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AMGCL —A C++ library for efficient solution of large sparse linear systems

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ABSTRACT

AMGCL is a header-only C++ library for the solution of large sparse linear systems with algebraic multigrid. The method may be used as a black-box solver for computational problems in various fields, since it does not require any information about the underlying geometry. AMGCL provides an efficient, flexible, and extensible implementation of several iterative solvers and preconditioners on top of different backends allowing the acceleration of the solution with the help of OpenMP, OpenCL, or CUDA technologies. Most algorithms have both shared memory and distributed memory implementations. The library is published under a permissive MIT license.

Code metadata

Current code version	1.3.99
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2020-51
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/4394229/tree/v1
Legal Code License	MIT
Code versioning system used	git
Software code languages, tools, and services used	C++, MPI, OpenMP, OpenCL, CUDA
Compilation requirements, operating environments	C++11 compiler, backend requirements
Link to developer documentation/manual	https://amgcl.readthedocs.io
Support email for questions	amgcl@googlegroups.com

1. Introduction

Most of the numerical simulation problems today involve solution of large sparse linear systems obtained from discretization of partial differential equations on either structured or unstructured meshes. The combination of a Krylov subspace method with algebraic multigrid (AMG) as a preconditioner is considered to be one the most effective choices for solution of such systems [1–3]. The AMG can be used as a black box solver for various computational problems, since it does not require any information about the underlying geometry, and is known to be robust and scalable [4].

AMGCL is a header-only C++ library implementing multiple Krylov subspace iterative solvers preconditioned with the algebraic multigrid method [5]. It has a minimal set of dependencies and provides both shared memory and distributed versions of the algorithms. The

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Listing 1: Composing a customized solver from AMGCL components

```
// GMRES preconditioned with AMG
typedef amgcl::make_solver<
  amgcl::amg<
    amgcl::backend::builtin<float>,
    amgcl::coarsening::smoothed_aggregation,
    amgcl::relaxation::ilu0
    >,
  amgcl::solver::gmres<
    amgcl::backend::builtin<double>
    >
  > Solver;
```

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. The library users may also provide their own backends which enables tight integration between AMGCL and the user code.

Although the initial focus of the library was the implementation of the algebraic multigrid, its modular architecture allowed to provide more specialized preconditioners, such as CPR [6] or Schur pressure correction [7]. The multigrid relaxation components may be used as single level preconditioners.

2. AMGCL design principles

The main drivers behind AMGCL design are usability, efficiency, and extensibility. The design principles that help to achieve the goals are described below.

Policy-based design [8] 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. Listing 1 illustrates this by defining a GMRES [9] iterative solver preconditioned with smoothed aggregation algebraic multigrid with ILU(0) relaxation [10]. The solver uses mixed precision, where double precision builtin backend (parallelized with OpenMP) is used for the solver, and single precision backend is used for 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.

Preference for *free functions* as opposed to member functions [11], 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. The *value types* are one level below the backends: 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.

3. Impact

AMGCL demonstrates performance comparable [5,12] with popular software packages, such as PETSC [13], Trilinos [14], CUSP [15], or PARDISO [16]. The fact that the library allows the user to easily switch to mixed precision approach or use block-valued system formulation may yield significant savings in both computation time and memory requirements [12]. Another advantage of AMGCL is that it has less steep learning curve and lower entry cost than such large-scale packages as PETSC or Trilinos, and is published under permissive MIT license which allows for commercial use of the library.

AMGCL is used as a default solver in the Kratos Multi-Physics framework [17] developed at CIMNE, Barcelona. Linear solvers based on AMGCL are also provided as part of the MATLAB Reservoir Simulation Toolbox (MRST) [18] developed by the Computational Geosciences group in the Department of Mathematics and Cybernetics at SINTEF Digital. The library was used in research on subsurface flow [19–37], fluid simulation [38–46], air flow [47–52], machine learning [53–55], micromagnetics [56–58], 3D printing [59,60], computer graphics [61,62], contact mechanics [63], elastodynamics [64], semiconductor device modeling [65], and topology optimization [66].

Declaration of competing interest

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

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