The system matrices resulting from the 3D elasticity equations usually have block structure with small $3 \times 3$ blocks. It has been shown in [8] that using block representation and block arithmetics for such systems may reduce both the computation time and the memory required for the preconditioner. In order to achieve good convergence, the AMG preconditioner or, more specifically, the tentative prolongation operator has to be constructing using geometry-specific information in form of zero-energy modes, or near nullspace components, which in case of elasticity problems consist of the six rigid body modes [16]. However, the tentative prolongation operator construction is expressed in terms of scalar arithmetics, which makes it hard to use block representation of the system matrix and block arithmetics during the preconditioner setup in general.

This paper proposes a couple of practical approaches allowing to combine the use of zero-energy modes with the block arithmetics in the smoothed aggregation AMG setup. The first approach converts the constructed matrices to the block representation as the final step of the setup. This allows to speed up the solution phase of the algorithm, but does not improve the efficiency of the method initialization. The second approach constructs the transfer operators using the near nullspace components in the scalar space, while keeping the rest of the setup in the block domain. On the example of two real-world elasticity problems it is shown that the latter approach allows to

* E-mail: dennis.demidov@gmail.com
speed up the overall computation by 40–50%, and reduce the memory footprint of the preconditioner by about 30%. The suggested modifications are implemented as part of the open-source C++ library AMGCL [5, 6].

The rest of the paper is organized as follows: Section 2 outlines the smoothed aggregation AMG and describes the block representation of the matrices; Section 3 shows how block arithmetics may be used in the smoothed aggregation AMG setup when zero-energy modes are provided by the user; Section 4 provides the benchmarking results for the proposed approaches on the example of two real-world 3D elasticity models.

2. SMOOTHED AGGREGATION ALGEBRAIC MULTIGRID

Algebraic multigrid method [2, 14] solves a system of linear algebraic equations

\[ Au = f, \]  

where \( A \) is a square matrix. Multigrid methods are based on recursive application of the two-grid scheme, which combines relaxation and coarse grid correction. Relaxation, or smoothing iteration \( S_i \), is a simple iterative method, such as damped Jacobi or Gauss–Seidel iteration [1]. Coarse grid correction solves the residual equation on the coarser grid, and improves the fine-grid approximation with the interpolated coarse-grid solution. Transfer between the grids is described with the transfer operators \( P \) (prolongation) and \( R \) (restriction).

In geometric multigrid methods the grid hierarchy, the matrices \( A_i \) and operators \( P_i \) and \( R_i \) on each level of the hierarchy are supplied by the user based on the problem geometry. In algebraic multigrid methods the grid hierarchy and the transfer operators are in general constructed automatically, based only on the algebraic properties of the matrix \( A \).

When solving elasticity problems, it is important to provide the rigid body modes, or the zero-energy modes, or in more generic terms, the near nullspace components for the linear system. The components are used during construction of the tentative prolongation operator in order to ensure optimal convergence of the solver. The near nullspace components are problem-specific and should be supplied by the user. In case of 3D elasticity, the six rigid body modes are computed from the discretization grid coordinates and provided in form of a \( n \times 6 \) matrix \( B \) [16].

Algorithm 1 Smoothed aggregation AMG setup.

Start with the square system matrix \( A_1 = A \) and the matrix \( B_1 = B \) containing the near nullspace components.

while the matrix \( A_i \) is too large to be solved directly do

Construct the prolongation operator \( P_i \) and the next level matrix \( B_{i+1} \) from \( A_i \) and \( B_i \),

obtain restriction operator \( R_i = P_i^T \).

Construct the smoother \( S_i \) from \( A_i \),

Construct the coarser system using Galerkin operator: \( A_{i+1} = R_i A_i P_i \),

end while

Construct a direct solver for the coarsest system \( A_L \).

Algorithm 1 describes the setup phase of the smoothed aggregation AMG method. Here, on each level of the AMG hierarchy, the prolongation operator \( P_i \) is constructed from the system matrix \( A_i \) and the matrix \( B_i \) containing the near nullspace components for the system. A common choice for the restriction operator \( R_i \) is the transpose of the prolongation operator \( R_i = P_i^T \). The next coarser level of the AMG hierarchy is fully defined by the transfer operators \( P_i \) and \( R_i \). After the AMG hierarchy has been constructed, it is used as preconditioner with a Krylov subspace iterative solver, where a single V-cycle shown in Algorithm 2 is used as the preconditioning step.

The AMGCL opensource C++ library (published at https://github.com/ddemidov/amgcl under permissive MIT license) provides a flexible and extensible AMG implementation [5, 6]. It has a minimal set of dependencies, targets both shared and distributed memory machines, and supports modern many-core architectures. The value type concept of the AMGCL library allows to generalize the provided algorithms for complex or non-scalar systems. A value type defines several overloads for common math operations and is specified as a template parameter for a backend, where backend is a class that defines matrix and vector types and implements parallel primitives that are used
Algorithm 2 AMG V-cycle.

Start at the finest level with an initial approximation $u_1 = u^0$.

while not converged do
  for each level of the hierarchy, finest-to-coarsest do
    Apply a couple of smoothing iterations to the current solution: $u_i = S_i(f_i, u_i)$.
    Find residual $e_i = f_i - A_iu_i$ and restrict it to the RHS on the coarser level: $f_{i+1} = R_i e_i$.
  end for
  Solve the coarsest system directly: $u_L = A^{-1}_L f_L$.
  for each level of the hierarchy, coarsest-to-finest do
    Update the current solution with the interpolated solution from the coarser level: $u_i = u_i + P_i u_{i+1}$.
    Apply a couple of smoothing iterations to the current solution: $u_i = S_i(f_i, u_i)$.
  end for
end while

during the solution phase of the algorithm. Most often, a value type is simply a plain double or float scalar, but it is also possible to use small statically sized matrices when the system matrix has block structure, which decreases the setup time and memory footprint of the algorithm, increases cache locality and may improve convergence rate in some cases [8, 11].

Switching to a block-valued backend has several advantages. First, the block representation of the matrix is more efficient memory-wise. This is demonstrated on the example of the following sparse matrix that has a $2 \times 2$ block structure:

$$
\begin{bmatrix}
0.71 & 0.65 & 0.26 & 0.79 \\
0.54 & 0.37 & 0.17 & 0.62 \\
0.89 & 0.05 \\
0.27 & 0.15 \\
0.52 & 0.34 \\
0.45 & 0.64
\end{bmatrix}
$$

Below is the standard scalar representation of the matrix in the CSR format:

ptr=[0, 4, 8, 10, 12, 14, 16]
col=[0, 1, 2, 3, 0, 1, 2, 3, 2, 3, 2, 3, 4, 5, 4, 5]
val=[0.71, 0.65, 0.26, 0.79, 0.54, 0.37, 0.17, 0.62, 0.89, 0.05, 0.27, 0.15, 0.52, 0.34, 0.45, 0.64]

Compare it to the block-valued representation of the same matrix:

ptr=[0, 2, 3, 4]
col=[0, 1, 1, 2]
val=[[0.71, 0.65; 0.54, 0.37], [0.26, 0.79; 0.17, 0.62], [0.89, 0.05; 0.27, 0.15], [0.52, 0.34; 0.45, 0.64]]

With the block representation, the matrix has twice fewer rows and columns, and four times fewer logical non-zero values. This means that the matrix representation needs twice less memory to store the ptr array, and four times less memory for the col array. Since most of the parallel primitives used in the AMG V-cycle and in iterative solvers in general are memory-bound, this improves the performance of the solution phase. The reduced logical size of the matrix also simplifies and speeds up the algorithm setup. Finally, using the block arithmetics improves cache efficiency, since block elements may be loaded and used all at once.

When the system matrix $A$ is obtained by discretization of a 3D elasticity problem, it has block structure with small $3 \times 3$ blocks, as illustrated by Figure 1(a) showing the non-zero pattern of the system matrix for the connecting rod model. When the six rigid body modes are used as near nullspace components, the matrices at the subsequent levels of the AMG hierarchy also have block...
structure with $6 \times 6$ blocks, as shown on Figure 1(b). This means that the system matrices at every level of the constructed hierarchy may be represented using the $3 \times 3$ block values. However, even though most of the steps in Algorithm 1 and all of the steps in Algorithm 2 may be expressed in terms of block arithmetics, the construction of the tentative prolongation operator $P_i$ together with the next level matrix $B_{i+1}$ has to be performed using scalar arithmetics. The next section outlines the proposed workarounds for this issue.
Listing 1. Implementation of the hybrid backend, converting the constructed matrices to the block format.

```cpp
template <class Block>
struct builtin_hybrid : public builtin<typename math::scalar_of<Block>::type>
{
    typedef builtin<typename math::scalar_of<Block>::type> Base;
    typedef crs<Block> matrix;

    static auto copy_matrix(
        std::shared_ptr<typename Base::matrix> As,
        const typename Base::params&
    )
    {
        return std::make_shared<matrix>(adapter::block_matrix<Block>(*As));
    }
};
```

3. ENABLING THE USE OF BLOCK ARITHMETICS IN AMGCL

The multigrid hierarchy in the AMGCL library is constructed using builtin data structures and then transferred into one of the provided backends. This allows for transparent acceleration of the solution phase with help of OpenMP, OpenCL, or CUDA technologies. This may also be used for transparently conversion of the constructed matrices at every level of the hierarchy into the block format. The implementation is shown in Listing 1. Here, the hybrid backend extends the builtin one and overrides the static function `copy_matrix()` that transfers a matrix into the backend format. This way, the AMG hierarchy is constructed in the scalar space, and the matrices are converted into the block representation afterwards. In Section 4 this method is shown as NS Hybrid1.

This approach has a couple of disadvantages. First, the setup is still performed using scalar arithmetics, and does not have any performance gains of using block arithmetics. Second, it may work well with simpler relaxation schemes, such as damped Jacobi or sparse approximate inverse, where the most time consuming operation is a sparse matrix-vector product, which is performed using block arithmetics automatically. But the more involved smoothers, such as the ones based on incomplete LU factorization [13], will still be constructed and applied using scalar arithmetics, which means there will be no performance gains for the most time-consuming part of the solution.

In order to deal with the latter drawback, a relaxation wrapper has to be introduced. The wrapper will first convert the input matrix into the block format and only then construct the underlying relaxation scheme. This is implemented in AMGCL as `amgcl::relaxation::as_block` helper class template. The implementation is straightforward and is not shown here for the sake of brevity. The NS Hybrid2 solver in Section 4 uses the hybrid backend with the incomplete LU relaxation wrapped into the `as_block` helper class.

The hybrid backend method is a half-measure in the sense that the preconditioner setup is still performed using the scalar arithmetics. As was discussed earlier, it should be possible to perform most of the setup operations in the block space except for the computation of the transfer operators. This may be implemented with the help of a coarsening scheme wrapper `amgcl::coarsening::as_scalar` presented on Listing 2. The wrapper converts the input system matrix from the block into the scalar format, applies the underlying coarsening scheme in the scalar space, and converts the computed transfer operators back into the block format. This way only the coarsening step is performed in the scalar space, and all of the other setup operations, including the time consuming Galerkin operator and the relaxation scheme construction, are done using block arithmetics. This solver is designated as NS Block in the next section.

4. MODEL PROBLEMS AND PERFORMANCE RESULTS

The proposed techniques for enabling the use of block arithmetics with smoothed aggregation AMG are benchmarked in this section on the examples of two 3D elasticity problems. The first problem models a connecting rod shown on Figure 2(a). The discretized system matrix has 81 657 unknowns and 3 171 111 nonzero elements and was kindly provided by David Herrero-Pérez in [12]. The second problem is a solid hook shape optimization example [9, 10] from Kratos Multi-Physics framework [3, 4]. The system matrix here is taken from the first iteration of the optimization...
Listing 2. Coarsening scheme wrapper that converts the input matrix from block into scalar format, applies the underlying coarsening scheme, and converts the results back to the block format.

```cpp
template <template <class> class Coarsening>
struct as_scalar {
    template <class Backend>
    struct type {
        typedef typename Backend::value_type Block;
        typedef typename math::scalar_of< Backend>::type Scalar;
        typedef Coarsening< backend::builtin<Scalar> > Base;

        typedef typename Base::params params;
        Base base;

        type(const params &prm = params()) : base(prm) {};
    
    template <class Matrix>
    auto transfer_operators(const Matrix &B) {
        auto [P, R] = base.transfer_operators(*adapter::unblock_matrix(B));
        return std::make_tuple(
            std::make_shared<Matrix>(adapter::block_matrix<Block>(*P)),
            std::make_shared<Matrix>(adapter::block_matrix<Block>(*R)));
    }
};
```

Listing 3. Declaration of the Scalar solver.

```cpp
typedef amgcl::backend::builtin<double> Backend;
typedef amgcl::make_solver<
    amgcl::amg<
        Backend,
        amgcl::coarsening::smoothed_aggregation,
        amgcl::relaxation::ilu0
    >,
    amgcl::solver::cg<Backend>
> Solver;
```

algorithm and contains 59,718 unknowns and 2,309,832 nonzero elements. The solid hook geometry is shown on Figure 2(b).

Each of the model systems is solved with the six solvers outlined below. Every version uses the conjugate gradient iterative solver with different variations of the smoothed aggregation AMG preconditioner. The incomplete LU factorization with zero fill-in (ILU(0)) is used as a smoother in every case. The relative residual threshold of $10^{-8}$ is used in all experiments. All tests were conducted on a 3.40GHz Intel Core i5-3570K CPU. The complete source code for the benchmarks is published in [7].

Scalar solver. Here the preconditioner is a standard smoothed aggregation AMG with the scalar double precision value type. Point-wise aggregation with block size of 3 is used to account for the fact that the system matrix has block structure. The near nullspace components for the problem are not used. The definition of the solver is presented in Listing 3. The `make_solver` class here binds together an iterative solver (CG) and a preconditioner (AMG). Both the solver and the preconditioner are parameterized on the backend, which in this case is the builtin backend with plain double as value type. The AMG preconditioner class has two other template parameters: coarsening (here `smoothed_aggregation`) and relaxation (here `ilu0`).

Block solver. This is similar to the Scalar solver, except that the block-valued backend is used instead of the scalar-valued one. Plain aggregation is used as opposed to the point-wise one, since the coarsening with block values automatically accounts for the block structure of the system matrix.
The solver is defined as shown in Listing 4. Both the Scalar and the Block solvers do not employ the near nullspace components of the problem and are only used here to show that providing rigid body modes is important to get good convergence in elasticity problems.

NS Scalar solver uses scalar arithmetics throughout and is used as a baseline reference for the rest of the solvers. The solver definition is identical to the Scalar solver, but the rigid body modes are computed from the grid coordinates and provided as near nullspace components to the solver constructor. All the solvers below also use the near nullspace components to construct the tentative prolongation operator.

NS Hybrid1 solver uses the hybrid backend introduced in the previous section. Here, the preconditioner is set up using scalar arithmetics, and then the constructed matrices are converted to the block format. The definition of the solver is shown in Listing 5.

NS Hybrid2 solver differs from NS Hybrid1 in the choice of the relaxation scheme. Here, the ILU(0) relaxation is wrapped into the relaxation::as_block helper class, so that the relaxation is constructed using block arithmetics. The solver is defined according to Listing 6.

NS Block solver uses the builtin block-valued backend similar to the Block solver, but the coarsening scheme here is wrapped into the coarsening::as_scalar helper class. This allows the
Listing 5. Declaration of the NS Hybrid1 solver.

```cpp
typedef amgcl::static_matrix<double, 3, 3> Block;
typedef amgcl::backend::builtin_hybrid<Block> Backend;
typedef amgcl::make_solver
  amgcl::amg
    Backend,
    amgcl::coarsening::smoothed_aggregation,
    amgcl::relaxation::ilu0
  >,
  amgcl::solver::cg<Backend>
> Solver;
```

Listing 6. Declaration of the NS Hybrid2 solver.

```cpp
typedef amgcl::static_matrix<double, 3, 3> Block;
typedef amgcl::backend::builtin_hybrid<Block> Backend;
typedef amgcl::make_solver
  amgcl::amg
    Backend,
    amgcl::coarsening::smoothed_aggregation,
    amgcl::relaxation::as_block<
      amgcl::backend::builtin<Block>,
      amgcl::relaxation::ilu0
  >::type
  >,
  amgcl::solver::cg<Backend>
> Solver;
```

Listing 7. Declaration of the NS Block solver.

```cpp
typedef amgcl::static_matrix<double, 3, 3> Block;
typedef amgcl::backend::builtin<Block> Backend;
typedef amgcl::make_solver
  amgcl::amg
    Backend,
    amgcl::coarsening::as_scalar<
      amgcl::coarsening::smoothed_aggregation
    >,
    amgcl::relaxation::ilu0
  >,
  amgcl::solver::cg<Backend>
> Solver;
```

complete preconditioner setup to be performed in block space except for the coarsening, which is
done using scalar arithmetics. Listing 7 shows the definition of the solver in this case.

The performance results for the above solvers are shown in Tables 1 and 2. The tables show
the preconditioner setup time and the solution time in seconds, the sum of the two times as the
total compute time, the number of iterations required for the solver to converge, and the memory
footprint of each preconditioner version in megabytes.

The Scalar solver, as expected, has the worst overall performance, since it does not use any
problem-specific information aside from the aggregation block size. The Block solver does not
rely on the near nullspace components either and behaves similar to the Scalar solver in terms of
convergence (the number of iterations for the solver is only slightly lower than that of the Scalar
one). However, using the block arithmetics allows to reduce the setup time by a factor of about
3, and the total compute time is almost twice lower. The memory footprint of the preconditioner
is also significantly reduced. The Block solver has the fastest setup time and the lowest memory
footprint among all of the considered solvers.
Table 1. Performance results for the connecting rod model.

| Solver     | Setup (s) | Solve (s) | Total (s) | Iterations | Memory (M) |
|------------|-----------|-----------|-----------|------------|------------|
| Scalar     | 0.330     | 1.942     | 2.271     | 96         | 138.86     |
| Block      | 0.117     | 1.065     | 1.182     | 74         | 83.68      |
| NS Scalar  | 0.673     | 0.771     | 1.444     | 29         | 205.16     |
| NS Hybrid1 | 0.699     | 0.621     | 1.321     | 29         | 147.38     |
| NS Hybrid2 | 0.454     | 0.501     | 0.955     | 29         | 114.19     |
| NS Block   | 0.300     | 0.503     | 0.803     | 29         | 114.19     |

Table 2. Performance results for the solid hook model.

| Solver     | Setup (s) | Solve (s) | Total (s) | Iterations | Memory (M) |
|------------|-----------|-----------|-----------|------------|------------|
| Scalar     | 0.227     | 1.366     | 1.594     | 82         | 110.68     |
| Block      | 0.067     | 0.672     | 0.739     | 73         | 61.89      |
| NS Scalar  | 0.591     | 0.500     | 1.091     | 21         | 179.47     |
| NS Hybrid1 | 0.613     | 0.421     | 1.034     | 21         | 129.52     |
| NS Hybrid2 | 0.355     | 0.283     | 0.638     | 21         | 99.76      |
| NS Block   | 0.230     | 0.279     | 0.509     | 21         | 99.76      |

The NS Scalar solver uses the rigid body modes provided with each of the models, but does not use the block arithmetics. The fact that the six near nullspace components are used for the construction of the tentative prolongation makes the AMG hierarchy much heavier in terms of the memory footprint: the preconditioner requires 50–60% more memory, and each iteration of the solver takes about 30–40% more time. However, the use of the rigid body modes results in the significant improvement of the solver performance. NS Scalar converges about 3 times faster and thus the overall compute time is about 50% lower than that of the Scalar solver. Interestingly, even with the improved convergence, the NS Scalar solver is still slower than the simple Block solver. Due to the much faster setup the Block solver is able to outperform the NS Scalar solver by 20–30%. This makes the Block solver a viable choice in cases where the problem is able to converge at all without the use of the near nullspace components.

NS Hybrid1 solver constructs the preconditioner in the scalar space and converts the constructed matrices into the block representation. Hence, its setup time is slightly higher than that of the NS Scalar solver. The solution time for the NS Hybrid1 is lower than NS Scalar, but not in a significant way. This is explained by the fact that about 75% of the solution time is spent on relaxation, and the ILU(0) relaxation here is both constructed and applied in the scalar space. This issue is resolved in the NS Hybrid2 solver, which uses as_block relaxation wrapper to move the construction and application of the ILU(0) relaxation into the block space. This reduces the setup time by 35–40%, and improves the solution time by 20–30% compared to the NS Hybrid1 solver, and by 35–40% compared to the NS Scalar solver. The memory footprint of the NS Hybrid2 solver is also reduced by 20–40%.

The best overall performance is shown by the NS Block solver. Here, the preconditioner is almost completely constructed using block arithmetics with the exception of the transfer operators computation, which is done in the scalar space with the help of the coarsening:as_scalar wrapper class. The setup time here is the best among the NS family of solvers, and is on par with the simple Scalar solver. The solution time is similar to the NS Hybrid2 solver, since both solvers, even though slightly different in terms of construction, result in identical internal data structures. This
is confirmed by the fact that both solvers have equivalent memory footprints. In terms of the overall compute time the NS Block solver is able to outperform the NS Scalar solver by almost 50%, and the simple Scalar solver — by about 65%.

5. SUMMARY

It has been shown that using block arithmetics may significantly speed up the solution of 3D elasticity problems with smoothed aggregation AMG. Two practical techniques of enabling the use of block arithmetics based on the open-source AMGCL library have been suggested. The first approach introduces a hybrid backend that constructs the complete AMG hierarchy using scalar values, and then converts the computed matrices into the block representation. The second technique uses block-valued backend with a coarsening wrapper that converts the input matrix into the scalar format, applies the standard coarsening using scalar arithmetics, and converts the computed transfer operators back to the block representation. The second technique turned out to be more effective. The NS Block solver is able to outperform the fully scalar method by about 50% and requires about 30% less memory for the preconditioner. Another advantage of the NS Block solver is that it does not need to introduce another backend, and the same code may be used with OpenMP or GPGPU backends. Both techniques have been made available to the scientific community as part of the open-source AMGCL library. The flexibility of the library allowed to implement the suggested methods with a minimal amount of code.

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