Accelerating linear solvers for Stokes problems with C++ metaprogramming

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Abstract

The efficient solution of large sparse saddle point systems is very important in computational fluid mechanics. The discontinuous Galerkin finite element methods have become increasingly popular for incompressible flow problems but their application is limited due to high computational cost. We describe C++ programming techniques that may help to accelerate linear solvers for such problems. The approach is based on the policy-based design pattern and partial template specialization, and is implemented in the open source AMGCL library. The efficiency is demonstrated with the example of accelerating an iterative solver of a discontinuous Galerkin finite element method for the Stokes problem. The implementation allows selecting algorithmic components of the solver by adjusting template parameters without any changes to the codebase. It is possible to switch the system matrix to use small statically sized blocks to store the nonzero values, or use a mixed precision solution, which results in up to 4 times speedup, and reduces the memory footprint of the algorithm by about 40%. We evaluate both monolithic and composite preconditioning strategies for 3 benchmark problems. The performance of the proposed solution is compared with a multithreaded direct Pardiso solver and a parallel iterative PETSc solver.

Keywords: Stokes problem, C++ metaprogramming, algebraic multigrid, scalability.

1. Introduction

Incompressible flow modeling has many applications in the scientific and engineering field [1, 2]. The discontinuous Galerkin (DG) finite element methods (FEM) have become increasingly popular for incompressible flow problems (Stokes or Navier-Stokes equations). Compared to the continuous Galerkin (CG) FEM, DG offers several attractive features for incompressible flow simulations: higher-order accuracy on arbitrary unstructured meshes, local mass and momentum conservation, pointwise divergence-free velocity solution, and ease of parallelization [3, 4, 5]. However, the high computational cost of DG methods limits their applicability. Recently, several hybridized DG methods (hybridizable discontinuous Galerkin and weak Galerkin methods) have been proposed to reduce the global degrees-of-freedom (DOFs) of DG while retaining many of the attractive features of DG methods [6, 7, 8]. In these hybridized DG methods, the

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number of global DOFs is significantly reduced by introducing facet variables and eliminating local DOFs via static condensation. However, to achieve the same level of accuracy, the DOFs and computational cost of the hybridized DG methods are still much higher than the conventional CG FEM [9, 10].

For a large 3D simulation, both memory footprint and the solution performance depends not only on the problem size but also on the linear solver configuration. For the Stokes problems, the discretization of the conventional CG FEM results in an indefinite saddle point linear system. There is a lot of research dedicated to the effective solution of such systems, see [11] for an extensive overview. Common approaches are direct solvers and preconditioned Krylov subspace iterative solvers. The direct methods are robust, but do not scale beyond a certain size, typically of the order of a few millions of unknowns [12, 13], due to their intrinsic memory requirements and sheer computational cost. Preconditioned iterative solvers may be further classified by the type of the preconditioner. The simplest choice would be a monolithic preconditioner that does not take the block structure of the linear system into consideration and treats the problem as an opaque linear system. This approach usually does not work very well for saddle point problems, but may still be considered as a viable solution in some cases. Another large class of preconditioners for saddle point problems takes the block structure of the system matrix into account. Well-known examples of such preconditioners are inexact Uzawa algorithm [14], SIMPLE schemes [15], or block-triangular preconditioners [16]. Here we are using the Schur complement pressure correction preconditioner [17, 18, 19]. To our best knowledge, the applicability and performance of the various iterative solvers for the Stokes problem that are commonly used by the CG FEM remains unknown for the new hybridized DG methods.

A lot of popular scientific software packages today are either developed with C or Fortran programming languages, or have C-compatible application programming interface (API). Notable examples are PETSc [20] software package, or BLAS and LAPACK standard programming interfaces with well known and efficient implementations such as Intel MKL [21], OpenBLAS [22], or NVIDIA CUBLAS [23]. The low-level API makes it easy to use the functionality, as most modern programming languages support interaction with external libraries with a C-compatible API. However, this also has some disadvantages: such packages usually have fixed interfaces and may only deal with the cases that the developers have thought about in advance. For example, BLAS has separate sets of similar functions that deal with single, double, complex, or double complex values, but it is impossible to work with mixed precision inputs or with user-defined custom types despite some previous efforts [24]. The PETSc framework, despite being extremely configurable and flexible, still does not support mixed precision solvers or non-standard value types, because switching a value type is done with a preprocessor definition and has a global effect.

In this work, we consider the C++ programming techniques that support creating flexible, extensible and efficient scientific software on the example of the open source $AMGCL^2$ library [25, 26] that implements the algebraic multigrid method (AMG) [27, 28] and other preconditioners for solution of large sparse linear systems of equations. The library uses the C++ metaprogramming so that its users may easily extend it or use it with their datatypes. The advantages of this approach are studied with an example of accelerating an iterative solver of a DG method, specifically the weak Galerkin method, for the Stokes problem. We show that static polymorphism allows reusing the same code in order to exploit the block structure of the matrix by switching to small statically sized matrices as value type, and to employ the mixed precision approach. This results in up to 4 times faster solution and up to 40% reduction of the memory footprint of the algorithm. The source code for the benchmarks is published in [29], and the dataset used in the benchmarks is made available in [30].

The rest of the paper is organized as follows. In Section 2 we discuss the design choices behind the AMGCL library that improve the flexibility and performance of the code. Section 3 describes the Stokes problem and weak Galerkin discretization. Section 4 provides an overview of the linear solvers used in this work. Section 5 presents the results of the numerical experiments and compares the performance of various solution approaches implemented in AMGCL with the performance of a direct MKL solver and an iterative PETSc solver.

²Published at https://github.com/ddemidov/amgcl under MIT license.

Listing 1: Policy-based design illustration: creating customized solvers from AMGCL components

```
// GMRES solver preconditioned with AMG
1
    typedef amgcl::make_solver<</pre>
2
      amgcl::amg<</pre>
3
        amgcl::backend::builtin<double>,
4
        amgcl::coarsening::smoothed_aggregation,
5
        amgcl::relaxation::spai0
6
        >,
7
      amgcl::solver::gmres<</pre>
        amgcl::backend::builtin<double>
9
        >
10
      > Solver;
11
```

2. AMGCL

AMGCL is a C++ header-only template library with a minimal set of dependencies and provides both shared-memory and distributed memory (MPI) versions of the algorithms. The multigrid hierarchy 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. Users may even provide their backends to enable a tight integration between AMGCL and the user code. The library uses the following design principles:

- *Policy-based design* [31] of public library classes such as amgcl::make_solver or amgcl::amg allows the library users to compose their customized version of the iterative solver and preconditioner from the provided components and easily extend and customize the library by providing their implementation of the algorithms.
- Preference for *free functions* as opposed to member functions [32], combined with *partial template specialization* allows extending the library operations onto user-defined datatypes and to introduce new algorithmic components when required.
- The *backend* system of the library allows expressing the algorithms such as Krylov iterative solvers or multigrid relaxation methods in terms of generic parallel primitives to facilitate a transparent acceleration of the solution phase with OpenMP, OpenCL, or CUDA technologies.
- One level below the backends are *value types*: AMGCL supports systems with scalar, complex, or block value types both in single and double precision. Arithmetic operations necessary for the library implementation may also be extended onto the user-defined types using template specialization.

2.1. Policy-based design

The solvers and preconditioners in AMGCL are composed by the library user from the provided components. For example, the most frequently used class template amgcl::make_solver<P,S> binds an iterative solver S to a preconditioner P chosen by the user. To illustrate this, Listing 1 defines a GMRES iterative solver preconditioned with the algebraic multigrid (AMG). Smoothed aggregation is used as the AMG coarsening strategy, and diagonal sparse approximate inverse (SPAI0) is used on each level of the multigrid hierarchy as the smoother. Similar to the solver and the preconditioner, the AMG components (coarsening and relaxation) are specified as template parameters and may be customized by the user. Here the double precision builtin backend (parallelized with OpenMP) is used both for the solver and the preconditioner. Choosing another backend like amgcl::backend::cuda<double> or amgcl::backend::vexcl<double> would make the solver use the CUDA or OpenCL for an acceleration of the solution. This approach allows the library users not only to select any of the solvers, preconditioners, or backends provided by AMGCL, but also to use their custom components, as long as they conform to the generic AMGCL interface.

Besides compile-time composition of the AMGCL algorithms described above, it may be necessary to specify runtime parameters for the constructed solvers. This is done with the parameters structure declared by

```
1 template <class Precond, class Solver>
2 struct make_solver {
3 struct params {
4 typename Precond::params precond;
5 typename Solver::params solver;
6 };
```

7 };

Listing 3: Setting parameters for AMGCL components

```
1 // Set the solver parameters
2 Solver::params prm;
3 prm.solver.M = 50;
4 prm.solver.tol = 1e-6;
5 prm.precond.coarsening.aggr.eps_strong = 1e-3;
6
7 // Instantiate the solver
8 Solver S(A, prm);
```

each of the components as a subtype. In general, each parameter has a reasonable default value. When a class is composed of several components, it includes the parameters of its dependencies into its own params struct. This allows providing a unified interface to the parameters for various AMGCL algorithms. Listing 2 shows that the parameters for the amgcl::make_solver<P,S> class are declared simply as a combination of the preconditioner and the solver parameters. Listing 3 shows an example of parameters specification for the solver from Listing 1. Namely, the number of the GMRES iterations before a restart is set to 50, the relative residual threshold is set to 10^{-6} , and the strong connectivity threshold ε_{str} for the smoothed aggregation is set to 10^{-3} . The rest of the parameters are left with their default values.

2.2. Free functions and partial template specialization

Using free functions as opposed to class methods allows us to decouple the library functionality from specific classes and enables support for third-party datatypes within the library [32]. Delegating the implementation of a free function to a struct template specialization provides more control over the mapping between the input datatype and the specific version of the algorithm. For example, class constructors in AMGCL may accept an arbitrary datatype as an input matrix, as long as the implementation of specific functions supporting the datatype has been provided. Some of the free functions that need to be implemented are amgcl::backend::rows(A) and amgcl::backend::cols(A) (returning the number of rows and columns for the matrix), or amgcl::backend::row_begin(A,i) (returning iterator over the nonzero entries for the matrix row). AMGCL provides adapters for several common input matrix formats, such as Eigen::SparseMatrix from Eigen [33], Epetra_CrsMatrix from Trilinos Epetra [34], or a generic tuple of the Compressed Sparse Row (CSR) arrays. It is also possible to adapt a user-defined datatype.

2.3. Backends

A backend in AMGCL is a class binding datatypes like matrix and vector to parallel primitives like matrix-vector product, linear combination of vectors, or inner product computation. The backend system is implemented using the free functions combined with a template specialization approach from the previous section, which decouples the implementation of common parallel primitives from specific datatypes used in the supported backends. For example, in order to switch to the CUDA backend in Listing 1, one just needs to replace amgcl::backend::builtin<double> with amgcl::backend::cuda<double>. The backend system allows non-intrusive adoption of third-party or user-defined datatypes for use within AMGCL.

An algorithm setup in AMGCL is performed using internal data structures. As soon as the setup is completed, the necessary objects (mostly matrices and vectors) are moved to the backend datatypes. The solution phase of an algorithm is expressed in terms of the predefined parallel primitives which makes it possible to select a parallelization technology (such as OpenMP, CUDA, or OpenCL) simply by changing the backend template parameter of the algorithm. For example, the L2 norm of the residual $\epsilon = ||f - Ax||$ in AMGCL is computed using amgcl::backend::residual() and amgcl::backend::inner_product() primitives:

```
1 backend::residual(f, A, x, r);
```

```
2 auto e = sqrt(backend::inner_product(r, r));
```

2.4. Value types

The value type concept allows generalizing AMGCL 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. Most often, a value type is simply a builtin **double** or **float** scalar, but it is also possible to use small statically sized matrices when the system matrix has a block structure, which decreases the setup time and memory footprint of the algorithm, increases cache locality and may improve convergence rate in some cases [35].

The value types are used during both the setup and the solution phases. Common value type operations are defined in amgcl::math namespace, similar to how backend operations are defined in amgcl::backend. Examples of such operations are math::norm() or math::adjoint(). Arithmetic operations like multiplication or addition are defined as operator overloads. AMGCL algorithms at the lowest level are expressed in terms of the value type interface, which makes it possible to transparently change the algorithm precision, or move to complex values by adjusting the template parameter of the selected backend.

The generic implementation of the value type operations also makes it possible to use efficient third party implementations of the block value arithmetics. For example, using statically sized Eigen matrices instead of the builtin amgcl::static_matrix as block value type may improve performance in case of relatively large blocks, since the Eigen library supports SIMD vectorization.

3. Stokes problem

Consider the equations for the steady incompressible Stokes flow in a bounded domain Ω :

$$-\mu \nabla^2 \mathbf{u} + \nabla p = \mathbf{f},$$

$$\nabla \cdot \mathbf{u} = 0,$$
 (1)

with the following Dirichlet (D) and Neumann (N) boundary conditions:

$$\mathbf{u}_D = [u_D, v_D], \text{ on } \partial\Omega_D$$

$$\mu \nabla \mathbf{u} \cdot \mathbf{n} - p \cdot \mathbf{n} = p_N \mathbf{n}, \text{ on } \partial\Omega_N$$
 (2)

where $\partial \Omega_D \cup \partial \Omega_N = \partial \Omega$ and $\partial \Omega_D \cap \partial \Omega_N = \emptyset$; μ is the fluid dynamic viscosity [Pas], **u** is the flow velocity $[m s^{-1}]$, p is the fluid pressure [Pa], and **f** is the body force term per unit volume $[N/m^3]$, such as electric force and gravity.

The discretization of the Stokes equations (1) is based on a locally divergence-free weak Galerkin finite element method (WGFEM) presented by Wang and Mu [7]. A brief introduction of this method is given below, see [7] for the detailed description and analysis. Let T be a simplex element and $e = \partial T$ the element boundary. Denote the finite element spaces as $V_h = \{(\mathbf{v}_0, \mathbf{v}_b) : \mathbf{v}_0 \in P_k(T), \mathbf{v}_b \in P_k(e)\}$ and $W_h := \{q \in L^2(\Omega) : q \in P_k(T)\}$, which are piecewise discontinuous polynomials with degree less or equal to k for any cell T in the triangulation. Besides, denote the subspace $V_h^{0,\partial\Omega_D}$ with the homogeneous boundary condition, i.e., $\mathbf{v}_b|_{\partial\Omega_D} = 0$. A numerical approximation for eqs. (1) and (2) is to find $\mathbf{u}_h = \{\mathbf{u}_0, \mathbf{u}_b\} \in V_h$ and $p_h \in W_h$ such that $\mathbf{u}_b|_{\partial\Omega_D} = \mathbf{u}_D$ and

$$\int_{\Omega} \mu \nabla_{w} \mathbf{u}_{h} \cdot \nabla_{w} \mathbf{v} - \int_{\Omega} p_{h} (\nabla_{w} \cdot \mathbf{v}) = \int_{\Omega} \mathbf{f} \cdot R_{T} (\mathbf{v}) + \int_{\partial \Omega_{N}} p_{N} \mathbf{n} \cdot \mathbf{v}, \ \forall \mathbf{v} = \{\mathbf{v}_{0}, \mathbf{v}_{b}\} \in V_{h}^{0, \partial \Omega_{D}}, \int_{\Omega} (\nabla_{w} \cdot \mathbf{u}_{h}) q = 0, \ \forall q \in W_{h}$$
(3)

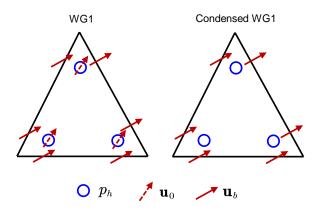


Figure 1: Illustration of the DOFs for the WGFEM method where the interior velocity DOFs can be eliminated via static condensation.

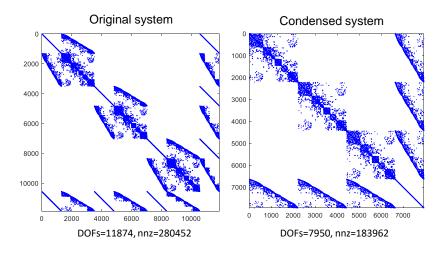


Figure 2: An example of the original and condensed linear system pattern of Stokes problem using WGFEM. Both linear systems are symmetric indefinite.

where ∇_w is the weak gradient operator used in WGFEM. R_T is a velocity reconstruction operator defined on the H(div)-conforming Raviart–Thomas (RT) element space. As shown in Figure 1, p_h and \mathbf{u}_0 are the discontinuous pressure and velocity DOFs defined on the interior of each element. \mathbf{u}_b are the continuous velocity DOFs defined on element facets.

The linear system arising from (3) can be expressed in block-matrix form:

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \left\{ \begin{array}{c} U \\ P \end{array} \right\} = \left\{ \begin{array}{c} L_U \\ L_P \end{array} \right\}$$
(4)

where velocity DOFs have a form of $U = [U_0, U_b]^T$ which corresponds to the interior and facet velocity coefficients of \mathbf{u}_0 and \mathbf{u}_b , respectively. Since \mathbf{u}_0 is defined on a discontinuous space, A has a block-diagonal structure. U_0 can be eliminated from the full linear system (4) via static condensation to produce a significantly smaller condensed system. The linear system (4) can be rearranged as:

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{01} & A_{11} \end{bmatrix} \left\{ \begin{array}{c} X_0 \\ X_1 \end{array} \right\} = \left\{ \begin{array}{c} F_0 \\ F_1 \end{array} \right\}$$
(5)

where $X_0 = [U_0]^T$ and $X_1 = [U_b, P]^T$. Substituting $X_0 = A_{00}^{-1} (F_0 - A_{01}X_1)$ into (5) yields the condensed

```
typedef amgcl::backend::builtin<double> Backend;
1
   typedef amgcl::make_solver<</pre>
2
     amgcl::relaxation::as_preconditioner<
3
       Backend,
4
       amgcl::relaxation::iluk
5
       >,
6
     amgcl::solver::idrs<Backend>
7
     > Solver;
8
9
   Solver::params prm;
10
   prm.solver.s = 5;
11
   prm.precond.k = 1;
12
```

system:

$$A_{11} - A_{10} \left(A_{00}^{-1} \right) A_{01} \right] X_1 = \left\{ F_1 - A_{10} \left(A_{00}^{-1} \right) F_0 \right\}.$$
(6)

The condensed linear system can be written in a block-matrix form as:

$$\begin{bmatrix} A_c & B_c^T \\ B_c & C \end{bmatrix} \left\{ \begin{array}{c} U_b \\ P \end{array} \right\} = \left\{ \begin{array}{c} L_{Uc} \\ L_{Pc} \end{array} \right\}.$$
(7)

The condensed linear system (7) is significantly smaller than the original system (4). Taking a 3D unit cube case (Figure 2) with a linear finite element approximation (k = 1) as an example, the number of global DOFs is reduced by about 30% via static condensation. All the linear systems benchmarked in Section 5 are assembled from the condensed system (7) with the linear pressure and velocity approximation (k = 1). The system is a saddle point problem. There is a lot of research dedicated to the effective solution of such systems, see [11] for an extensive overview. Common approaches are direct solvers and preconditioned Krylov subspace iterative solvers. The following section provides an overview of the solvers studied in this work.

4. Linear solvers for the Stokes problem

The PARDISO solver from MKL [36] is used as a direct solver example. Specifically, the LU factorization solver for real and nonsymmetric matrices is used with the default parameters. The direct solver is robust, but it does not scale well. Both the solution time and the memory requirements grow non-linearly with the system matrix size.

The performance of the preconditioned iterative solvers is tested with AMGCL and PETSc libraries. The simplest choice for the preconditioner is a monolithic one, which does not take the structure of the system into account. We use the IDR(s) solver [37] preconditioned with an incomplete LU factorization with the first order fill-in [38]. The implementation uses amgcl::relaxation::iluk smoother from AMGCL wrapped into amgcl::relaxation::as_preconditioner class. The complete definition for the solver class is shown in Listing 4. The solver is labeled as AMGCL V1 in Section 5.

A preconditioner that takes the structure of the system into account should be a better choice performancewise. As an example of such approach, we consider the Schur complement pressure correction preconditioner [17, 19]. The preconditioning step consists of solving two linear systems:

$$SP = L_{P_c} - B_c A_c^{-1} L_{U_c}, (8a)$$

$$A_c U_b = L_{U_c} - B_c^T P.$$
(8b)

Here S is the Schur complement $S = C - B_c A_c^{-1} B_c^T$. Note that explicitly forming the Schur complement matrix is prohibitively expensive, and the following approximation is used to create the preconditioner for (8a):

$$\hat{S} = C - \operatorname{diag}\left(B_c \operatorname{diag}(A_c)^{-1} B_c^T\right).$$
(9)

```
KSPSetType(solver, KSPBCGSL):
1
   KSPBCGSLSetEll(solver, 5);
2
3
   KSPGetPC(solver,&prec);
4
   PCSetType(prec, PCFIELDSPLIT);
\mathbf{5}
   PCFieldSplitSetType(prec, PC_COMPOSITE_SCHUR);
6
   PCFieldSplitSetSchurPre(prec, PC_FIELDSPLIT_SCHUR_PRE_SELFP, 0);
7
   PCFieldSplitSetSchurFactType(prec, PC_FIELDSPLIT_SCHUR_FACT_LOWER);
8
   PCFieldSplitGetSubKSP(prec, &nsplits, &subksp);
10
   KSPSetType(subksp[0], KSPPREONLY);
11
   KSPSetType(subksp[1], KSPPREONLY);
12
   KSPGetPC(subksp[0], &pc_u);
13
14
   KSPGetPC(subksp[1], &pc_p);
   PCSetType(pc_u, PCGAMG);
15
   PCSetType(pc_p, PCJACOBI);
16
```

There is no need to solve the equations (8) exactly. In our experiments, we perform a single application of the corresponding preconditioner as an approximation to S^{-1} and A_c^{-1} . This means that the overall preconditioner is linear, and we can use a non-flexible iterative solver with it. The matrix (9) has a simple band diagonal structure, and a diagonal preconditioner (Jacobi in case of PETSc, and SPAI(0) [39] in case of AMGCL) shows reasonable performance. The A_c matrix has more interesting structure, and we found that algebraic multigrid with incomplete LU decomposition [38] as a smoother has the best performance as a preconditioner for (8b). This approach was implemented both with AMGCL and PETSc libraries.

The PETSc implementation uses FieldSplit preconditioner of type PC_COMPOSITE_SCHUR with LOWER approximate block factorization type. The preconditioner for the Schur complement is generated from an explicitly-assembled approximation $\hat{S} = C - B_c \operatorname{diag}(A_c)^{-1}B_c^T$. This is more expensive than (9), but it is the best choice available in PETSc in terms of performance for our test problems. The Jacobi and Geometric Algebraic Multigrid (GAMG) preconditioners are used for (8a) and (8b) accordingly. The GAMG preconditioner is used with the default options (smoothed aggregation coarsening with Chebyshev relaxation on each level). Listing 5 shows the definition of the PETSc solver.

The AMGCL implementation (labeled AMGCL V2 in Section 5) is shown in Listing 6, where line 30 enables the approximation (9) for the Schur complement in the preconditioner for the system (8a). This version of the solver has reasonable performance already, but there is still some room for improvement. Note that the nested solvers for systems (8a) and (8b) in lines 18 and 10 of Listing 6 explicitly specify the backend they use. This may seem like redundancy in the library API, but in fact it enables the solver tuning. The matrix A_c has a block structure with 3×3 blocks, where each block corresponds to a single tetrahedron face. We can exploit this with the value type system of AMGCL. The modified nested solver declaration for (8b) is shown in Listing 7. Namely, we declare a block-valued backend with amgcl::static_matrix<3,3,double> as the value type, and use it for the solver. We have to use amgcl::make_block_solver
>instead of amgcl::make_solver
>to automatically convert the matrix A_c to the block format during setup and mix the scalar and block-valued vectors during the preconditioning step. The resulting solver is labeled as AMGCL V3 in Section 5. Switching to the 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 2×2 block structure:

$$\begin{bmatrix} 0.71 & 0.65 & 0.26 & 0.79 \\ 0.54 & 0.37 & 0.17 & 0.62 \\ & 0.89 & 0.05 \\ & 0.27 & 0.15 \\ & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & &$$

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

```
typedef amgcl::backend::builtin<double> Backend;
1
2
    typedef amgcl::make_solver<</pre>
3
      amgcl::amg<
4
        Backend,
\mathbf{5}
        amgcl::coarsening::aggregation,
6
        amgcl::relaxation::ilut
7
        >,
8
      amgcl::solver::preonly<Backend>
9
      > USolver; // Solver for (8b)
10
11
    typedef amgcl::make_solver<</pre>
12
      amgcl::relaxation::as_preconditioner<</pre>
13
        Backend,
14
        amgcl::relaxation::spai0
15
        >,
16
      amgcl::solver::preonly<Backend>
17
        PSolver; // Solver for (8a)
      >
18
19
    typedef amgcl::make_solver<</pre>
20
      amgcl::preconditioner::schur_pressure_correction<
^{21}
        USolver,
22
        PSolver
^{23}
        >,
^{24}
      amgcl::solver::idrs<Backend>
25
      > Solver;
^{26}
27
    Solver::params prm;
28
    prm.solver.s = 5;
29
    prm.precond.adjust_p = 1;
30
```

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 (because each row and column now spans two scalar unknowns), 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. The reduced logical size of the matrix also speeds up the algorithm setup. Finally, the block-valued backend improves cache efficiency during the solution phase. Our experiments show that the setup phase is around 85% faster, the memory footprint is reduced by 15% to 30%, and the overall speedup of 30% to 40% is achieved over the V2 solver.

Another possibility to improve the solver performance is to use the mixed precision approach. A preconditioner only needs to approximate the inverse of the system matrix, which makes the single precision values a natural choice for the preconditioning step. It is enough to use the single precision valued backends with the nested solvers for (8), as shown in Listing 8. The outer iterative solver still uses the double precision

Listing 7: Nested solver declaration for (8b) using the block-valued backend (AMGCL V3)

```
typedef amgcl::backend::builtin<amgcl::static_matrix<3,3,double>> BlockBackend;
1
   typedef amgcl::make_block_solver<</pre>
2
     amgcl::amg<
3
       BlockBackend,
4
       amgcl::coarsening::aggregation,
5
       amgcl::relaxation::ilut
6
       >,
7
     amgcl::solver::preonly<BlockBackend>
8
     > USolver;
9
```

Listing 8: Declaration of single-precision backends for the nested solvers in Listing 6 (AMGCL V4)

```
typedef amgcl::backend::builtin<amgcl::static_matrix<3,3,float>> BlockBackend;
typedef amgcl::backend::builtin<float> SBackend;
```

backend which makes sure the final result has the desired accuracy. The mixed precision version of the solver is labeled as AMGCL V4 in Section 5. As shown in our experiments, using the mixed-precision approach does not increase the number of iterations, and further reduces the memory footprint of the algorithm by around 30% and speeds up the solution phase by 30% to 40% with respect to the V3 solver. The latter is explained by the fact that most iterative solvers are memory-bound, and switching to the single precision effectively doubles the available memory bandwidth.

Note that AMGCL V2, V3, and V4 solvers use the same source code on all stages of the solution, and only differ by the value type of the nested solver backends. The C++ templating system combined with the value type concept in AMGCL allows the compiler to generate efficient machine code for each of the cases.

5. Performance study

In this section, we evaluate the performance of the direct MKL Pardiso solver v2020 and the five iterative solvers introduced in Section 3 and listed in Table 1. The solvers are benchmarked using the three problems described in the following subsections. All tests were conducted on a workstation with 3.30GHz 10-core Intel I9-9820X processor and 64GB of RAM. The Pardiso and the AMGCL solvers use thread parallelism with the OpenMP technology, and the PETSc solver is parallelized using MPI with a single MPI process per CPU core. The source code for the benchmarks is published in [29], and the dataset used in the benchmarks is available in [30]. The AMGCL tests were compiled with g++ v9.2.0 compiler with the 03 optimization level. The PETSc tests were linked against PETSc v3.14.0.

5.1. Unit cube problem

Consider a rotating flow driven by an external force **f** in a closed unit cube $\Omega = [0, 1]^3$ with the constant viscosity $\mu = 1$ as in [40]. The external force **f** and the analytical solution **u** and *p* for this problem can be

	Table 1: Iterative solvers used in the performance tests.				
	Solver	Preconditioner	Value type	Mixed Precision	
AMGCL V1	IDR(5)	ILU(1)	Scalar	No	
AMGCL V2	IDR(5)	SchurPC	Scalar	No	
AMGCL V3	IDR(5)	SchurPC	Block $(3x3)$	No	
AMGCL V4	IDR(5)	SchurPC	Block $(3x3)$	Yes	
PETSc	BCGSL(5)	FieldSplit	Scalar	No	

Table 1: Iterative solvers used in the performance tests

Table 2: Linear system size (DOFs), number of non-zeros (NNZs), and linear system CSR storage memory for the unit cube problem.

Cells	DOFs	NNZs	CSR Memory
384	$9\ 312$	195000	$6.40 { m ~Mb}$
3 072	71 040	$1\ 710\ 000$	$52.64 { m ~Mb}$
24 576	$554 \ 496$	$14 \ 300 \ 000$	$427.65~\mathrm{Mb}$
$131 \ 712$	$2 \ 940 \ 000$	$78 \ 400 \ 000$	$2.27~{ m Gb}$
196 608	$4 \ 380 \ 672$	$117 \ 429 \ 672$	$3.39~{ m Gb}$

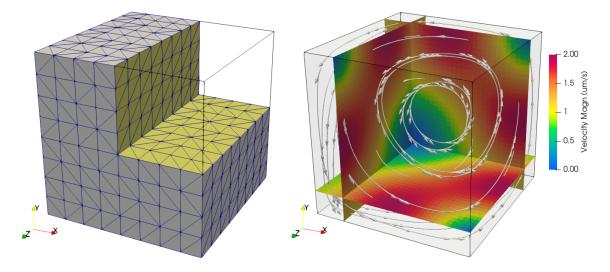


Figure 3: Mesh and velocity field for the unit cube problem

expressed as:

$$\mathbf{f} = \pi \begin{bmatrix} 2\pi \sin(\pi x)\cos(\pi y) - 2\pi \sin(\pi x)\cos(\pi z) + \sin(\pi y)\sin(\pi z)\cos(\pi x) \\ -2\pi \sin(\pi y)\cos(\pi x) + 2\pi \sin(\pi y)\cos(\pi z) + \sin(\pi x)\sin(\pi z)\cos(\pi y) \\ 2\pi \sin(\pi z)\cos(\pi x) - 2\pi \sin(\pi z)\cos(\pi y) + \sin(\pi x)\sin(\pi y)\cos(\pi z) \\ \mathbf{u} = \pi \begin{bmatrix} \sin(\pi x)\cos(\pi y) - \sin(\pi x)\cos(\pi z) \\ \sin(\pi y)\cos(\pi z) - \sin(\pi y)\cos(\pi x) \\ \sin(\pi z)\cos(\pi x) - \sin(\pi z)\cos(\pi y) \end{bmatrix},$$
(10)
$$\mathbf{p} = \sin(\pi x)\sin(\pi y)\sin(\pi z) - \frac{8}{\pi^3}.$$

The domain is partitioned into an unstructured tetrahedral mesh in 5 levels of refinement using Gmsh [41]. The mesh and the computed velocity field are shown in Figure 3. The number of elements, DOFs, non-zeros, and the memory occupied by the system matrix in the CSR format on each level is presented in Table 2.

Figure 4 shows the solution time and the memory usage for the AMGCL, PETSc, and Pardiso solvers. The top left plot shows the solution time in seconds, the top right plot shows the memory footprint of each solver scaled by the size of the system CSR matrix. The plots in the bottom row present the solution time and the memory footprint scaled by the AMGCL V4 solver results. Here the results for AMGCL V1 and V3 are omitted for the sake of readability.

As expected, the direct Pardiso solver scales worse than any of the iterative solvers with respect to both the solution time and especially the memory footprint. In fact, the memory requirements of the Pardiso are so high that it was not able to process the largest problem $(4.4 \times 10^6 \text{ DOFs})$ on the workstation with 64 Gb of RAM. The system with $2.9 \times 10^6 \text{ DOFs}$ consumed 61.1 Gb with the Pardiso solver, as opposed to 5.1 Gb with the AMGCL V4 solver.

Among the iterative solvers, the monolithic AMGCL V1 appears to be the least scalable. The convergence rate of AMGCL V1 deteriorates with the problem size and the number of iterations increases from 20 for the

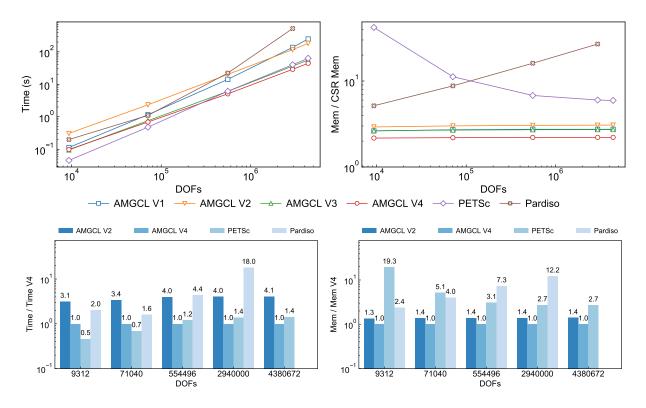


Figure 4: Solution time and memory usage for the unit cube problem.

smallest problem to 1004 for the largest one. However, the memory requirements of this simple method are low (comparable to AMGCL V3), and each iteration is cheap with respect to the composite preconditioners, which allows AMGCL V1 to outperform V2 for problems smaller than 2.9×10^6 DOFs.

All solvers using the Schur pressure correction preconditioner show similar scalability in terms of the compute time. The PETSc version has the best performance for problems below 0.5×10^6 DOFs, and consistently outperforms AMGCL V2 for all problem sizes. Memory-wise, the PETSc version apparently has a constant overhead of around 200 Mb, which explains its relatively high memory usage for the smaller problems. AMGCL solvers stay the most memory-efficient even for the largest problem, where PETSc uses 20.6 Gb, and AMGCL solvers consume from 7.6 Gb (V4) to 10.6 Gb (V2). AMGCL V3 and V4 outperform PETSc for the three largest problems. The switch to the block-valued backend for (8b) has the largest impact on performance, since the V3 and V4 solution times are very close. AMGCL V4 is up to 4.1 times faster than V2 and only about 25% faster than V3. Due to the mixed precision approach, V4 memory requirements are 40% less than V2, and 25% less than V1 and V3. Although the AMGCL V2, V3, and V4 solvers use exactly the same code, the block-valued backend combined with the mixed precision approach allows the AMGCL V4 to outperform PETSc by about 40% for the largest problem sizes.

5.2. Converging-diverging tube problem

In this case, the solution performance is evaluated with the example of a pressure-driven tube flow (Figure 5). Consider the Stokes flow through a 3D converging-diverging tube under a pressure drop of 1Pa. The Neumann boundary conditions are imposed at the top $(z = -3.75\mu m)$ and the bottom $(z = 1.25\mu m)$ walls. The no-slip wall boundary conditions of $\mathbf{u} = (0, 0, 0)^T$ are imposed on the surface of the varying radius tube. The fluid dynamics viscosity is uniformly set as 1Pas. Given the tube length $L = 5\mu m$ and the average tube radius of $R_0 = 1\mu m$, the radius of the axisymmetric tube can be expressed as:

$$R(z) = 1.0 + 0.6 \sin\left(\frac{2\pi z}{5.0}\right).$$
(11)

Table 3: Linear system size (DOFs), number of non-zeros (NNZs), and linear system CSR storage memory for the convergingdiverging tube problem.

Cells	DOFs	NNZs	CSR Memory
327	7 950	184000	$6.07 { m ~Mb}$
$1 \ 203$	28 653	710 000	$22.78 \mathrm{~Mb}$
5 319	$125\ 028$	$3\ 220\ 000$	$101.43~{\rm Mb}$
40 488	$921\ 129$	$25 \ 300 \ 000$	$766.66~{\rm Mb}$
144 995	$3\ 262\ 682$	95 300 000	$2.81~{\rm Gb}$
296 823	$6\ 648\ 114$	$196\ 657\ 124$	$5.78~{ m Gb}$

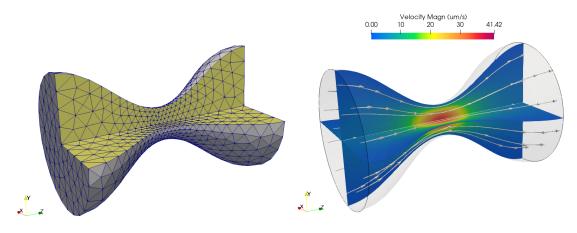


Figure 5: Mesh and velocity field for the converging-diverging tube problem

The 6 mesh refinement levels are generated using Gmsh. The mesh and the computed velocity field are shown in Figure 5. Table 3 shows the problem size at each level, and Figure 6 presents the solution time and the memory usage scaled by the CSR matrix size and by the AMGCL V4 solver results.

The main trends here are similar to the unit cube problem case. The direct Pardiso solver shows the worst scaling both in solution time and memory, and is not able to solve the largest system of 6.6×10^6 DOFs due to the memory limitations. The iterative AMGCL V1 solver with a simple monolithic preconditioner has low memory usage but scales badly with respect to the solution time. Both Pardiso and the AMGCL V1 solvers are outperformed by AMGCL V2 starting with the 0.9×10^6 DOFs problem.

The AMGCL V3 and V4 solvers, and the PETSc solver show similar performance, although this time PETSc has slightly lower solution time everywhere except the 0.9×10^6 DOFs problem, where it is outperformed by both AMGCL V3 and V4. Again, PETSc has a large constant memory overhead of approximately 250 Mb, and is overall more expensive memory-wise. At the largest problem of 6.6×10^6 DOFs PETSc needs 31.2 Gb, while AMGCL only requires from 12.6 Gb (V4) to 17.2 Gb (V2). AMGCL V4 is 3–4 times faster than V2 and is consistently the most memory-efficient solver.

5.3. Sphere packing problem

The final case we consider is a complex sphere packing flow problem with non-uniform cell size distribution and large cell size contrast (Figure 7). A box-shaped domain of $85 \times 85 \times 85\mu$ m is used where the 21 spheres with a radius of 22µm are packed randomly with the resulting porosity of 36.4%. Similar to the convergingdiverging tube problem, a pressure drop of 1Pa is applied on both ends of the domain in z direction ($z = 0\mu$ m and $z = 85\mu$ m). The no-slip wall boundary conditions of $\mathbf{u} = (0, 0, 0)^T$ are imposed on all sphere surfaces and box surfaces in Y and X directions. The 7 refinement mesh levels are generated using Gmsh. The mesh and the computed velocity field are shown in Figure 7. Table 4 shows the problem size at each level, and Figure 8 presents the solution time and the memory usage scaled by the CSR matrix size and by the AMGCL V4 solver results.

The matrix structure in this case is favorable to the direct Pardiso solver, since the solver shows the relatively low memory usage of approximately 10 times the size of the CSR matrix, as opposed to 21 and

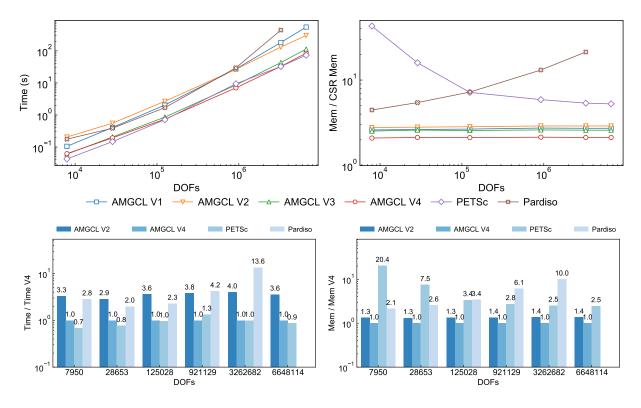


Figure 6: Solution time and memory usage for the converging-diverging tube problem.

Table 4: Linear system size (DOFs), number of non-zeros (NNZs), and linear system CSR storage memory for the sphere packing problem.

Cells	DOFs	NNZs	CSR Memory
$9\ 487$	238 810	$5\ 021\ 060$	$176.87 \mathrm{~Mb}$
19 373	483 509	$10 \ 400 \ 000$	$397.01 { m ~Mb}$
36 430	$896\ 257$	$20\ 200\ 000$	$687.07~{\rm Mb}$
$63 \ 382$	$1 \ 537 \ 891$	$36\ 100\ 000$	$1.18~{\rm Gb}$
$100 \ 255$	$2\ 405\ 788$	$58\ 400\ 000$	$1.87~{\rm Gb}$
259 009	$6\ 089\ 212$	$157\ 000\ 000$	$4.90~{\rm Gb}$
$404 \ 019$	$9\ 420\ 534$	$248\ 874\ 496$	$7.96~{ m Gb}$

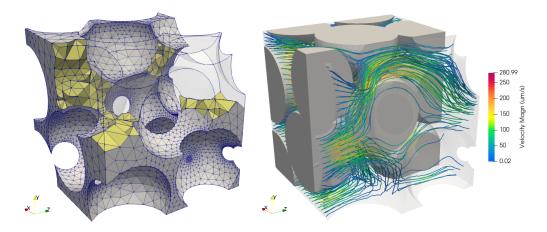


Figure 7: Mesh and velocity field for the sphere packing problem

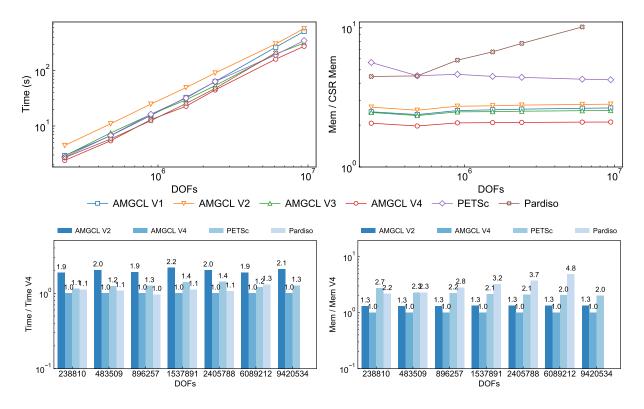


Figure 8: Solution time and memory usage for the sphere packing problem.

27 times for the unit cube and the converging-diverging tube problems at the largest problem sizes. This could possibly be explained by the significant amount of tetrahedron faces with the Dirichlet boundaries modeling the no-slip conditions at the sphere walls. As a result, the direct Pardiso solver shows almost linear scalability and only starts to slow down at the largest problem size it can handle on our machine. Up to that point, it shows the solution times comparable with AMGCL V4, which shows the best solution times among the iterative solvers for this problem. However, the high memory requirements still remain an issue for the Pardiso solver.

The simplest AMGCL V1 version with the monolithic preconditioner shows worse than linear scalability, but still is able to outperform V2 even for the largest problem. Its efficiency is explained by the fact that AMGCL V1 makes twice fewer iterations for the sphere packing problem than in the cases of the unit cube and converging-diverging tube problems, which probably has the same reasons the Pardiso solver is working so well here.

Among the rest of the iterative solvers, AMGCL V2 shows the worst performance throughout the whole range of the problem sizes, while AMGCL V4 consistently has the best solution times and is about 2 times faster than V2 and 10–30% faster than PETSc. Memory-wise, AMGCL solvers are still the most efficient. The V4 version requires about twice less memory than the PETSc solver for all problem sizes starting with the 0.4×10^6 DOFs one. As in the previous cases, the constant memory overhead inherent to PETSc skews the ratio for the smallest problem size.

6. Discussion

We have analyzed the efficiency of several solvers for large sparse linear systems obtained from discretization of the Stokes equations with a discontinuous Galerkin finite element method. As expected, the direct Pardiso solver from MKL demonstrated the worst scalability in terms of both the solution time and the memory footprint of the solution. A Krylov subspace iterative method preconditioned with a monolithic preconditioner ignoring the system structure scales linearly with the system size with respect to memory, but the solution time has faster than linear growth. The solvers that use the Schur pressure correction preconditioner accounting for the problem structure show equally good scalability. However, the PETSc version is 2–4 times faster than the AMGCL V2 version, even though both versions work with scalar matrices and use a full precision approach. AMGCL is able to outperform PETSc for two out of three benchmarks by up to 40% with versions V3 (using the blockvalued backend for the flow subsystem), and V4 (using both the block-valued backend and mixed precision approach). This means that if the performance of the baseline AMGCL V2 could be improved to be on par with the PETSc implementation, then the performance of the AMGCL V4 solver could be considerably faster than the PETSc version. This, however, is out of scope of the current work.

Comparing the baseline AMGCL V2 performance to V3 shows that the switch from the scalar to the block value type reduces the setup complexity by 85%, the memory footprint of the method by about 20% and achieves the total speedup of 30% to 40%. Further, using a mixed precision approach (single precision preconditioner with double precision iterative solver) the memory footprint of the method is further reduced by 30% and the total solution time is decreased by another 30%. Overall, the V4 solver requires approximately 40% less memory and is 2 to 4 times faster than the V2 solver, even though the number of iterations between versions V2 - V4 of the solver stays practically constant. In other words, as long as using the single precision preconditioning does not affect the convergence of the solution, the improvements described here should not change the algorithmic scalability of the method, but should simply accelerate the underlying operations.

It should be noted that AMGCL versions from V2 to V4 are using the same code. By using the C++ metaprogramming techniques such as policy-based design, partial template specialization, and free functions in the library code, we are able to select the most efficient implementation simply by changing the backend definition in the solver template parameters. Of course, the C++ metaprogramming does not guarantee high performance by itself, and the same approach could be implemented in a pure C library, but it would require much bigger effort from the library developers. The results in this work were presented for the new DG FEM method, but we believe the same techniques could be used to accelerate the solution of any Stokes-like system.

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