Accelerating linear solvers for large-scale Stokes problems with C++ metaprogramming

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Abstract

Ability to solve large sparse linear systems of equations is very important in modern numerical methods. Creating a solver with a user-friendly interface that can work in many specific scenarios is a challenging task. We describe the C++ programming techniques that can help in creating flexible and extensible programming interfaces for linear solvers. The approach is based on policy-based design and partial template specialization, and is implemented in the open source AMGCL library. Convenience for the user and efficiency is demonstrated on the example of accelerating a large-scale Stokes problem solution with a Schur pressure correction preconditioner. The user may select algorithmic components of the solver by adjusting template parameters without any change to the codebase. It is also possible to switch to block values, or use mixed precision solution, which results in up to 4 times speedup, and reduces the memory footprint of the algorithm by about 50%.

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

1. Introduction

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 [1] software package, or BLAS and LAPACK standard programming interfaces with well known and efficient implementations such as Intel MKL [2], OpenBLAS [3], or NVIDIA CUBLAS [4]. 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 [5]. The PETSC framework, despite being extremely configurable and flexible, still does not support using mixed precision or non-standard value types, because switching a value type is done with a preprocessor definition and has global effect. Another common drawback of large scientific

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packages is that users have to adopt the datatypes provided by the framework in order to work with it, which steepens the learning curve and introduces additional integration costs. Admittedly, most of such libraries are the low level linear algebra packages, but even more modern and user-friendly frameworks, like Python SciPy [6] or the Fenics project [7] are often based on these libraries and thus inherit the restrictions.

Using C++ programming language with capabilities for generic programming may help to overcome these issues while staying highly effective [8]. Well-known examples of C++-based software packages are Trilinos [9], OpenFOAM [10], or Kratos Multiphysics [11].

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 library [12] that implements the algebraic multigrid method (AMG) [13, 14] and other preconditioners for solution of large sparse linear systems of equations. The library uses C++ metaprogramming so that its users may easily extend it or use it with their own datatypes. The advantages of this approach are studied on the example of solving a Stokes system using Schur pressure correction preconditioner [15]. We show how static polymorphism allows to reuse the same code in order to exploit 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 50% reduction of the memory footprint of the algorithm.

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 possible solution options. Section 4 presents the results of our numerical experiments and compares the performance of various solution approaches implemented in AMGCL with the performance of a direct MKL solver as a baseline.

2. AMGCL

The AMGCL C++ library is a header-only template library with a minimal set of dependencies [12] and provides both shared-memory and distributed memory (MPI) versions of the algorithms. The multigrid hierarchy is constructed using built-in 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 own backends which enables tight integration between AMGCL and the user code. The library uses the following design principles:

- **Policy-based design** [16] of public library classes such as amgcl::make_solver or amgcl::amg allows the library users to compose their own customized version of the iterative solver and preconditioner from the provided components and easily extend and customize the library by providing their own implementation of the algorithms.

- Preference for **free functions** as opposed to member functions [17], combined with **partial template specialization** allows to extend 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 which facilitates 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 work may also be extended onto the user-defined types using template specialization.

2.1. Policy-based design

Available 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 together an iterative solver S and a preconditioner P chosen by the user. To illustrate this, listing 1 defines a conjugate

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\[2\] Published at https://github.com/ddemidov/amgcl under MIT license.
Listing 1: Policy-based design illustration: creating customized solvers from AMGCL components

```cpp
// CG solver preconditioned with ILU0
typedef amgcl::make_solver<
    amgcl::relaxation::as_preconditioner<
        amgcl::backend::builtin<double>,
        amgcl::relaxation::ilu0
    >,
    amgcl::solver::cg<
        amgcl::backend::builtin<double>
    >
> Solver1;

// GMRES solver preconditioned with AMG
typedef amgcl::make_solver<
    amgcl::amg<
        amgcl::backend::builtin<double>,
        amgcl::coarsening::smoothed_aggregation,
        amgcl::relaxation::spai0
    >,
    amgcl::solver::gmres<
        amgcl::backend::builtin<double>
    >
> Solver2;
```

Listing 2: Example of parameter declaration in AMGCL components

```cpp
template <class P, class S>
struct make_solver {
    struct params {
        typename P::params precond;
        typename S::params solver;
    };
};
```

gradient iterative solver preconditioned with an incomplete LU decomposition with zero fill-in in lines 2 to 10. The builtin backend (parallelized with OpenMP) with double precision is used both for the solver and the preconditioner. This approach allows the user not only to select any of the preconditioners/solvers provided by AMGCL, but also to use their own custom components, as long they conform to the generic AMGCL interface. In particular, the preconditioner class has to provide a constructor that takes the system matrix, the preconditioner parameters (defined as a subtype of the class, see below), and the backend parameters. The iterative solver constructor should take the size of the system matrix, the solver parameters, and the backend parameters.

This approach is used not only at the user-facing level of the library, but in any place where using interchangeable components makes sense. Lines 13 to 22 in listing 1 show the declaration of GMRES iterative solver preconditioned with the algebraic multigrid (AMG). Smoothed aggregation is used as the AMG coarsening strategy, and diagonal sparse approximate inverse is used on each level of the multigrid hierarchy as a 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.

Besides compile-time composition of the AMGCL algorithms described above, the library user may need to specify runtime parameters for the constructed algorithms. This is done with the params structure declared by each of the components as its subtype. In general, each parameter usually has a reasonable default value. When a class is composed from several components, it includes the parameters of its dependencies into its own params struct. This allows to provide a unified interface to the parameters of various AMGCL algorithms.
// Set the solver parameters
Solver2::params prm;
prm.solver.M = 50;
prm.solver.tol = 1e-6;
prm.precond.coarsening.aggr.eps_strong = 1e-3;

// Instantiate the solver
Solver2 S(A, prm);

Listing 3 shows an example of how the parameters for the preconditioned GMRES solver from listing 1 may be specified. Namely, the number of the GMRES iterations before restart is set to 50, the relative residual threshold is set to $10^{-6}$, and the strong connectivity threshold $\varepsilon_{str}$ 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 to decouple the library functionality from specific classes and enables support for third-party datatypes within the library [17]. Moving the implementation from the free function into a struct template specialization provides more control over the mapping between the input datatype and the specific specific version of the algorithm. For example, constructors of AMGCL classes may accept an arbitrary datatype as input matrix, as long as the implementations of several basic functions supporting the datatype have been provided. Some of the free functions that need to be implemented are amgcl::backend::rows(A), 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 values for the matrix row). Listing 4 shows implementation of amgcl::backend::rows() function for the case when the input matrix is specified as a std::tuple(n,ptr,col,val) or matrix size n, pointer vector ptr containing row offsets into the column index and value vectors, and the column index and values vectors col and val for the nonzero matrix entries. AMGCL provides adapters for several common input matrix formats, such as Eigen::SparseMatrix from Eigen [18], Epetra_CrsMatrix from Trilinos Epetra [9], and it is easy to adapt a user-defined datatype.

2.3. Backends

A backend in AMGCL is a class binding datatypes like matrix and vector with 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 template specialization approach from the previous section, which decouples implementation of common parallel primitives from specific datatypes used in the supported backends. This allows to adopt third-party or user-defined datatypes for use within AMGCL without any modification. For example, in order to switch to the CUDA backend in listing 1, we just need to replace amgcl::backend::builtin<double> with amgcl::backend::cuda<double>.

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 transferred to the backend datatypes. Solution phase of the algorithms is expressed in terms of the predefined parallel primitives which makes it possible to switch parallelization technology (such as OpenMP, CUDA, or OpenCL) simply by changing the backend template parameter of the algorithm. For example, the residual norm $\|f - Ax\|$ in AMGCL is computed using amgcl::backend::residual() and amgcl::backend::inner_product() primitives:

```cpp
backend::residual(f, A, x, r);
auto e = sqrt(backend::inner_product(r, r));
```
// Generic implementation of the rows() function.
// Works as long as the matrix type provides rows() member function.

template <class Matrix, class Enable = void>
struct rows_impl {
  static size_t get(const Matrix &A) {
    return A.rows();
  }
};

// Returns the number of rows in a matrix.
template <class Matrix>
size_t rows(const Matrix &matrix) {
  return rows_impl<Matrix>::get(matrix);
}

// Specialization of rows_impl template for a CRS tuple.
template <typename N, typename PRng, typename CRng, typename VRng>
struct rows_impl< std::tuple<N, PRng, CRng, VRng> > {
  static size_t get(const std::tuple<N, PRng, CRng, VRng> &A) {
    return std::get<0>(A);
  }
};

2.4. Value types

Value type concept allows to generalize AMGCL algorithms onto complex or non-scalar systems. A value type defines a number of overloads for common math operations, and is used as a template parameter for a backend. Most often, a value type is simply a builtin double or float atomic value, but it is also possible to use small statically sized matrices when the system matrix has a block structure, which may decrease the setup time and the overall memory footprint, increase cache locality, or improve convergence ratio [19].

Value types are used during both setup and 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 switch precision of the algorithms, or move to complex values, simply by adjusting 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 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 a numerical scheme of the steady incompressible Stokes equations in a bounded domain Ω:

\[-\mu \nabla^2 u + \nabla p = f,\]
\[\nabla \cdot u = 0,\]

with the following boundary conditions:

\[u_D = [u_D, v_D], \text{ on } \partial \Omega_D\]
\[\mu \nabla u \cdot n - p \cdot n = p_N n, \text{ on } \partial \Omega_N\]
where \(\partial \Omega_D \cup \partial \Omega_N = \partial \Omega\) and \(\partial \Omega_D \cap \partial \Omega_N = \emptyset\); \(\mu\) is the fluid dynamic viscosity \([\text{Pa s}]\), \(\mathbf{u}\) is the flow velocity \([\text{m s}^{-1}]\), \(p\) is the fluid pressure \([\text{Pa}]\), and \(\mathbf{f}\) is the body force term per unit volume \([\text{N/m}^3]\), such as electric force and gravity.

The discretization of the Stokes equation of (1) is based on locally divergence-free weak Galerkin finite element method (WGFEM) presented by Wang and Mu \([20]\). A brief introduction of this method is given below, see \([20]\) for a detailed description and analysis. Denote the finite element spaces as \(V_h = \{(v_0, v_b) : v_0 \in P_k(T), v_b \in P_k(e)\}\) and \(W_h = \{q \in L^2(\Omega) : q \in P_k(T)\}\), which are piece-wise discontinuous polynomials with degree less or equal to \(k\) for any cell \(T\) in the triangulation. Besides, denote the subspace \(V_0, \partial \Omega_D h\) with the homogeneous boundary condition, i.e., \(v_b|_{\partial \Omega_D} = 0\).

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

\[
\int_{\Omega} \mu \nabla w \cdot \mathbf{u}_h \, d\Omega - \int_{\Omega} p_h (\nabla w \cdot \mathbf{v}) \, d\Omega = \int_{\Omega} \mathbf{f} \cdot R_T (\mathbf{v}) + \int_{\partial \Omega_N} p_N n \cdot \mathbf{v}, \quad \forall \mathbf{v} = \{\mathbf{v}_0, \mathbf{v}_b\} \in V_h^{0, \partial \Omega_D},
\]

\[
\int_{\Omega} (\nabla w \cdot \mathbf{u}_h) \, q = 0, \quad \forall q \in W_h
\]

where \(R_T\) is a velocity reconstruction operator defined on the \(H(\text{div})\)-conforming Raviart–Thomas (RT) element space. As shown in fig. 1, \(p_h\) and \(\mathbf{u}_h\) are the discontinuous pressure and velocity degree-of-freedoms (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 as block-matrix form:

\[
\begin{bmatrix}
A & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
U \\
P
\end{bmatrix}
= \begin{bmatrix}
L_U \\
L_P
\end{bmatrix}
\]  

\[ (4) \]

where velocity DOFs has a form of \(U = [U_0, U_b]^T\) which is corresponding to the interior and facet velocity coefficients of \(\mathbf{u}_0\) and \(\mathbf{u}_b\), respectively. As \(\mathbf{u}_0\) is defined on 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 system. The linear system (4) can be rearranged as:

\[
\begin{bmatrix}
A_{00} & A_{01} \\
A_{01} & A_{11}
\end{bmatrix}
\begin{bmatrix}
X_0 \\
X_1
\end{bmatrix}
= \begin{bmatrix}
F_0 \\
F_1
\end{bmatrix}
\]  

\[ (5) \]

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) we obtain the condensed system:

\[
\begin{bmatrix}
A_{11} - A_{10} (A_{00}^{-1}) A_{01}
\end{bmatrix}
X_1 = \{ F_1 - A_{10} (A_{00}^{-1}) F_0 \}.
\]  

\[ (6) \]
The condensed linear system can be written in block-matrix form as:

\[
\begin{bmatrix}
A_c & B_c^T \\
B_c & C
\end{bmatrix}
\begin{bmatrix}
U_b \\
P
\end{bmatrix}
= 
\begin{bmatrix}
L_{U_c} \\
L_{P_c}
\end{bmatrix}.
\]  

(7)

The condensed linear system (7) is significantly smaller than (4). Taking a 3D unit cube case (fig. 2) with the linear finite element approximation ($k = 1$), the number of global DOFs is reduced by about 30% via static condensation. In this paper, all testing linear systems are assembled from condensed system (7) with linear pressure and velocity approximation ($k = 1$). The system is a saddle point problem. There is a lot of research dedicated to effective solution of such systems, see [21] for an extensive overview. Common approaches are direct solvers, and preconditioned Krylov subspace iterative solvers.

Direct methods are robust, but do not scale beyond a certain size, typically of the order of a few millions of unknowns [22, 23], due to their intrinsic memory requirements and sheer computational cost. In this work we are using a direct solution with a PARDISO solver from MKL [24] as a baseline.

Preconditioned iterative solvers may be further divided by the type of the preconditioner. The simplest choice would be a monolithic preconditioner that does not take the block structure of (7) 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. Here we are using conjugate gradient iterative solver [25] preconditioned with an incomplete LU factorization with the first order fill-in [26]. The implementation uses \texttt{amgcl::relaxation::iluk} smoother from AMGCL wrapped into \texttt{amgcl::relaxation::as_preconditioner} class. The complete definition for the solver class is shown in listing 5. The solver is labeled as V1 in section 4.

Another large class of preconditioners for saddle point type problems takes the block structure of the system matrix into account. Well-known examples of such preconditioners are inexact Uzawa algorithm [27],
Listing 6: FGMRES preconditioned with SchurPC (V2)

```c
typedef amgcl::backend::builtin<double> Backend;
typedef amgcl::make_solver<
    amgcl::preconditioner::schur_pressure_correction<
        amgcl::make_solver< // Solver for (8b)
            Backend,
            amgcl::coarsening::aggregation,
            amgcl::relaxation::ilut
        >,
        amgcl::solver::cg<Backend>
    >,
    amgcl::make_solver< // Solver for (8a)
        amgcl::relaxation::as_preconditioner<
            Backend,
            amgcl::relaxation::spai0
        >,
        amgcl::solver::cg<Backend>
    >
    >,
    amgcl::solver::fgmres<Backend>
>
Solver;
```

SIMPLE schemes [28], or block-triangular preconditioners [29]. Here we are using Schur complement pressure correction preconditioner [30, 31]. The preconditioning step consists of solving two linear systems:

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

$$A_c U_b = L_{U_c} - B_c^T P.$$  \hspace{1cm} (8b)

Here $S$ is the Schur complement $S = C - B_c A_c^{-1} B_c^T$. Note that explicitly forming the Schur complement system is prohibitively expensive, and matrix-free iterative solver is used to solve (8a), where each application of matrix vector product $Sp$ involves an approximate solution of the system

$$A_c u = f.$$  \hspace{1cm} (9)

Thus, we need to solve the system (9) once to form the right-hand side for (8a), once to solve (8b), and on each iteration of the matrix-free solution of (8a). This makes the possibility to find an approximate solution to the system (9) extremely important for the overall algorithm efficiency. In our experiments the system is solved with conjugate gradient iterative solver preconditioned with non-smoothed aggregation AMG. Incomplete LU with thresholding [26] is used as a smoother on each level of the AMG hierarchy.

Another important detail is the preconditioner that is used for the matrix-free solution of (8a). Here we are using the matrix

$$\hat{S} = C - \text{diag}(B_c \text{diag}(A_c)^{-1} B_c^T)^{-1}$$  \hspace{1cm} (10)

as an approximation to the Schur complement [32]. $\hat{S}$ is easy to construct explicitly, and keeps the block-diagonal structure (with $4 \times 4$ blocks) of the matrix $C$. We use conjugate gradient preconditioned with SPAI(0) [33] as an iterative solver for the system (8a). The SPAI(0) preconditioner is constructed for the approximated Schur complement (10).
Listing 7: FGMRES preconditioned with SchurPC, with block matrix $A_c$ (V3)

```cpp
typedef amgcl::backend::builtin<
double> Backend;
typedef amgcl::backend::builtin<amgcl::static_matrix<3,3,double>> BBackend;
typedef amgcl::make_solver<
  amgcl::preconditioner::schur_pressure_correction<
    amgcl::make_block_solver<
      // Solver for (8b)
      amgcl::amg<
        BBackend,
        amgcl::coarsening::aggregation,
        amgcl::relaxation::ilut
      >,
      amgcl::solver::cg<BBackend>
    >,
    amgcl::make_solver<
      // Solver for (8a)
      amgcl::relaxation::as_preconditioner<
        Backend,
        amgcl::relaxation::spai0
      >,
      amgcl::solver::cg<Backend>
    >,
    amgcl::solver::fgmres<Backend>
  >
> Solver;
```

Since the approach described above results in a preconditioner that may vary from iteration to iteration, we use flexible GMRES [26] as the outer iterative solver for the system (7). The solver is labeled as V2 in section 4, and its complete definition is shown in listing 6. Here we construct the solver from readily available components in AMGCL, and then adjust some of the runtime parameters to get the optimal performance. Namely, we limit the number of iterations and tolerance in the inner solvers for eqs. (8a) and (8b) (lines 26 to 29). Line 24 disables the default optimization where $\text{diag}(A_c)^{-1}$ is used instead of $A_c^{-1}$ in the matrix-free implementation of the Schur complement, which turned out to be counterproductive in our experiments, and line 25 enables approximation (10) 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 12 and 4 of listing 6 explicitly specify the backend they use. This may seem like a redundancy in the library API, but in fact it allows us to further tune the solver. We note that the matrix $A_c$ has block structure with small $3 \times 3$ blocks, where each block corresponds to a single tetrahedron face. This can be used to our advantage by employing the value type system of AMGCL. The modified solver declaration is shown in listing 7. Namely, we declare block-valued backend using `amgcl::static_matrix<3,3,double>` and use it with the inner solver for the system (8b). We also need to use `amgcl::make_block_solver<>` instead of `amgcl::make_solver<>` here which implicitly converts the input matrix to the block format during setup and allows to mix scalar and block-valued vectors during the preconditioning step.

Switching to a block-valued backend has several advantages. First, the block representation of the matrix is more efficient memory-wise. The matrix $A_c$ in block format has three times fewer rows and columns which reduces the sizes of book-keeping arrays of the CRS format. Row pointer array becomes three times smaller, and the column index arrays becomes nine times smaller with respect to the scalar matrix. The reduced logical size of the matrix matrix also speeds up the setup phase of the algorithm. Finally, block-valued backend improves cache efficiency during the solution phase. Our experiments showed that the setup phase was around 85% faster, the memory footprint was reduced by 15% to 30%, and the overall speedup of 31% to 41% was achieved over the V2 solver.

Another possibility to improve the performance of the solver is to use mixed precision for the solution. A preconditioner only needs to be an approximation to the system matrix inverse, which makes using single
typedef amgcl::backend::builtin<double> Backend;
typedef amgcl::backend::builtin<float> SBackend;
typedef amgcl::backend::builtin<amgcl::static_matrix<3,3,float>> BBackend;
typedef amgcl::make_solver<
    amgcl::preconditioner::schur_pressure_correction<
        amgcl::make_block_solver<
            // Solver for (8b)
            amgcl::amg<
                BBackend,
                amgcl::coarsening::aggregation,
                amgcl::relaxation::ilut
            >,
            amgcl::solver::cg<BBackend>
        >,
        // Solver for (8a)
        amgcl::relaxation::as_preconditioner<
            SBackend,
            amgcl::relaxation::spai0
        >,
        amgcl::solver::cg<SBackend>
    >,
    amgcl::solver::fgmres<Backend>
> Solver;

Table 1: Iterative solvers used in the performance tests

| Solver | Preconditioner | Value type | Mixed Precision |
|--------|----------------|------------|-----------------|
| V1 CG  | ILU(1)         | Scalar     | N               |
| V2 FGMRES | SchurPC  | Scalar     | N               |
| V3 FGMRES | SchurPC  | Block (3x3) | N               |
| V4 FGMRES | SchurPC  | Block (3x3) | Y               |

precision floating point numbers for preconditioning step a natural choice. In order to implement this, as shown in listing 8, we change the block-valued backend used in the solver for (8b) to use single precision arithmetic, and we declare a single precision scalar backend that we use for the solution of (8a). The outer FGMRES solver still uses the double precision backend which makes sure the final result has the desired accuracy. As shown in our experiments, using mixed-precision solver does not increase the number of iterations required for convergence, but further reduces the memory footprint of the algorithm by around 30% and speeds up the solution phase by 60% to 70% with respect to the V3 solver. The latter is explained by the fact that performance of most iterative solvers is memory-bound, and switching to the single precision numbers effectively doubles the available memory bandwidth.

4. Performance study

In this section, we evaluate the performance of 4 iterative solvers (introduced in section 3 and listed in table 1) for three benchmark problems and compare the results against the multi-threaded direct solver of MKL Pardiso v2020. The LU factorization solver (mtype=11) in MKL is used with the default PARDISO solver parameters (iparm). The relative residual threshold for all iterative solvers is set to $10^{-12}$. All tests are conducted on a workstation with 3.30GHz 10-core Intel I9-9820X processor and 64GB of RAM. We compiled AMGCL using Intel Compiler v19.1 with the O3 optimization level.
4.1. Unit cube problem

Consider a rotating flow driven by an external force $f$ in a closed unit cube $\Omega = [0,1]^3$ with constant viscosity of $\mu = 1$ as in [34]. The external force $f$ and analytical solution $u$ and $p$ for this problem can be expressed as:

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

The domain is partitioned into unstructured tetrahedral mesh in 6 levels of refinement using Gmsh [35]. Table 2 shows the baseline performance results by using the multi-threaded direct solver using 10 cores. Results show that the direct solver memory usage is increased much faster than the linear system storage memory usage. In this example problem, a workstation with 64 Gb RAM is limited to solve a problem with about 0.13 million cells.

Figure 4 shows the relative memory usage and runtime performance for iterative solvers against the direct solver for the unit cube problem. The memory usage of the iterative solvers becomes significantly lower than the direct solver with increasing problem size. For the largest case of 0.13 million cells the memory usage of the iterative solver V4 and of the Intel MKL Pardiso are 3.7 Gb and 61.1 Gb, respectively. Also, with the help of block value backend and mixed-precision, the AMG solver of V4 saves additional 30-50% memory.
4.2. Converging-diverging tube problem

In this case, the performance of AMGCL is evaluated on a pressure-driven tube flow (fig. 5). Consider 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 wall \((z = 1.25\mu m)\). The no-slip wall boundary conditions of \(u = \{0, 0, 0\}^T\) are imposed on the surface of varying radius tube. The fluid dynamics viscosity is uniformly set as 1Pa.s. Given the tube length \(L = 5\mu m\) and average tube radius of \(R_0 = 1\mu m\), the radius of the axisymmetric tube can be expressed as:

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

(12)

In this case, 6 levels of refinement mesh are generated using Gmsh [35]. Table 3 shows the baseline performance results for the direct solver. Note that a workstation with 64 Gb RAM is limited to solve a problem with about 0.14 million cells. Figure 6 shows that for large problems the iterative solvers have significantly lower relative memory usage and better runtime performance compared to the direct solver. By
### Table 3: Test2: Linear system size (DOFs), number of non-zeros (NNZs), linear system CSR storage memory, peak memory usage and the solution time for the direct solver (MKL Pardiso)

| Cells  | DOFs   | NNZs   | CSR Mem  | Direct Mem | Direct time |
|--------|--------|--------|----------|------------|-------------|
| 327    | 7550   | 184000 | 6.07 Mb  | 27.1 Mb    | 0.18 s      |
| 1203   | 28653  | 710000 | 22.78 Mb | 124.2 Mb   | 0.39 s      |
| 5319   | 125028 | 3220000| 101.43 Mb| 733.77 Mb  | 1.69 s      |
| 40488  | 921129 | 2530000| 766.66 Mb| 9.81 Gb    | 29.60 s     |
| 144995 | 3262682| 95300000|         | 59.82 Gb   | 445.00 s    |
| 296823 | 6648114| 196657124|        | Out-of-Mem | NA          |

### Figure 6: Test2: Relative memory usage and performance of AMGCL versus Intel MKL Pardiso

Comparing the memory and run time performance among iterative solvers (V1 – V4), V1 and V4 have the best overall performance. Note that V4 performs better than V1 for large problem sizes but is slower for smaller problems. This is due to the fact that V4 is preconditioned with AMG which is relatively expensive for simple problems but offers better scalability. This is consistent with our observations in section 4.1.

### 4.3. Sphere packing problem

In order to further evaluate the performance of AMGCL, a complex sphere packing flow problem with non-uniform cell size distribution and large cell size contrast is considered (fig. 7). A box-shape domain of $85 \times 85 \times 85 \mu m$ is considered where 21 spheres with a radius of $22 \mu m$ are packed randomly. The porosity is 36.4%. Similar to the converging-diverging tube problem, a pressure drop of 1 Pa 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. 6 levels of refinement mesh are generated using Gmsh [35].

### Table 4: Test3: Linear system size (DOFs), number of non-zeros (NNZs), linear system CSR storage memory, peak memory usage and the solution time for the direct solver (MKL Pardiso)

| Cells  | DOFs   | NNZs   | CSR Mem  | Direct Mem | Direct time |
|--------|--------|--------|----------|------------|-------------|
| 9487   | 238810 | 5021060| 176.87 Mb| 791.22 Mb  | 2.70 s      |
| 19373  | 483509 | 10400000| 397.01 Mb| 1.75 Gb    | 5.83 s      |
| 36430  | 896257 | 20200000| 687.07 Mb| 3.93 Gb    | 12.50 s     |
| 63382  | 1537891| 36100000| 1.18 Gb  | 7.93 Gb    | 25.50 s     |
| 100255 | 2405788| 58400000| 1.87 Gb  | 14.46 Gb   | 47.80 s     |
| 259009 | 6089212| 157000000| 4.90 Gb  | 49.76 Gb   | 211.00 s    |
| 404019 | 9420534| 24887496| 7.96 Gb  | Out-of-Mem | NA          |
Table 4 shows the baseline memory usage and runtime performance of Intel MKL Pardiso. Due to the significant amount of tetrahedron faces with the Dirichlet boundary conditions (no-slip wall), the linear system in this case has much less non-zero entries and memory usage compared to tests from the previous sections. A workstation with 64 Gb RAM now can solve a problem with about 0.28 million cells which is about 2 times larger than the maximum problem sizes from sections 4.1 and 4.2. As shown in fig. 8, iterative solvers still have great advantage in memory usage for large problems. However, the direct solver shows almost linear runtime growth before it runs out of memory. Among iterative solvers of V1 – V4, V4 still shows good scalability and has performance comparable with the direct solver for larger problem sizes.

5. Conclusion

We demonstrated that using C++ programming techniques such as policy-based design or partial template specialization may help in developing efficient, flexible and composeable scientific software. The open source AMGCL library allows to use the same code to create iterative solvers with scalar, complex (not tested in this paper), or block values, or use the solver and the preconditioner with mixed precision. Switching from the scalar to the block value type reduces the setup complexity by 85%, the memory footprint of the method by 15% to 30% and achieves the total speedup of 30% to 40%. Further, using 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 that uses block value type for the velocity subsystem and mixed precision approach, requires approximately 50% 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. Notably, the only change we had to make as users of the library, was to adjust template parameters of the solver. AMGCL is using the same code for all three versions of the FGMRES solver preconditioned with Schur pressure correction.

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