AMGCL Documentation

Release 0.0.1

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Mar 02, 2022

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AMGCL is a header-only C++ library for solving large sparse linear systems with algebraic multigrid (AMG) method. AMG is one of the most effective iterative methods for solution of equation systems arising, for example, from discretizing PDEs on unstructured grids [BrMH85], [Stue99], [TrOS01]. The method can be used as a black-box solver for various computational problems, since it does not require any information about the underlying geometry. AMG is often used not as a standalone solver but as a preconditioner within an iterative solver (e.g. Conjugate Gradients, BiCGStab, or GMRES).

The library has minimal dependencies, and provides both shared-memory and distributed memory (MPI) versions of the algorithms. The AMG hierarchy is constructed on a CPU and then is transferred into one of the provided backends. This allows for transparent acceleration of the solution phase with help of OpenCL, CUDA, or OpenMP technologies. Users may provide their own backends which enables tight integration between AMGCL and the user code.

The source code is available under liberal MIT license at https://github.com/ddemidov/amgcl.

CHAPTER 1

Referencing

CHAPTER 2

Contents:

2.1 Algebraic Multigrid

Here we outline the basic principles behind the Algebraic Multigrid (AMG) method [BrMH85], [Stue99]. Consider a system of linear algebraic equations in the form

$$Au = f$$

where A is an $n \times n$ matrix. Multigrid methods are based on the recursive use of two-grid scheme, which combines

- *Relaxation*, or *smoothing iteration*: a simple iterative method such as Jacobi or Gauss-Seidel; and
- *Coarse grid correction*: solving residual equation on a coarser grid. Transfer between grids is described with *transfer operators* P (*prolongation* or *interpolation*) and R (*restriction*).

A setup phase of a generic algebraic multigrid (AMG) algorithm may be described as follows:

- Start with a system matrix $A_1 = A$.
- **While the matrix A_i is too big to be solved directly:**
    1. Introduce prolongation operator P_i, and restriction operator R_i.
    2. Construct coarse system using Galerkin operator: $A_{i+1} = R_i A_i P_i$.
- Construct a direct solver for the coarsest system A_L.

Note that in order to construct the next level in the AMG hierarchy, we only need to define transfer operators P and R. Also, the restriction operator is often chosen to be a transpose of the prolongation operator: $R = P^T$.

Having constructed the AMG hierarchy, we can use it to solve the system as follows:

- Start at the finest level with initial approximation $u_1 = u^0$.
- **Iterate until convergence (*V-cycle*):**
    - **At each level of the grid hiearchy, finest-to-coarsest:**
        1. Apply a couple of smoothing iterations (*pre-relaxation*) to the current solution $u_i = S_i(A_i, f_i, u_i)$.

2. Find residual $e_i = f_i - A_i u_i$ and restrict it to the RHS on the coarser level: $f_{i+1} = R_i e_i$.

– Solve the corasest system directly: $u_L = A_L^{-1} f_L$.

– **At each level of the grid hiearchy, coarsest-to-finest:**

1. Update the current solution with the interpolated solution from the coarser level: $u_i = u_i + P_i u_{i+1}$.
2. Apply a couple of smoothing iterations (*post-relaxation*) to the updated solution: $u_i = S_i(A_i, f_i, u_i)$.

More often AMG is not used standalone, but as a preconditioner with an iterative Krylov subspace method. In this case single V-cycle is used as a preconditioning step.

So, in order to fully define an AMG method, we need to choose transfer operators P and R, and smoother S.

2.2 Design Principles

A lot of linear solver software packages are either developed in C or Fortran, or provide C-compatible application programming interface (API). The low-level API is stable and compatible with most of the programming languages. However, this also has some disadvantages: the fixed interfaces usually only support the predefined set of cases that the developers have thought of in advance. For an example, BLAS specification has separate sets of functions that deal with single, double, complex, or double complex precision values, but it is impossible to work with mixed precision inputs or with user-defined or third-party custom types. Another common drawback of large scientific 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, such as the necessity to copy the data between various formats.

AMGCL is using modern C++ programming techniques in order to create flexible and efficient API. The users may easily extend the library or use it with their own datatypes. The following design pronciples are used throughout the code:

- *Policy-based design* [Alex00] 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 [Meye05], 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.

2.2.1 Policy-based design

Listing 2.1: Policy-based design illustration: creating customized solvers from AMGCL components

```
1  // CG solver preconditioned with ILU0
2  typedef amgcl::make_solver<
3      amgcl::relaxation::as_preconditioner<
4          amgcl::backend::builtin<double>,
5          amgcl::relaxation::ilu0
6          >,
7      amgcl::solver::cg<
8          amgcl::backend::builtin<double>
9          >
10     > Solver1;
11
12 // GMRES solver preconditioned with AMG
13 typedef amgcl::make_solver<
14     amgcl::amg<
15         amgcl::backend::builtin<double>,
16         amgcl::coarsening::smoothed_aggregation,
17         amgcl::relaxation::spai0
18         >,
19     amgcl::solver::gmres<
20         amgcl::backend::builtin<double>
21         >
22     > Solver2;
```

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 2.1 defines a conjugate 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 paticular, 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 2.1 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.

Listing 2.2: Example of parameter declaration in AMGCL components

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

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. 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. Listing 2.2 shows how the parameters are declared for the `amgcl::make_solver<P,S>` class. Listing 2.3 shows an example of how the parameters for the preconditioned GMRES solver from Listing 2.1 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 ε_{str} for the smoothed aggregation is set to 10^{-3}. The rest of the parameters are left with their default values.

Listing 2.3: Setting parameters for AMGCL components

```
// 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);
```

2.2.2 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 [Meye05]. 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 2.4 shows an implementation of `amgcl::backend::rows()` function for the case when the input matrix is specified as a `std::tuple(n,ptr,col,val)` of 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, `Epetra_CrsMatrix` from Trilinos Epetra, and it is easy to adapt a user-defined datatype.

Listing 2.4: Implementation of `amgcl::backend::rows()` free function for the CRS tuple

```
// 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 >
```

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```
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);
    }
};
```

2.2.3 Backends

A backend in AMGCL is a class that binds 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 the implementation of common parallel primitives from the 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 2.1, 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 $\epsilon = ||f - Ax||$ in AMGCL is computed using `amgcl::backend::residual()` and `amgcl::backend::inner_product()` primitives:

```
backend::residual(f, A, x, r);
auto e = sqrt(backend::inner_product(r, r));
```

2.2.4 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.

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 `amgcl::math::norm()` or `amgcl::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.

2.2.5 Runtime interface

The compile-time configuration of AMGCL solvers is not always convenient, especially if the solvers are used inside a software package or another library. The runtime interface allows to shift some of the configuraton decisions to

runtime. The classes inside `amgcl::runtime` namespace correspond to their compile-time alternatives, but the only template parameter you need to specify is the backend.

Since there is no way to know the parameter structure at compile time, the runtime classes accept parameters only in form of `boost::property_tree::ptree`. The actual components of the method are set through the parameter tree as well. For example, the solver above could be constructed at runtime in the following way:

```
#include <amgcl/backend/builtin.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/runtime.hpp>
#include <amgcl/relaxation/runtime.hpp>
#include <amgcl/solver/runtime.hpp>

typedef amgcl::backend::builtin<double> Backend;

typedef amgcl::make_solver<
    amgcl::amg<
        Backend,
        amgcl::runtime::coarsening::wrapper,
        amgcl::runtime::relaxation::wrapper
        >,
    amgcl::runtime::solver::wrapper<Backend>
    > Solver;

boost::property_tree::ptree prm;

prm.put("solver.type", "bicgstab");
prm.put("solver.tol", 1e-3);
prm.put("solver.maxiter", 10);
prm.put("precond.coarsening.type", "smoothed_aggregation");
prm.put("precond.relax.type", "spai0");

Solver solve( std::tie(n, ptr, col, val), prm );
```

2.3 Components

AMGCL defines the following algorithmic components:

2.3.1 Backends

A backend in AMGCL is a class that binds 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 free functions and partial template specializations, which allows to decouple the implementation of common parallel primitives from the specific datatypes used in the supported backends. This makes it possible to adopt third-party or user-defined datatypes for use within AMGCL without any modification of the core library code.

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 norm of the residual $\epsilon = ||f - Ax||$ in AMGCL is computed with `amgcl::backend::residual()` and `amgcl::backend::inner_product()` primitives:

```
backend::residual(f, A, x, r);
auto e = sqrt(backend::inner_product(r, r));
```

The backends currenly supported by AMGCL are listed below.

OpenMP (builtin) backend

template<class **ValueType**>
class amgcl::backend::**builtin**
Include <amgcl/backend/builtin.hpp>.

This is the bultin backend that does not have any external dependencies and uses OpenMP-parallelization for its primitives. As with any backend in AMGCL, it is defined with a *value type* template parameter, which specifies the type of the system matrix elements. The backend is also used internally by AMGCL during construction phase, and so moving the constructed datatypes (matrices and vectors) to the backend has no overhead. The backend has no parameters (the `params` subtype is an empty struct).

class params

OpenMP (builtin) hybrid backend

template<class **ScalarType**, class **BlockType**>
class amgcl::backend::**builtin_hybrid**
Include <amgcl/backend/builtin_hybrid.hpp>.

The hybrid builtin backend uses the scalar value type to build the hierarchy in the same way the builtin backend does. But before the constructed matrices are moved to the backend, they are converted to the block-wise format in order to improve the solution performance. This is especially helpful when a set of near null-space vectors is provided to the AMG preconditioner. In this case it is impossible to use block value type during the preconditioner construction, but the matrices still have block-wise structure.

See *Using near null-space vectors* and issue #215 for more details.

Similar to the builtin backend, the hybrid builtin backend has no parameters.

class params

NVIDIA CUDA backend

template<class **ValueType**>
class amgcl::backend::**cuda**
Include <amgcl/backend/cuda.hpp>.

The backend uses the NVIDIA CUDA technology for the parallelization of its primitives. It depends on the Thrust and cuSPARSE libraries. The code using the backend has to be compiled with NVIDIA's nvcc compiler. The user needs to initialize the cuSPARSE library with a call to the *cusparseCreate()* function and pass the returned handle to AMGCL in the backend parameters.

class params
The backend parameters

cusparseHandle_t **cusparse_handle**
cuSPARSE handle created with the cusparseCreate() function.

VexCL backend

template<class **ValueType**>
class amgcl::backend::**vexcl**
Include <amgcl/backend/vexcl.hpp>.

The backend uses the VexCL library for the implementation of its primitives. VexCL provides OpenMP, OpenCL, or CUDA parallelization, selected at compile time with a preprocessor definition. The user has to initialize the VexCL context and pass it to AMGCL via the backend parameter.

class params
The backend parameters

std::vector<vex::backend::command_queue> **q**
VexCL command queues identifying the compute devices in the compute context.

bool **fast_matrix_setup** = true
Transform the CSR matrices into the internal VexCL format on the GPU. This is faster, but temporarily requires more memory on the GPU.

VexCL hybrid backend

template<class **ScalarType**, class **BlockType**>
class amgcl::backend::**vexcl_hybrid**
Include <amgcl/backend/vexcl.hpp>.

The hybrid VexCL backend, similar to the hybrid OpenMP backend, uses scalar value type during the method setup, and converts the constructed matrices to block-wise format before moving them to the backend.

class params
The backend parameters

std::vector<vex::backend::command_queue> **q**
VexCL command queues identifying the compute devices in the compute context.

bool **fast_matrix_setup** = true
Transform the CSR matrices into the internal VexCL format on the GPU. This is faster, but temporarily requires more memory on the GPU.

ViennaCL backend

template<class **Matrix**>
class amgcl::backend::**viennacl**
Include <amgcl/backend/viennacl.hpp>.

The backend uses the ViennaCL library for the implementation of its primitives. ViennaCL is a free open-source linear algebra library for computations on many-core architectures (GPUs, MIC) and multi-core CPUs. The library is written in C++ and supports CUDA, OpenCL, and OpenMP (including switches at runtime). The template parameter for the backend specifies ViennaCL matrix class to use. Possible choices are viannacl::compressed_matrix<T>, viennacl::ell_matrix<T>, and viennacl::hyb_matrix<T>. The backend has no runtime parameters.

class params
The backend parameters

Eigen backend

template<class **ValueType**>
class amgcl::backend::**eigen**
Include <amgcl/backend/eigen.hpp>.

The backend uses Eigen library datatypes for implementation of its primitives. It could be useful in case the user already works with the Eigen library, for example, to assemble the linear system to be solved with AMGCL. AMGCL also provides an Eigen *matrix adapter*, so that Eigen matrices may be transparently used with AMGCL solvers.

class params
The backend parameters

Blaze backend

template<class **ValueType**>
class amgcl::backend::**blaze**
Include <amgcl/backend/blaze.hpp>.

The backend uses Blaze library datatypes for implementation of its primitives. It could be useful in case the user already works with the Blaze library, for example, to assemble the linear system to be solved with AMGCL.

class params
The backend parameters

2.3.2 Value Types

The value type concept allows to generalize AMGCL algorithms for the systems with complex or non-scalar coeffiecients. 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 `std::complex<T>`, or small statically sized matrices when the system matrix has a block structure. The latter may decrease the setup time and the overall memory footprint, increase cache locality, or improve convergence ratio.

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 `amgcl::math::norm()` or `amgcl::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 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.

Scalar values

All backends support `float` and `double` as value type. CPU-based backends (e.g. `amgcl::backend::builtin`) may also use `long double`. The use of non-trivial value types depends on whether the value type is supported by the selected backend.

Complex values

Data type: `std::complex<T>`

Include:

- `<amgcl/value_type/complex.hpp>`

Supported by backends:

- *amgcl::backend::builtin*
- *amgcl::backend::vexcl*
- *amgcl::backend::eigen*
- *amgcl::backend::blaze*

Statically sized matrices

Data type: `amgcl::static_matrix<T,N,N>`

Include:

- `<amgcl/value_type/static_matrix.hpp>`
- `<amgcl/backend/vexcl_static_matrix.hpp>` (in case VexCL is used as the backend)

Supported by backends:

- *amgcl::backend::builtin*
- *amgcl::backend::vexcl*

Eigen static matrices

Data type: `Eigen::Matrix<T,N,N>`

Include:

- `<amgcl/value_type/eigen.hpp>`

Supported by backends:

- *amgcl::backend::builtin*
- *amgcl::backend::eigen*

2.3.3 Matrix Adapters

A matrix adapter allows AMGCL to construct a solver from some common matrix formats. Internally, the CRS format is used, but it is easy to adapt any matrix format that allows row-wise iteration over its non-zero elements.

Tuple of CRS arrays

Include <amgcl/adapter/crs_tuple.hpp>

It is possible to use a `std::tuple` of CRS arrays as input matrix for any of the AMGCL algorithms. The CRS arrays may be stored either as STL containers:

```
std::vector<int>    ptr;
std::vector<int>    col;
std::vector<double> val;

Solver S( std::tie(n, ptr, col, val) );
```

or as `amgcl::iterator_range`, which makes it possible to adapt raw pointers:

```
int    *ptr;
int    *col;
double *val;

Solver S( std::make_tuple(n,
                      amgcl::make_iterator_range(ptr, ptr + n + 1),
                      amgcl::make_iterator_range(col, col + ptr[n]),
                      amgcl::make_iterator_range(val, val + ptr[n])
                      ) );
```

Zero copy

Include <amgcl/adapter/zero_copy.hpp>

template<class **Ptr**, class **Col**, class **Val**>
std::shared_ptr<amgcl::backend::crs<*Val*>> **zero_copy**(size_t *n*, **const** *Ptr* **ptr*, **const** *Col* **col*, **const** *Val* **val*)

Returns a shared pointer to the sparse matrix in internal AMGCL format. The matrix may be directly used for constructing AMGCL algorithms. `Ptr` and `Col` have to be 64bit integral datatypes (signed or unsigned). In case the *amgcl::backend::builtin* backend is used, no data will be copied from the CRS arrays, so it is the user's responsibility to make sure the pointers are alive until the AMGCL algorithm is destroyed.

Block matrix

Include <amgcl/adapter/block_matrix.hpp>

template<class **BlockType**, class **Matrix**>
block_matrix_adapter<*Matrix*, *BlockType*> **block_matrix**(**const** *Matrix* &*A*)

Converts scalar-valued matrix to a block-valued one on the fly. The adapter allows to iterate the rows of the scalar-valued matrix as if the matrix was stored using the block values. The rows of the input matrix have to be sorted column-wise.

Scaled system

Include <amgcl/adapter/scaled_problem.hpp>

template<class **Backend**, class **Matrix**>

auto **scaled_diagonal**(**const** *Matrix* &*A*, **const typename** *Backend*::params &*bprm* = **typename** *Backend*::params())

Returns a scaler object that may be used to scale the system so that the matrix has unit diagonal:

$$A_s = D^{1/2} A D^{1/2}$$

where D is the matrix diagonal. This keeps the matrix symmetrical. The RHS also needs to be scaled, and the solution of the system has to be postprocessed:

$$D^{1/2} A D^{1/2} y = D^{1/2} b, \quad x = D^{1/2} y$$

The scaler object may be used to scale both the matrix:

```
auto A = std::tie(rows, ptr, col, val);
auto scale = amgcl::adapter::scale_diagonal<Backend>(A, bprm);

// Setup solver
Solver solve(scale.matrix(A), prm, bprm);
```

and the RHS:

```
// option 1: rhs is untouched
solve(*scale.rhs(b), x);

// option 2: rhs is prescaled in-place
scale(b);
solve(b, x);
```

The solution vector has to be postprocessed afterwards:

```
// postprocess the solution in-place:
scale(x);
```

Reordered system

Include <amgcl/adapter/reorder.hpp>

template<class **ordering** = amgcl::reorder::cuthill_mckee<false>>
class amgcl::adapter::**reorder**

Reorders the matrix to reduce its bandwidth. Example:

```
// Prepare the reordering:
amgcl::adapter::reorder<> perm(A);

// Create the solver using the reordered matrix:
Solver solve(perm(A), prm);

// Reorder the RHS and solve the system:
solve(perm(rhs), x_ord);

// Postprocess the solution vector to get the original ordering:
perm.inverse(x_ord, x);
```

Eigen matrix

Simply including <amgcl/adapter/eigen.hpp> allows to use Eigen sparse matrices in AMGCL algorithm constructors. The Eigen matrix has to be stored with the RowMajor ordering.

Epetra matrix

Including `<amgcl/adapter/epetra.hpp>` allows to use Trilinos Epetra distributed sparse matrices in AMGCL MPI algorithm constructors.

uBlas matrix

Including `<amgcl/adapter/ublas.hpp>` allows to use uBlas sparse matrices in AMGCL algorithm constructors, and directly use uBlas vectors as the RHS and solution arrays.

2.3.4 Iterative Solvers

An iterative solver is a Krylov subspace method that may be combined with a *preconditioner* in order to solve the linear system.

All iterative solvers in AMGCL have two template parameters, `Backend` and `InnerProduct`. The `Backend` template parameter specifies the *backend* to target, and the `InnerProduct` parameter is used to select the implementation of the inner product to use with the solver. The correct implementation should be automatically selected by the library depending on whether the solver is used in a shared or distributed memory setting.

All solvers provide similar interface described below:

constructor(size_t *n*, **const** params &*prm* = params(), **const** backend_params &*bprm* = backend_params())
: The solver constructor. Takes the size of the system to solve, the solver parameters and the backend parameters.

template<class **Matrix**, class **Precond**, class **VectorRHS**, class **VectorX**>
std::tuple<size_t, scalar_type> **operator()**(**const** *Matrix* &*A*, **const** *Precond* &*P*, **const** *VectorRHS* &*rhs*, **const** *VectorX* &*x*)
: Computes the solution for the given system matrix `A` and the right-hand side `rhs`.

  Returns the number of iterations made and the achieved relative residual as a `std::tuple<size_t, scalar_type>`. The solution vector `x` provides initial approximation on input and holds the computed solution on output.

template<class **Precond**, class **VectorRHS**, class **VectorX**>
std::tuple<size_t, scalar_type> **operator()**(**const** *Precond* &*P*, **const** *VectorRHS* &*rhs*, **const** *VectorX* &*x*)
: Computes the solution for the given right-hand side `rhs`. The matrix that was used to create the preconditioner `P` is used as the system matrix.

  Returns the number of iterations made and the achieved relative residual as a `std::tuple<size_t, scalar_type>`. The solution vector `x` provides initial approximation on input and holds the computed solution on output.

AMGCL implementats the following iterative solvers:

CG

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class amgcl::solver::**cg**

Include `<amgcl/solver/cg.hpp>`

The Conjugate Gradient method is an effective method for symmetric positive definite systems. It is probably the oldest and best known of the nonstationary methods [Barr94], [Saad03].

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

BiCGStab

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::bicgstab`

Include `<amgcl/solver/bicgstab.hpp>`

The BiConjugate Gradient Stabilized method (BiCGStab) was developed to solve nonsymmetric linear systems while avoiding the often irregular convergence patterns of the Conjugate Gradient Squared method [Barr94].

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

bool **check_after** = false
Always do at least one iteration

amgcl::preconditioner::side::type **pside** = amgcl::preconditioner::side::right
Preconditioner kind (left/right)

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

BiCGStab(L)

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::bicgstabl`

Include `<amgcl/solver/bicgstabl.hpp>`

This is a generalization of the BiCGStab method [SlDi93], [Fokk96]. For $L = 1$, this algorithm coincides with BiCGStab. In some situations it may be profitable to take $L > 2$. Although the steps of BiCGStab(L) are more expensive for larger L, numerical experiments indicate that, in certain situations, due to a faster convergence, for instance, BiCGStab(4) performs better than BiCGStab(2).

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

int **L** = 2
The order of the method

scalar_type **delta** = 0
Threshold used to decide when to refresh computed residuals.

bool **convex** = true
Use a convex function of the MinRes and OR polynomials after the BiCG step instead of default MinRes

amgcl::preconditioner::side::type **pside** = amgcl::preconditioner::side::right
Preconditioner kind (left/right)

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

GMRES

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class amgcl::solver::**gmres**

Include <amgcl/solver/gmres.hpp>

The Generalized Minimal Residual method is an extension of MINRES (which is only applicable to symmetric systems) to unsymmetric systems. Like MINRES, it generates a sequence of orthogonal vectors, but in the absence of symmetry this can no longer be done with short recurrences; instead, all previously computed vectors in the orthogonal sequence have to be retained. For this reason, "restarted" versions of the method are used [Barr94].

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

int **M** = 30
The number of iterations before restart

amgcl::preconditioner::side::type **pside** = amgcl::preconditioner::side::right
Preconditioner kind (left/right)

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

"Loose" GMRES (LGMRES)

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class amgcl::solver::**lgmres**

Include <amgcl/solver/lgmres.hpp>

The residual vectors at the end of each restart cycle of restarted GMRES often alternate direction in a cyclic fashion, thereby slowing convergence. LGMRES is an implementation of a technique for accelerating the convergence of restarted GMRES by disrupting this alternating pattern. The new algorithm resembles a full conjugate gradient method with polynomial preconditioning, and its implementation requires minimal changes to the standard restarted GMRES algorithm [BaJM05].

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

unsigned **K** = 3
Number of vectors to carry between inner GMRES iterations. According to [BaJM05], good values are in the range of 1-3. However, if you want to use the additional vectors to accelerate solving multiple similar problems, larger values may be beneficial.

bool **always_reset** = true
Reset augmented vectors between solves. If the solver is used to repeatedly solve similar problems, then keeping the augmented vectors between solves may speed up subsequent solves. This flag, when set, resets the augmented vectors at the beginning of each solve.

int **M** = 30
The number of iterations before restart

amgcl::preconditioner::side::type **pside** = amgcl::preconditioner::side::right
Preconditioner kind (left/right)

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

Flexible GMRES (FGMRES)

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::` **fgmres**

Include `<amgcl/solver/fgmres.hpp>`

Often, the application of the preconditioner P is a result of some unspecified computation, possibly another iterative process. In such cases, it may well happen that P is not a constant operator. The preconditioned iterative solvers may not converge if P is not constant. There are a number of variants of iterative procedures developed in the literature that can accommodate variations in the preconditioner, i.e., that allow the preconditioner to vary from step to step. Such iterative procedures are called "flexible" iterations. The method implements flexible variant of the GMRES algorithm [Saad03].

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

int **M** = 30
The number of iterations before restart

size_t **maxiter** = 100
The maximum number of iterations

scalar_type **tol** = 1e-8
Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
Output the current iteration number and relative residual during solution.

IDR(s)

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::idrs`

Include `<amgcl/solver/idrs.hpp>`

This is a very stable and efficient IDR(s) variant as described in [GiSo11]. The Induced Dimension Reduction method, IDR(s), is a robust and efficient short-recurrence Krylov subspace method for solving large nonsymmetric systems of linear equations.

IDR(s) compared to BI-CGSTAB/BiCGStab():

- Faster.
- More robust.
- More flexible.

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The solver parameters.

unsigned **s** = 4
Dimension of the shadow space in IDR(s).

scalar_type **omega** = 0.7
Computation of omega.

- If omega = 0, a standard minimum residual step is performed.
- If omega > 0, omega is increased if the cosine of the angle between Ar and r < omega.

bool **smoothing** = false
: Specifies if residual smoothing must be applied.

bool **replacement** = false
: Residual replacement. Determines the residual replacement strategy. If true, the recursively computed residual is replaced by the true residual.

size_t **maxiter** = 100
: The maximum number of iterations

scalar_type **tol** = 1e-8
: Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
: Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
: Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
: Output the current iteration number and relative residual during solution.

Richardson iteration

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::`**richardson**

Include <amgcl/solver/richardson.hpp>

The preconditioned Richardson iterative method

$$x^{i+1} = x^i + \omega P(f - Ax^i)$$

typedef typename *Backend*::value_type **value_type**
: The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
: The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
: The solver parameters.

scalar_type **damping** = 1.0
: The damping factor ω

size_t **maxiter** = 100
: The maximum number of iterations

scalar_type **tol** = 1e-8
: Target relative residual error $\varepsilon = \frac{||f-Ax||}{||f||}$

scalar_type **abstol** = std::numeric_limits<*scalar_type*>::min()
: Target absolute residual error $\varepsilon = ||f - Ax||$

bool **ns_search** = false
: Ignore the trivial solution `x=0` when the RHS is zero. Useful when searching for the null-space vectors of the system.

bool **verbose** = false
: Output the current iteration number and relative residual during solution.

PreOnly

template<class **Backend**, class **InnerProduct** = amgcl::detail::default_inner_product>
class `amgcl::solver::`**preonly**

Include `<amgcl/solver/preonly.hpp>`

Only apply the preconditioner once. This is not very useful as a standalone solver, but may be used in composite preconditioners as a nested solver, so that the composite preconditioner itself remains linear and may be used with a non-flexible iterative solver.

typedef typename *Backend*::value_type **value_type**
: The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
: The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
: The solver parameters.

2.3.5 Preconditioners

Aside from the AMG, AMGCL implements preconditioners for some common problem types. For example, there is a Schur complement pressure correction preconditioner for Navie-Stokes type problems, or CPR preconditioner for reservoir simulations. Also, it is possible to use single level relaxation method as a preconditioner.

General preconditioners

These preconditioners do not take the origin or structure of matrix into account, and may be useful both on their own, as well as building blocks for the composite preconditioners.

AMG

template<class **Backend**, template<class> class **Coarsening**, template<class> class **Relax**>
class `amgcl::`**amg**

Include `<amgcl/amg.hpp>`

AMG is one the most effective methods for the solution of large sparse unstructured systems of equations, arising, for example, from discretization of PDEs on unstructured grids [TrOS01]. The method may be used as a black-box solver for various computational problems, since it does not require any information about the underlying geometry.

The three template parameters allow the user to select the exact components of the method:

- The *Backend* to transfer the constructed hierarchy to,
- The *Coarsening* strategy for the hierarchy construction, and
- The *Relaxation* scheme (smoother to use during the solution phase).

typedef typename *Backend*::params **backend_params**
The backend parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

typedef *Coarsening*<*Backend*> **coarsening_type**
The coarsening class instantiated for the specified backend

typedef *Relax*<*Backend*> **relax_type**
The relaxation class instantiated for the specified backend

class params
The AMG parameters. The coarsening and the relaxation parameters are encapsulated as part of the AMG parameters.

typedef typename *coarsening_type*::params **coarsening_params**
The type of the coarsening parameters

typedef typename *relax_type*::params **relax_params**
The type of the relaxation parameters

coarsening_params **coarsening**
The coarsening parameters

relax_params **relax**
The relaxation parameters

unsigned **coarse_enough** = *Backend*::direct_solver::coarse_enough()
Specifies when a hierarchy level is coarse enough to be solved directly. If the number of variables at the level is lower than this threshold, then the hierarchy construction is stopped and the linear system is solved directly at this level. The default value comes from the direct solver class defined as part of the backend.

bool **direct_coarse** = true
Use direct solver at the coarsest level. When set, the coarsest level is solved with a direct solver. Otherwise a smoother is used as a solver. This may be useful when the system is singular, but is still possible to solve with an iterative solver.

unsigned **max_levels** = std::numeric_limits<unsigned>::max()
The maximum number of levels. If this number is reached even when the size of the last level is greater that `coarse_enough`, then the hierarchy construction is stopped. The coarsest level will not be solved directly, but will use a smoother.

unsigned **npre** = 1
The number of pre-relaxations.

unsigned **npost** = 1
The number of post-relaxations.

unsigned **ncycle** = 1
The shape of AMG cycle (1 for V-cycle, 2 for W-cycle, etc).

unsigned **pre_cycles** = 1
The number of cycles to make as part of preconditioning.

bool **allow_rebuild** = false
Keep transfer operator matrices (P and R) in internal format to allow for quick rebuild of the hierarchy. See *amgcl::amg::rebuild()*.

template<class **Matrix**>
void **rebuild**(**const** *Matrix* &*A*, **const** *backend_params* &*bprm* = *backend_params*())
Rebuild the hierarchy using the new system matrix. Requires `allow_rebuild` to be set in parameters. The transfer operators created during the initial setup are reused in order to create the coarse system matrices: $A_c^{\text{new}} = RA^{new}P$.

Single-level relaxation

template<class **Backend**, template<class> class **Relax**>
class amgcl::relaxation::**as_preconditioner**

Include <amgcl/relaxation/as_preconditioner.hpp>

Allows to use a *relaxation* method as a standalone preconditioner.

Relax<backend> smoother;
The relaxation class instantiated for the specified backend

typedef typename smoother::params **params**
The relaxation params are inherited as the parameters for the preconditioner

Dummy

template<class **Backend**>
class amgcl::preconditioner::**dummy**

Include <amgcl/preconditioner/dummy.hpp>

The dummy preconditioner, equivalent to an identity matrix. May be used to test the convergence of unpreconditioned iterative solvers.

class params
There are no parameters

Composite preconditioners

The preconditioners in this section take the into account the block structure of the system and properties of the individual blocks. Most often the preconditioners are used for the solution of saddle point or Stokes-like systems, where the system matrix may be represented in the following form:

$$\begin{pmatrix} A & B_1^T \\ B_2 & C \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} b_u \\ b_p \end{pmatrix} \tag{2.1}$$

CPR

template<class **PPrecond**, class **SPrecond**>
class amgcl::preconditioner::**cpr**

Include <amgcl/preconditioner/cpr.hpp>

The Constrained Pressure Residual (CPR) preconditioner [Stue07]. The CPR preconditioners are based on the idea that coupled system solutions are mainly determined by the solution of their elliptic components (i.e., pressure). Thus, the procedure consists of extracting and accurately solving pressure subsystems. Residuals associated with this solution are corrected with an additional preconditioning step that recovers part of the global information contained in the original system.

The template parameters `PPrecond` and `SPrecond` for the CPR preconditioner specify which preconditioner to use with the pressure subblock (the C matrix in (2.1)), and with the complete system.

The system matrix should be ordered by grid nodes, so that the pressure and suturation/concentration unknowns belonging to the same grid node are compactly located together in the vector of unknowns. The pressure should be the first unknown in the block of unknowns associated with a grid node.

class params
The CPR preconditioner parameters

typedef typename *SPrecond*::value_type **value_type**
The value type of the system matrix

typedef typename *PPrecond*::params **pprecond_params**
The type of the pressure preconditioner parameters

typedef typename *SPrecond*::params **sprecond_params**
The type of the global preconditioner parameters

pprecond_params **pprecond**
The pressure preconditioner parameters

sprecond_params **sprecond**
The global preconditioner parameters

int **block_size** = 2
The number of unknowns associated with each grid node. The default value is 2 when the system matrix has scalar value type. Otherwise, the block size of the system matrix value type is used.

size_t **active_rows** = 0
When non-zero, only unknowns below this number are considered to be pressure. May be used when a system matrix contains unstructured tail block (for example, the unknowns associated with wells).

CPR (DRS)

template<class **PPrecond**, class **SPrecond**>
class amgcl::preconditioner::**cpr_drs**

Include <amgcl/preconditioner/cpr.hpp>

The Constrained Pressure Residual (CPR) preconditioner with weighted dynamic row sum (WDRS) [Grie14], [BrCC15].

The template parameters `PPrecond` and `SPrecond` for the CPR WDRS preconditioner specify which preconditioner to use with the pressure subblock (the C matrix in (2.1)), and with the complete system.

The system matrix should be ordered by grid nodes, so that the pressure and suturation/concentration unknowns belonging to the same grid node are compactly located together in the vector of unknowns. The pressure should be the first unknown in the block of unknowns associated with a grid node.

class params

The CPR preconditioner parameters

typedef typename *SPrecond*::value_type **value_type**

The value type of the system matrix

typedef typename *PPrecond*::params **pprecond_params**

The type of the pressure preconditioner parameters

typedef typename *SPrecond*::params **sprecond_params**

The type of the global preconditioner parameters

pprecond_params **pprecond**

The pressure preconditioner parameters

sprecond_params **sprecond**

The global preconditioner parameters

int **block_size** = 2

The number of unknowns associated with each grid node. The default value is 2 when the system matrix has scalar value type. Otherwise, the block size of the system matrix value type is used.

size_t **active_rows** = 0

When non-zero, only unknowns below this number are considered to be pressure. May be used when a system matrix contains unstructured tail block (for example, the unknowns associated with wells).

double **eps_dd** = 0.2

Controls the severity of the violation of diagonal dominance. See [Grie14] for more details.

double **eps_ps** = 0.02

Controls the pressure/saturation coupling. See [Grie14] for more details.

std::vector<double> **weights**

The weights for the weighted DRS method. See [BrCC15] for more details.

Schur Pressure Correction

template<class **USolver**, class **PSolver**>
class `amgcl::preconditioner::schur_pressure_correction`

Include `<amgcl/preconditioner/schur_pressure_correction.hpp>`

The system (2.1) may be rewritten as

$$\begin{pmatrix} A & B_1^T \\ 0 & S \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} b_u \\ b_p - B_2 A^{-1} b_u \end{pmatrix}$$

where $S = C - B_2 A^{-1} B_1^T$ is the Schur complement. The Schur complement pressure correction preconditioner uses this representation and an approximation to the Schur complement matrix in order to decouple the pressure and the velocity parts of the system [ElHS08].

The two template parameters for the method, `USolver` and `PSolver`, specify the *preconditioned solvers* for the A and S blocks.

class params
The parameters for the Schur pressure correction preconditioner

typedef typename *USolver*::params **usolver_params**
The type of the USolver parameters

typedef typename *PSolver*::params **psolver_params**
The type of the PSolver parameters

usolver_params **usolver**
The USolver parameters

psolver_params **psolver**
The PSolver parameters

std::vector<char> **pmask**
The indicator vector, containing 1 for pressure unknowns, and 0 otherwise.

int **type** = 1
The variant of the block preconditioner to use.
- When `type = 1`:

$$Sp = b_p - B_2 A^{-1} b_u$$
$$Au = b_u - B_1^T p$$

- When `type = 2`:

$$Sp = b_p$$
$$Au = b_u - B_1^T p$$

bool **approx_schur** = false
When set, approximate A^{-1} as $\mathrm{diag}(A)^{-1}$ during computation of the matrix-less Schur complement when solving the $Sp = b_p$ system. Otherwise, the full solve using `USolver` is used.

int **adjust_p** = 1
Adjust the matrix used to construct the preconditioner for the Schur complement system.
- When `adjust_p = 0`, use the unmodified C matrix;
- When `adjust_p = 1`, use $C - \mathrm{diag}(B_2 \mathrm{diag}(A)^{-1} B_1^T)$;
- When `adjust_p = 2`, use $C - B_2 \mathrm{diag}(A)^{-1} B_1^T$.

bool **simplec_dia** = true
When set, use $\frac{1}{\sum_j \|A_{i,j}\|}$ instead of $\mathrm{diag}(A)^{-1}$ as the approximation for A^{-1} (similar to the SIMPLEC algorithm).

int **verbose** = 0
- When `verbose >= 1`, show the number of iterations and the relative residual achieved after each nested solve.
- When `verbose >= 2`, save the A and C submatrices as `Kuu.mtx` and `Kpp.mtx`.

2.3.6 Relaxation

A relaxation method or a smoother is used on each level of the AMG hierarchy during solution phase.

Damped Jacobi

template<class **Backend**>
class `amgcl::relaxation::damped_jacobi`

Include <amgcl/relaxation/damped_jacobi.hpp>

The damped Jacobi relaxation

class params
Damped Jacobi relaxation parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

scalar_type **damping** = 0.72
The damping factor

Gauss-Seidel

template<class **Backend**>
class `amgcl::relaxation::`**gauss_seidel**

Include <amgcl/relaxation/gauss_seidel.hpp>

The Gauss-Seidel relaxation. The relaxation is only available for the backends where the matrix supports row-wise iteration over its non-zero values.

class params
Gauss-Seidel relaxation parameters

bool **serial** = false
Use the serial version of the algorithm

Chebyshev

template<class **Backend**>
class `amgcl::relaxation::`**chebyshev**

Include <amgcl/relaxation/chebyshev.hpp>

Chebyshev iteration is an iterative method for the solution of a system of linear equations, and unlike Jacobi, it is not a stationary method. However, it does not require inner products like many other nonstationary methods (most Krylov methods). These inner products can be a performance bottleneck on certain distributed memory architectures. Furthermore, Chebyshev iteration is, like Jacobi, easier to parallelize than for instance Gauss–Seidel smoothers. The Chebyshev iteration requires some information about the spectrum of the matrix. For symmetric matrices, it needs an upper bound for the largest eigenvalue and a lower bound for the smallest eigenvalue [GhKK12].

class params
Chebyshev relaxation parameters

unsigned **degree** = 5
The degree of Chebyshev polynomial

float **higher** = 1.0
: The highest eigen value safety upscaling. use boosting factor for a more conservative upper bound estimate [ABHT03].

float **lower** = 1.0 / 30
: Lowest-to-highest eigen value ratio.

int **power_iters** = 0
: The number of power iterations to apply for the spectral radius estimation. When 0, use Gershgorin disk theorem to estimate the spectral radius.

bool **scale** = false
: Scale the system matrix

Incomplete LU relaxation

The incomplete LU factorization process computes a sparse lower triangular matrix L and a sparse upper triangular matrix U so that the residual matrix $R = LU - A$ satisfies certain constraints, such as having zero entries in some locations. The relaxations in this section use various approaches to computation of the triangular factors L and U, but share the triangular system solution implementation required in order to apply the relaxation. The parameters for the triangular solution algorithm are defined as follows:

template<class **Backend**>
class amgcl::relaxation::detail::**ilu_solve**
: For the builtin OpenMP backend the incomplete triangular factors are solved using the OpenMP-parallel level scheduling approach. For the GPGPU backends, the triangular factors are solved approximately, using multiple damped Jacobi iterations [ChPa15].

class params

bool **serial** = false
: Use the serial version of the algorithm. This parameter is only used with the *amgcl::backend::builtin* backend.

unsigned **iters** = 2
: The number of Jacobi iterations to approximate the triangular system solution. This parameter is only used with GPGPU backends.

scalar_type **damping** = 1.0
: The damping factor for the triangular solve approximation. This parameter is only used with GPGPU backends.

ILU0

template<class **Backend**>
class amgcl::relaxation::**ilu0**

Include <amgcl/relaxation/ilu0.hpp>

The incomplete LU factorization with zero fill-in [Saad03]. The zero pattern for the triangular factors L and U is taken to be exactly the zero pattern of the system matrix A.

class params
: ILU0 relaxation parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

scalar_type **damping** = 1.0
The damping factor

typename amgcl::relaxation::detail::*ilu_solve*<*Backend*>::params **solve**
The parameters for the triangular factor solver

ILUK

template<class **Backend**>
class `amgcl::relaxation::iluk`

Include `<amgcl/relaxation/iluk.hpp>`

The ILU(k) relaxation.

The incomplete LU factorization with the level of fill-in [Saad03]. The accuracy of the ILU0 incomplete factorization may be insufficient to yield an adequate rate of convergence. More accurate incomplete LU factorizations are often more efficient as well as more reliable. These more accurate factorizations will differ from ILU(0) by allowing some fill-in. Thus, ILUK(k) keeps the 'k-th order fill-ins' [Saad03].

The ILU(1) factorization results from taking the zero pattern for triangular factors to be the zero pattern of the product L_0U_0 of the factors L_0, U_0 obtained from ILU(0). This process is repeated to obtain the higher level of fill-in factorizations.

class params
ILUK relaxation parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

int **k** = 1
The level of fill-in

scalar_type **damping** = 1.0
The damping factor

typename amgcl::relaxation::detail::*ilu_solve*<*Backend*>::params **solve**
The parameters for the triangular factor solver

ILUP

template<class **Backend**>
class `amgcl::relaxation::ilup`

Include <amgcl/relaxation/ilup.hpp>

The ILUP(k) relaxation.

This variant of the ILU relaxation is similar to ILUK, but differs in the way the zero pattern for the triangular factors is determined. Instead of the recursive definition using the product LU of the factors from the previous level of fill-in, ILUP uses the powers of the boolean matrix S sharing the zero pattern with the system matrix A [MiKu03]. ILUP(0) coinsides with ILU0, ILUP(1) has the same zero pattern as S^2, etc.

class params
ILUP relaxation parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

int **k** = 1
The level of fill-in

scalar_type **damping** = 1.0
The damping factor

typename amgcl::relaxation::detail::*ilu_solve*<*Backend*>::params **solve**
The parameters for the triangular factor solver

ILUT

template<class **Backend**>
class `amgcl::relaxation::ilut`

Include <amgcl/relaxation/ilut.hpp>

The ILUT(p, τ) relaxation.

Incomplete factorizations which rely on the levels of fill are blind to numerical values because elements that are dropped depend only on the structure of A. This can cause some difficulties for realistic problems that arise in many applications. A few alternative methods are available which are based on dropping elements in the Gaussian elimination process according to their magnitude rather than their locations. With these techniques, the zero pattern P is determined dynamically.

A generic ILU algorithm with threshold can be derived from the IKJ version of Gaussian elimination by including a set of rules for dropping small elements. In the factorization ILUT(p, τ), the following rule is used:

1. an element is dropped (i.e., replaced by zero) if it is less than the relative tolerance τ_i obtained by multiplying τ by the original 2-norm of the i-th row.
2. Only the pl_i largest elements are kept in the L part of the row and the pu_i largest elements in the U part of the row in addition to the diagonal element, which is always kept. l_i and u_i are the number of nonzero elements in the i-th row of the system matrix A below and above the diagonal.

class params
ILUT relaxation parameters

typedef typename *Backend*::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

scalar_type **p** = 2
The fill factor

scalar_type **tau** = 1e-2
The minimum magnitude of non-zero elements relative to the current row norm.

scalar_type **damping** = 1.0
The damping factor

typename amgcl::relaxation::detail::*ilu_solve*<*Backend*>::params **solve**
The parameters for the triangular factor solver

Sparse Approximate Inverse relaxation

Sparse approximate inverse (SPAI) smoothers based on the SPAI algorithm by Grote and Huckle [GrHu97]. The SPAI algorithm computes an approximate inverse M explicitly by minimizing $I - MA$ in the Frobenius norm. Both the computation of M and its application as a smoother are inherently parallel. Since an effective sparsity pattern of M is in general unknown a priori, the computation cost can be greatly reduced by choosing an a priori sparsity pattern for M. For SPAI-0 and SPAI-1 the sparsity pattern of M is fixed: M is diagonal for SPAI-0, whereas for SPAI-1 the sparsity pattern of M is that of A [BrGr02].

SPAI0

template<class **Backend**>
class `amgcl::relaxation::spai0`

Include `<amgcl/relaxation/spai0.hpp>`

The SPAI-0 variant of the sparse approximate inverse smother [BrGr02].

class params
The SPAI-0 has no parameters

SPAI1

template<class **Backend**>
class `amgcl::relaxation::spai1`

Include `<amgcl/relaxation/spai1.hpp>`

The SPAI-1 variant of the sparse approximate inverse smother [BrGr02].

class params
The SPAI-1 has no parameters

Scalar to Block convertor

template<class **BlockBackend**, template<class> class **Relax**>
class amgcl::relaxation::**as_block**

Include <amgcl/relaxation/as_block.hpp>

Wrapper for the specified relaxation. Converts the input matrix from scalar to block format before constructing an amgcl smoother. See the *Using near null-space vectors* tutorial.

template <class Backend>
class type
The resulting relaxation class.

2.3.7 Coarsening Strategies

A coarsening strategy defines various options for creating coarse systems in the AMG hierarchy. A coarsening strategy takes the system matrix A at the current level, and returns prolongation operator P and the corresponding restriction operator R.

Ruge-Stuben

template<class **Backend**>
class amgcl::coarsening::**ruge_stuben**

Include <amgcl/coarsening/ruge_stuben>

The classic Ruge-Stuben coarsening with direct interpolation [Stue99].

class params

float **eps_strong** = 0.25
Parameter ε_{str} defining strong couplings.

Variable i is defined to be strongly negatively coupled to another variable, j, if

$$-a_{ij} \geq \varepsilon_{str} \max_{a_{ik}<0} |a_{ik}| \quad \text{with fixed} \quad 0 < \varepsilon_{str} < 1.$$

In practice, a value of $\varepsilon_{str} = 0.25$ is usually taken.

bool **do_trunc** = true
Prolongation operator truncation. Interpolation operators, and, hence coarse operators may increase substantially towards coarser levels. Without truncation, this may become too costly. Truncation ignores all interpolatory connections which are smaller (in absolute value) than the largest one by a factor of ε_{tr}. The remaining weights are rescaled so that the total sum remains unchanged. In practice, a value of $\varepsilon_{tr} = 0.2$ is usually taken.

float **eps_trunc** = 0.2
Truncation parameter ε_{tr}.

Aggregation-based coarsening

The aggregation-base class of coarsening methods split the nodes at the fine grid into disjoint sets of nodes, the so-called aggregates that act as nodes on the coarse grid. The prolongation operators are then built by first constructing a tentative prolongator using the knowledge of zero energy modes of the principal part of the differential operator with natural boundary conditions (e.g., near null-space vectors, or rigid body modes for elasticity). In case of smoothed aggregation the prolongation operator is then smoothed by a carefully selected iteration.

All of the aggregation based methods take the aggregation and the nullspace parameters:

class amgcl::coarsening::**pointwise_aggregates**

Pointwise aggregation. When the system matrix has a block structure, it is converted to a poinwise matrix (single value per block), and the aggregates are created for this reduced matrix instead.

class params

The aggregation parameters.

float **eps_strong** = 0.08

Parameter ε_{strong} defining strong couplings. Connectivity is defined in a symmetric way, that is, two variables i and j are considered to be connected to each other if $\frac{a_{ij}^2}{a_{ii}a_{jj}} > \varepsilon_{strong}$ with fixed $0 < \varepsilon_{strong} < 1$.

int **block_size** = 1

The block size in case the system matrix has a block structure.

class amgcl::coarsening::**nullspace_params**

The nullspace parameters.

int **cols** = 0

The number of near nullspace vectors.

std::vector<double> **B**

The near nullspace vectors. The vectors are represented as columns of a 2D matrix stored in row-major order.

Aggregation

template<class **Backend**>
class amgcl::coarsening::**aggregation**

Include <amgcl/coarsening/aggregation.hpp>

The non-smoothed aggregation coarsening [Stue99].

class params

The aggregation coarsening parameters

amgcl::coarsening::pointwise_aggregates::params aggr;

The aggregation parameters

amgcl::coarsening::*nullspace_params* **nullspace**

The near nullspace parameters

float **over_interp** = 1.5

Over-interpolation factor α [Stue99]. In case of aggregation coarsening, coarse-grid correction of smooth error, and by this the overall convergence, can often be substantially improved by using

"over-interpolation", that is, by multiplying the actual correction (corresponding to piecewise constant interpolation) by some factor $\alpha > 1$. Equivalently, this means that the coarse-level Galerkin operator is re-scaled by $1/\alpha$:

$$I_h^H A_h I_H^h \to \frac{1}{\alpha} I_h^H A_h I_H^h.$$

Smoothed Aggregation

template<class **Backend**>
class amgcl::coarsening::**smoothed_aggregation**

Include <amgcl/coarsening/smoothed_aggregation.hpp>

The smoothed aggregation coarsening [VaMB96].

class params
The smoothed aggregation coarsening parameters

amgcl::coarsening::pointwise_aggregates::params aggr;
The aggregation parameters

amgcl::coarsening::*nullspace_params* **nullspace**
The near nullspace parameters

float **relax** = 1.0
The relaxation factor r. Used as a scaling for the damping factor ω. When `estimate_spectral_radius` is set, then

$$\omega = r * (4/3)/\rho.$$

where ρ is the spectral radius of the system matrix. Otherwise

$$\omega = r * (2/3).$$

The tentative prolongation $\tilde{P}$ from the non-smoothed aggregation is improved by smoothing to get the final prolongation matrix P. Simple Jacobi smoother is used here, giving the prolongation matrix

$$P = \left(I - \omega D^{-1} A^F\right) \tilde{P}.$$

Here $A^F = (a_{ij}^F)$ is the filtered matrix given by

$$a_{ij}^F = \begin{cases} a_{ij} & \text{if } j \in N_i \\ 0 & \text{otherwise} \end{cases}, \quad \text{if } i \neq j,$$

$$a_{ii}^F = a_{ii} - \sum_{j=1, j\neq i}^{n} \left(a_{ij} - a_{ij}^F\right),$$

where N_i is the set of variables strongly coupled to variable i, and D denotes the diagonal of A^F.

bool **estimate_spectral_radius** = false
Estimate the matrix spectral radius. This usually improves the convergence rate and results in faster solves, but costs some time during setup.

int **power_iters** = 0
The number of power iterations to apply for the spectral radius estimation. Use Gershgorin disk theorem when `power_iters = 0`.

Smoothed Aggregation with Energy Minimization

template<class **Backend**>
class amgcl::coarsening::**smoothed_aggr_emin**

Include <amgcl/coarsening/smoothed_aggr_emin.hpp>

The smoothed aggregation with energy minimization coarsening [SaTu08].

class params
The smoothed aggregation with energy minimization coarsening parameters

amgcl::coarsening::pointwise_aggregates::params aggr;
The aggregation parameters

amgcl::coarsening::*nullspace_params* **nullspace**
The near nullspace parameters

Block to Scalar convertor

template<template<class> class **Coarsening**>
class amgcl::coarsening::**as_scalar**

Include <amgcl/coarsening/as_scalar.hpp>

Wrapper for the specified coarsening. Converts the input matrix from block to scalar format, applies the base coarsening, converts the resulting transfer operators back to block format. See the *Using near null-space vectors* tutorial.

template <class Backend>
class type
The resulting coarsening class.

2.3.8 Coupling Solvers with Preconditioners

These classes provide a convenient way to couple an iterative solver and a preconditioner. This may be used both for convenience and as a building block for a composite *preconditioner*.

make_solver

template<class **Precond**, class **IterSolver**>
class amgcl::**make_solver**

Include <amgcl/make_solver.hpp>

The class has two template parameters: `Precond` and `IterSolver`, which specify the preconditioner and the iterative solver to use. During construction of the class, instances of both components are constructed and are ready to use as a whole.

typedef typename Backend::params **backend_params**
The backend parameters

typedef typename Backend::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The coupled solver parameters

typename *Precond*::params **precond**
The preconditioner parameters

IterSolver::params **solver**
The iterative solver parameters

template<class **Matrix**>
make_solver(**const** *Matrix* &*A*, **const** *params* &*prm* = *params*(), **const** *backend_params* &*bprm* = *backend_params*())
The constructor

template<class **Matrix**, class **VectorRHS**, class **VectorX**>
std::tuple<size_t, *scalar_type*> **operator()**(**const** *Matrix* &*A*, **const** *VectorRHS* &*rhs*, *VectorX* &*x*) **const**
Computes the solution for the given system matrix `A` and the right-hand side `rhs`. Returns the number of iterations made and the achieved residual as a `std::tuple`. The solution vector `x` provides initial approximation on input and holds the computed solution on output.

The system matrix may differ from the matrix used during initialization. This may be used for the solution of non-stationary problems with slowly changing coefficients. There is a strong chance that a preconditioner built for a time step will act as a reasonably good preconditioner for several subsequent time steps [DeSh12].

template<class **VectorRHS**, class **VectorX**>
std::tuple<size_t, *scalar_type*> **operator()**(**const** *VectorRHS* &*rhs*, *VectorX* &*x*) **const**
Computes the solution for the given right-hand side `rhs`. Returns the number of iterations made and the achieved residual as a `std::tuple`. The solution vector `x` provides initial approximation on input and holds the computed solution on output.

const *Precond* &**precond**() **const**
Returns reference to the constructed preconditioner

const *IterSolver* &**solver**() **const**
Returns reference to the constructed iterative solver

make_block_solver

template<class **Precond**, class **IterSolver**>
class `amgcl::`**make_block_solver**

Include <amgcl/make_block_solver.hpp>

Creates coupled solver which targets a block valued backend, but may be initialized with a scalar system matrix, and used with scalar vectors.

The scalar system matrix is transparently converted to the block-valued on using the `amgcl::adapter::block_matrix()` adapter in the class constructor, and the scalar vectors are reinterpreted to the block-valued ones upon application.

This class may be used as a building block in a composite preconditioner, when one (or more) of the subsystems has block values, but has to be computed as a scalar matrix.

The interface is the same as that of *amgcl::make_solver*.

deflated_solver

template<class **Precond**, class **IterSolver**>
class amgcl::**deflated_solver**

Include <amgcl/deflated_solver.hpp>

Creates preconditioned deflated solver. Deflated Krylov subspace methods are supposed to solve problems with large jumps in the coefficients on layered domains. It appears that the convergence of a deflated solver is independent of the size of the jump in the coefficients. The specific variant of the deflation method used here is A-DEF2 from [TNVE09].

typedef typename Backend::params **backend_params**
The backend parameters

typedef typename Backend::value_type **value_type**
The value type of the system matrix

typedef typename amgcl::math::scalar_of<*value_type*>::type **scalar_type**
The scalar type corresponding to the value type. For example, when the value type is `std::complex<double>`, then the scalar type is `double`.

class params
The deflated solver parameters

int **nvec** = 0
The number of deflation vectors

scalar_type ***vec** = nullptr
The deflation vectors stored as a [nvec x n] matrix in row-major order

typename *Precond*::params **precond**
The preconditioner parameters

IterSolver::params **solver**
The iterative solver parameters

2.4 Tutorial

In this section we demonstrate the solution of some common types of problems. The first three problems are matrices from the SuiteSparse Matrix Collection, which is a widely used set of sparse matrix benchmarks. The Stokes problem may be downloaded from the dataset accompanying the [DeMW20] paper. The solution timings used in the sections below were obtained on an Intel Core i5-3570K CPU. The timings for the GPU backends were obtained with the NVIDIA GeForce GTX 1050 Ti GPU.

2.4.1 Poisson problem

This system may be downloaded from the poisson3Db page (use the Matrix Market download option). The system matrix has 85,623 rows and 2,374,949 nonzeros (which is on average is about 27 non-zero elements per row). The matrix has an interesting structure, presented on the figure below:

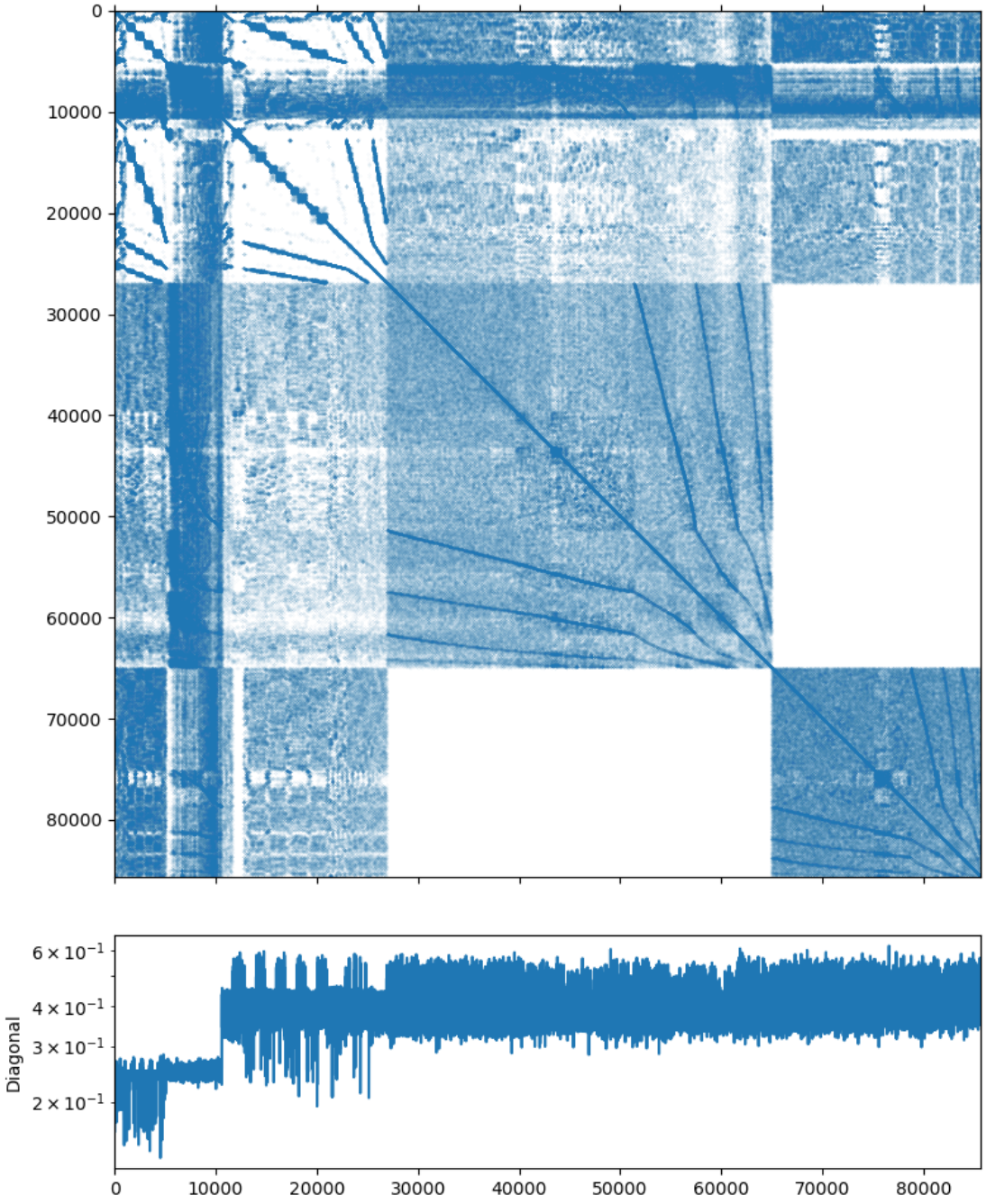

Fig. 2.1: Poisson3Db matrix portrait

A Poisson problem should be an ideal candidate for a solution with an AMG preconditioner, but before we start writing any code, let us check this with the examples/solver utility provided by AMGCL. It can take the input matrix and the RHS in the Matrix Market format, and allows to play with various solver and preconditioner options.

Note: The examples/solver is convenient not only for testing the systems obtained elsewhere. You can also save your own matrix and the RHS vector into the Matrix Market format with `amgcl::io::mm_write()` function. This way you can find the AMGCL options that work for your problem without the need to rewrite the code and recompile the program.

The default options of BiCGStab iterative solver preconditioned with a smoothed aggregation AMG (a simple diagonal SPAI(0) relaxation is used on each level of the AMG hierarchy) should work very well for a Poisson problem:

```
$ solver -A poisson3Db.mtx -f poisson3Db_b.mtx
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    58.93 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     50.07 M (83.20%)
    1         6361         446833      7.78 M (15.65%)
    2          384          32566      1.08 M ( 1.14%)

Iterations: 24
Error:      8.33789e-09

[Profile:       2.351 s] (100.00%)
[  reading:     1.623 s] ( 69.01%)
[  setup:       0.136 s] (  5.78%)
[  solve:       0.592 s] ( 25.17%)
```

As we can see from the output, the solution converged in 24 iterations to the default relative error of 1e-8. The solver setup took 0.136 seconds and the solution time is 0.592 seconds. The iterative solver used 4.57M of memory, and the preconditioner required 58.93M. This looks like a well-performing solver already, but we can try a couple of things just in case. We can not use the simpler CG solver, because the matrix is reported as a non-symmetric on the poisson3Db page. Using the GMRES solver seems to work equally well (the solution time is just slightly lower, but the solver requires more memory to store the orthogonal vectors). The number of iterations seems to have grown, but keep in mind that each iteration of BiCGStab requires two matrix-vector products and two preconditioner applications, while GMRES only makes one of each:

```
$ solver -A poisson3Db.mtx -f poisson3Db_b.mtx solver.type=gmres
Solver
======
Type:             GMRES(30)
Unknowns:         85623
Memory footprint: 20.91 M
```

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```
Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    58.93 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     50.07 M (83.20%)
    1         6361         446833      7.78 M (15.65%)
    2          384          32566      1.08 M ( 1.14%)

Iterations: 39
Error:      9.50121e-09

[Profile:       2.282 s] (100.00%)
[  reading:     1.612 s] ( 70.66%)
[  setup:       0.135 s] (  5.93%)
[  solve:       0.533 s] ( 23.38%)
```

We can also try differrent relaxation options for the AMG preconditioner. But as we can see below, the simplest SPAI(0) works well enough for a Poisson problem. The incomplete LU decomposition with zero fill-in makes less iterations, but is more expensive to setup:

```
$ solver -A poisson3Db.mtx -f poisson3Db_b.mtx precond.relax.type=ilu0
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    103.44 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     87.63 M (83.20%)
    1         6361         446833     14.73 M (15.65%)
    2          384          32566      1.08 M ( 1.14%)

Iterations: 12
Error:      7.99207e-09

[Profile:       2.510 s] (100.00%)
[ self:         0.005 s] (  0.19%)
[  reading:     1.614 s] ( 64.30%)
[  setup:       0.464 s] ( 18.51%)
[  solve:       0.427 s] ( 17.01%)
```

On the other hand, the Chebyshev relaxation has cheap setup but its application is expensive as it involves multiple matrix-vector products. So, even though it requires less iterations, the overall solution time does not improve that

much:

```
$ solver -A poisson3Db.mtx -f poisson3Db_b.mtx precond.relax.type=chebyshev
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    59.63 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     50.72 M (83.20%)
    1         6361         446833      7.83 M (15.65%)
    2          384          32566      1.08 M ( 1.14%)

Iterations: 8
Error:      5.21588e-09

[Profile:       2.316 s] (100.00%)
[  reading:     1.607 s] ( 69.39%)
[  setup:       0.134 s] (  5.78%)
[  solve:       0.574 s] ( 24.80%)
```

Now that we have the feel of the problem, we can actually write some code. The complete source may be found in tutorial/1.poisson3Db/poisson3Db.cpp and is presented below:

Listing 2.5: The source code for the solution of the poisson3Db problem.

```
#include <vector>
#include <iostream>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/solver/bicgstab.hpp>

#include <amgcl/io/mm.hpp>
#include <amgcl/profiler.hpp>

int main(int argc, char *argv[]) {
    // The matrix and the RHS file names should be in the command line options:
    if (argc < 3) {
        std::cerr << "Usage: " << argv[0] << " <matrix.mtx> <rhs.mtx>" << std::endl;
        return 1;
    }

    // The profiler:
    amgcl::profiler<> prof("poisson3Db");
```

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```
24
25      // Read the system matrix and the RHS:
26      ptrdiff_t rows, cols;
27      std::vector<ptrdiff_t> ptr, col;
28      std::vector<double> val, rhs;
29
30      prof.tic("read");
31      std::tie(rows, cols) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
32      std::cout << "Matrix " << argv[1] << ": " << rows << "x" << cols << std::endl;
33
34      std::tie(rows, cols) = amgcl::io::mm_reader(argv[2])(rhs);
35      std::cout << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;
36      prof.toc("read");
37
38      // We use the tuple of CRS arrays to represent the system matrix.
39      // Note that std::tie creates a tuple of references, so no data is actually
40      // copied here:
41      auto A = std::tie(rows, ptr, col, val);
42
43      // Compose the solver type
44      //   the solver backend:
45      typedef amgcl::backend::builtin<double> SBackend;
46      //   the preconditioner backend:
47  #ifdef MIXED_PRECISION
48      typedef amgcl::backend::builtin<float> PBackend;
49  #else
50      typedef amgcl::backend::builtin<double> PBackend;
51  #endif
52
53      typedef amgcl::make_solver<
54          amgcl::amg<
55              PBackend,
56              amgcl::coarsening::smoothed_aggregation,
57              amgcl::relaxation::spai0
58              >,
59          amgcl::solver::bicgstab<SBackend>
60          > Solver;
61
62      // Initialize the solver with the system matrix:
63      prof.tic("setup");
64      Solver solve(A);
65      prof.toc("setup");
66
67      // Show the mini-report on the constructed solver:
68      std::cout << solve << std::endl;
69
70      // Solve the system with the zero initial approximation:
71      int iters;
72      double error;
73      std::vector<double> x(rows, 0.0);
74
75      prof.tic("solve");
76      std::tie(iters, error) = solve(A, rhs, x);
77      prof.toc("solve");
78
79      // Output the number of iterations, the relative error,
80      // and the profiling data:
```

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```
81      std::cout << "Iters: " << iters << std::endl
82                << "Error: " << error << std::endl
83                << prof << std::endl;
84  }
```

In lines 4–10 we include the necessary AMGCL headers: the builtin backend uses the OpenMP threading model; the `crs_tuple` matrix adaper allows to use a `std::tuple` of CRS arrays as an input matrix; the *`amgcl::make_solver`* class binds together a preconditioner and an iterative solver; *`amgcl::amg`* class is the AMG preconditioner; *`amgcl::coarsening::smoothed_aggregation`* defines the smoothed aggreation coarsening strategy; *`amgcl::relaxation::spai0`* is the sparse approximate inverse relaxation used on each level of the AMG hierarchy; and *`amgcl::solver::bicgstab`* is the BiCGStab iterative solver. In lines 12–13 we include the Matrix Market reader and the AMGCL profiler.

After checking the validity of the command line arguments (lines 16–20), and initializing the profiler (line 23), we read the system matrix and the RHS vector from the Matrix Market files specified on the command line (lines 30–36).

Now we are ready to actually solve the system. First, we define the backends that we use with the iterative solver and the preconditioner (lines 44–51). The backend have to belong to the same class (in this case, *`amgcl::backend::builtin`*), but may have different value type precision. Here we use a double precision backend for the iterative solver, but choose either a double or a single precision for the preconditioner backend, depending on whether the preprocessor macro `MIXED_PRECISION` was defined during compilation. Using a single precision preconditioner may be both more memory efficient and faster, since the iterative solvers performance is usually memory-bound.

The defined backends are used in the solver definition (lines 53–60). Here we are using the *`amgcl::make_solver`* class to couple the AMG preconditioner with the BiCGStab iterative solver. We istantiate the solver in line 64.

In line 76 we solve the system for the given RHS vector, starting with a zero initial approximation (the `x` vector acts as an initial approximation on input, and contains the solution on output).

Below is the output of the program when compiled with a double precision preconditioner. The results are close to what we have seen with the examples/solver utility above, which is a good sign:

```
$ ./poisson3Db poisson3Db.mtx poisson3Db_b.mtx
Matrix poisson3Db.mtx: 85623x85623
RHS poisson3Db_b.mtx: 85623x1
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    58.93 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     50.07 M (83.20%)
    1         6361         446833      7.78 M (15.65%)
    2          384          32566      1.08 M ( 1.14%)

Iters: 24
Error: 8.33789e-09
```

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```
[poisson3Db:     2.412 s] (100.00%)
[  read:         1.618 s] ( 67.08%)
[  setup:        0.143 s] (  5.94%)
[  solve:        0.651 s] ( 26.98%)
```

Looking at the output of the mixed precision version, it is apparent that it uses less memory for the preconditioner (43.59M as opposed to 58.93M in the double-precision case), and is slightly faster during both the setup and the solution phases:

```
$ ./poisson3Db_mixed poisson3Db.mtx poisson3Db_b.mtx
Matrix poisson3Db.mtx: 85623x85623
RHS poisson3Db_b.mtx: 85623x1
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    43.59 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        85623        2374949     37.23 M (83.20%)
    1         6361         446833      5.81 M (15.65%)
    2          384          32566    554.90 K ( 1.14%)

Iters: 24
Error: 7.33493e-09

[poisson3Db:     2.234 s] (100.00%)
[  read:         1.559 s] ( 69.78%)
[  setup:        0.125 s] (  5.59%)
[  solve:        0.550 s] ( 24.62%)
```

We may also try to switch to the CUDA backend in order to accelerate the solution using an NVIDIA GPU. We only need to use the *amgcl::backend::cuda* instead of the `builtin` backend, and we also need to initialize the CUSPARSE library and pass the handle to AMGCL as the backend parameters. Unfortunately, we can not use the mixed precision approach, as CUSPARSE does not support that (we could use the VexCL backend though, see *Poisson problem (MPI version)*). The source code is very close to what we have seen above and is available at tutorial/1.poisson3Db/poisson3Db_cuda.cu. The listing below has the differences highligted:

Listing 2.6: The source code for the solution of the poisson3Db problem using the CUDA backend.

```
1 #include <vector>
2 #include <iostream>
3
4 #include <amgcl/backend/cuda.hpp>
5 #include <amgcl/adapter/crs_tuple.hpp>
6 #include <amgcl/make_solver.hpp>
```

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```
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/solver/bicgstab.hpp>

#include <amgcl/io/mm.hpp>
#include <amgcl/profiler.hpp>

int main(int argc, char *argv[]) {
    // The matrix and the RHS file names should be in the command line options:
    if (argc < 3) {
        std::cerr << "Usage: " << argv[0] << " <matrix.mtx> <rhs.mtx>" << std::endl;
        return 1;
    }

    // Show the name of the GPU we are using:
    int device;
    cudaDeviceProp prop;
    cudaGetDevice(&device);
    cudaGetDeviceProperties(&prop, device);
    std::cout << prop.name << std::endl;

    // The profiler:
    amgcl::profiler<> prof("poisson3Db");

    // Read the system matrix and the RHS:
    ptrdiff_t rows, cols;
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val, rhs;

    prof.tic("read");
    std::tie(rows, cols) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << cols << std::endl;

    std::tie(rows, cols) = amgcl::io::mm_reader(argv[2])(rhs);
    std::cout << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::backend::cuda<double> Backend;
    typedef amgcl::make_solver<
        amgcl::amg<
            Backend,
            amgcl::coarsening::smoothed_aggregation,
            amgcl::relaxation::spai0
            >,
        amgcl::solver::bicgstab<Backend>
        > Solver;

    // We need to initialize the CUSPARSE library and pass the handle to AMGCL
    // in backend parameters:
    Backend::params bprm;
```

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```
64      cusparseCreate(&bprm.cusparse_handle);
65
66      // There is no way to pass the backend parameters without passing the
67      // solver parameters, so we also need to create those. But we can leave
68      // them with the default values:
69      Solver::params prm;
70
71      // Initialize the solver with the system matrix:
72      prof.tic("setup");
73      Solver solve(A, prm, bprm);
74      prof.toc("setup");
75
76      // Show the mini-report on the constructed solver:
77      std::cout << solve << std::endl;
78
79      // Solve the system with the zero initial approximation.
80      // The RHS and the solution vectors should reside in the GPU memory:
81      int iters;
82      double error;
83      thrust::device_vector<double> f(rhs);
84      thrust::device_vector<double> x(rows, 0.0);
85
86      prof.tic("solve");
87      std::tie(iters, error) = solve(f, x);
88      prof.toc("solve");
89
90      // Output the number of iterations, the relative error,
91      // and the profiling data:
92      std::cout << "Iters: " << iters << std::endl
93                << "Error: " << error << std::endl
94                << prof << std::endl;
95  }
```

Using the consumer level GeForce GTX 1050 Ti GPU, the solution phase is almost 4 times faster than with the OpenMP backend. On the contrary, the setup is slower, because we now need to additionally initialize the GPU-side structures. Overall, the complete solution is about twice faster (comparing with the double precision OpenMP version):

```
$ ./poisson3Db_cuda poisson3Db.mtx poisson3Db_b.mtx
GeForce GTX 1050 Ti
Matrix poisson3Db.mtx: 85623x85623
RHS poisson3Db_b.mtx: 85623x1
Solver
======
Type:             BiCGStab
Unknowns:         85623
Memory footprint: 4.57 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08
Memory footprint:    44.81 M

level     unknowns       nonzeros      memory
```

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```
----------------------------------------
    0        85623        2374949     37.86 M (83.20%)
    1         6361         446833      5.86 M (15.65%)
    2          384          32566      1.09 M ( 1.14%)

Iters: 24
Error: 8.33789e-09

[poisson3Db:     2.253 s] (100.00%)
[ self:          0.223 s] (  9.90%)
[  read:         1.676 s] ( 74.39%)
[  setup:        0.183 s] (  8.12%)
[  solve:        0.171 s] (  7.59%)
```

2.4.2 Poisson problem (MPI version)

In section *Poisson problem* we looked at the solution of the 3D Poisson problem (available for download at poisson3Db page) using the shared memory approach. Lets solve the same problem using the Message Passing Interface (MPI), or the distributed memory approach. We already know that using the smoothed aggregation AMG with the simple SPAI(0) smoother is working well, so we may start writing the code immediately. The following is the complete MPI-based implementation of the solver (tutorial/1.poisson3Db/poisson3Db_mpi.cpp). We discuss it in more details below.

Listing 2.7: The MPI solution of the poisson3Db problem

```
#include <vector>
#include <iostream>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>

#include <amgcl/mpi/distributed_matrix.hpp>
#include <amgcl/mpi/make_solver.hpp>
#include <amgcl/mpi/amg.hpp>
#include <amgcl/mpi/coarsening/smoothed_aggregation.hpp>
#include <amgcl/mpi/relaxation/spai0.hpp>
#include <amgcl/mpi/solver/bicgstab.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

#if defined(AMGCL_HAVE_PARMETIS)
#  include <amgcl/mpi/partition/parmetis.hpp>
#elif defined(AMGCL_HAVE_SCOTCH)
#  include <amgcl/mpi/partition/ptscotch.hpp>
#endif

//---------------------------------------------------------------------------
int main(int argc, char *argv[]) {
    // The matrix and the RHS file names should be in the command line options:
    if (argc < 3) {
        std::cerr << "Usage: " << argv[0] << " <matrix.bin> <rhs.bin>" << std::endl;
        return 1;
    }
```

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```
30
31      amgcl::mpi::init mpi(&argc, &argv);
32      amgcl::mpi::communicator world(MPI_COMM_WORLD);
33
34      // The profiler:
35      amgcl::profiler<> prof("poisson3Db MPI");
36
37      // Read the system matrix and the RHS:
38      prof.tic("read");
39      // Get the global size of the matrix:
40      ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);
41      ptrdiff_t cols;
42
43      // Split the matrix into approximately equal chunks of rows
44      ptrdiff_t chunk = (rows + world.size - 1) / world.size;
45      ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
46      ptrdiff_t row_end = std::min(rows, row_beg + chunk);
47      chunk = row_end - row_beg;
48
49      // Read our part of the system matrix and the RHS.
50      std::vector<ptrdiff_t> ptr, col;
51      std::vector<double> val, rhs;
52      amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);
53      amgcl::io::read_dense(argv[2], rows, cols, rhs, row_beg, row_end);
54      prof.toc("read");
55
56      if (world.rank == 0)
57          std::cout
58              << "World size: " << world.size << std::endl
59              << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl
60              << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;
61
62      // Compose the solver type
63      typedef amgcl::backend::builtin<double> DBackend;
64      typedef amgcl::backend::builtin<float>  FBackend;
65      typedef amgcl::mpi::make_solver<
66          amgcl::mpi::amg<
67              FBackend,
68              amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
69              amgcl::mpi::relaxation::spai0<FBackend>
70              >,
71          amgcl::mpi::solver::bicgstab<DBackend>
72          > Solver;
73
74      // Create the distributed matrix from the local parts.
75      auto A = std::make_shared<amgcl::mpi::distributed_matrix<DBackend>>(
76              world, std::tie(chunk, ptr, col, val));
77
78      // Partition the matrix and the RHS vector.
79      // If neither ParMETIS not PT-SCOTCH are not available,
80      // just keep the current naive partitioning.
81  #if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
82  #  if defined(AMGCL_HAVE_PARMETIS)
83      typedef amgcl::mpi::partition::parmetis<DBackend> Partition;
84  #  elif defined(AMGCL_HAVE_SCOTCH)
85      typedef amgcl::mpi::partition::ptscotch<DBackend> Partition;
86  #  endif
```

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```
87
88      if (world.size > 1) {
89          prof.tic("partition");
90          Partition part;
91
92          // part(A) returns the distributed permutation matrix:
93          auto P = part(*A);
94          auto R = transpose(*P);
95
96          // Reorder the matrix:
97          A = product(*R, *product(*A, *P));
98
99          // and the RHS vector:
100         std::vector<double> new_rhs(R->loc_rows());
101         R->move_to_backend(typename DBackend::params());
102         amgcl::backend::spmv(1, *R, rhs, 0, new_rhs);
103         rhs.swap(new_rhs);
104
105         // Update the number of the local rows
106         // (it may have changed as a result of permutation):
107         chunk = A->loc_rows();
108         prof.toc("partition");
109     }
110 #endif
111
112     // Initialize the solver:
113     prof.tic("setup");
114     Solver solve(world, A);
115     prof.toc("setup");
116
117     // Show the mini-report on the constructed solver:
118     if (world.rank == 0)
119         std::cout << solve << std::endl;
120
121     // Solve the system with the zero initial approximation:
122     int iters;
123     double error;
124     std::vector<double> x(chunk, 0.0);
125
126     prof.tic("solve");
127     std::tie(iters, error) = solve(*A, rhs, x);
128     prof.toc("solve");
129
130     // Output the number of iterations, the relative error,
131     // and the profiling data:
132     if (world.rank == 0)
133         std::cout
134             << "Iters: " << iters << std::endl
135             << "Error: " << error << std::endl
136             << prof << std::endl;
137 }
```

In lines 4–21 we include the required components. Here we are using the builtin (OpenMP-based) backend and the CRS tuple adapter. Next we include MPI-specific headers that provide the distributed-memory implementation of AMGCL algorithms. This time, we are reading the system matrix and the RHS vector in the binary format, and include `<amgcl/io/binary.hpp>` header intead of the usual `<amgcl/io/mm.hpp>`. The binary format is not only faster to read, but it also allows to read the matrix and the RHS vector in chunks, which is what we need for the

distributed approach.

After checking the validity of the command line parameters, we initialize the MPI context and communicator in lines 31–32:

```
31      amgcl::mpi::init mpi(&argc, &argv);
32      amgcl::mpi::communicator world(MPI_COMM_WORLD);
```

The `amgcl::mpi::init` is a convenience RAII wrapper for `MPI_Init()`. It will call `MPI_Finalize()` in the destructor when its instance (`mpi`) goes out of scope at the end of the program. We don't have to use the wrapper, but it simply makes things easier. `amgcl::mpi::communicator` is an equally thin wrapper for `MPI_Comm`. `amgcl::mpi::communicator` and `MPI_Comm` may be used interchangeably both with the AMGCL MPI interface and the native MPI functions.

The system has to be divided (partitioned) between multiple MPI processes. The simplest way to do this is presented on the following figure:

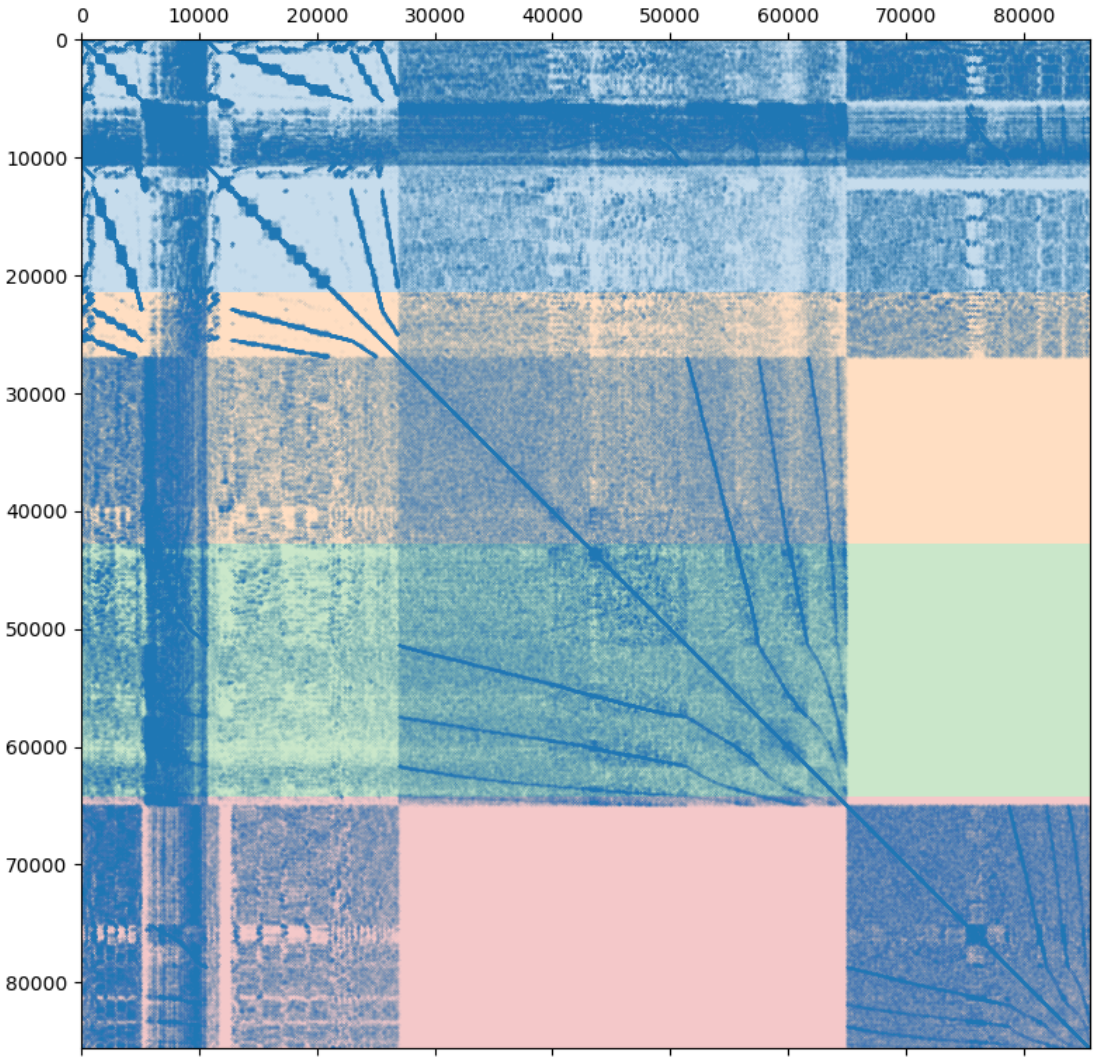

Fig. 2.2: Poisson3Db matrix partitioned between the 4 MPI processes

Assuming we are using 4 MPI processes, the matrix is split into 4 continuous chunks of rows, so that each MPI process owns approximately 25% of the matrix. This works well enough for a small number of processes, but as the size of the compute cluster grows, the simple partitioning becomes less and less efficient. Creating efficient partitioning is outside of AMGCL scope, but AMGCL does provide wrappers for the ParMETIS and PT-SCOTCH libraries specializing in this. The difference between the naive and the optimal partitioning is demonstrated on the next figure:

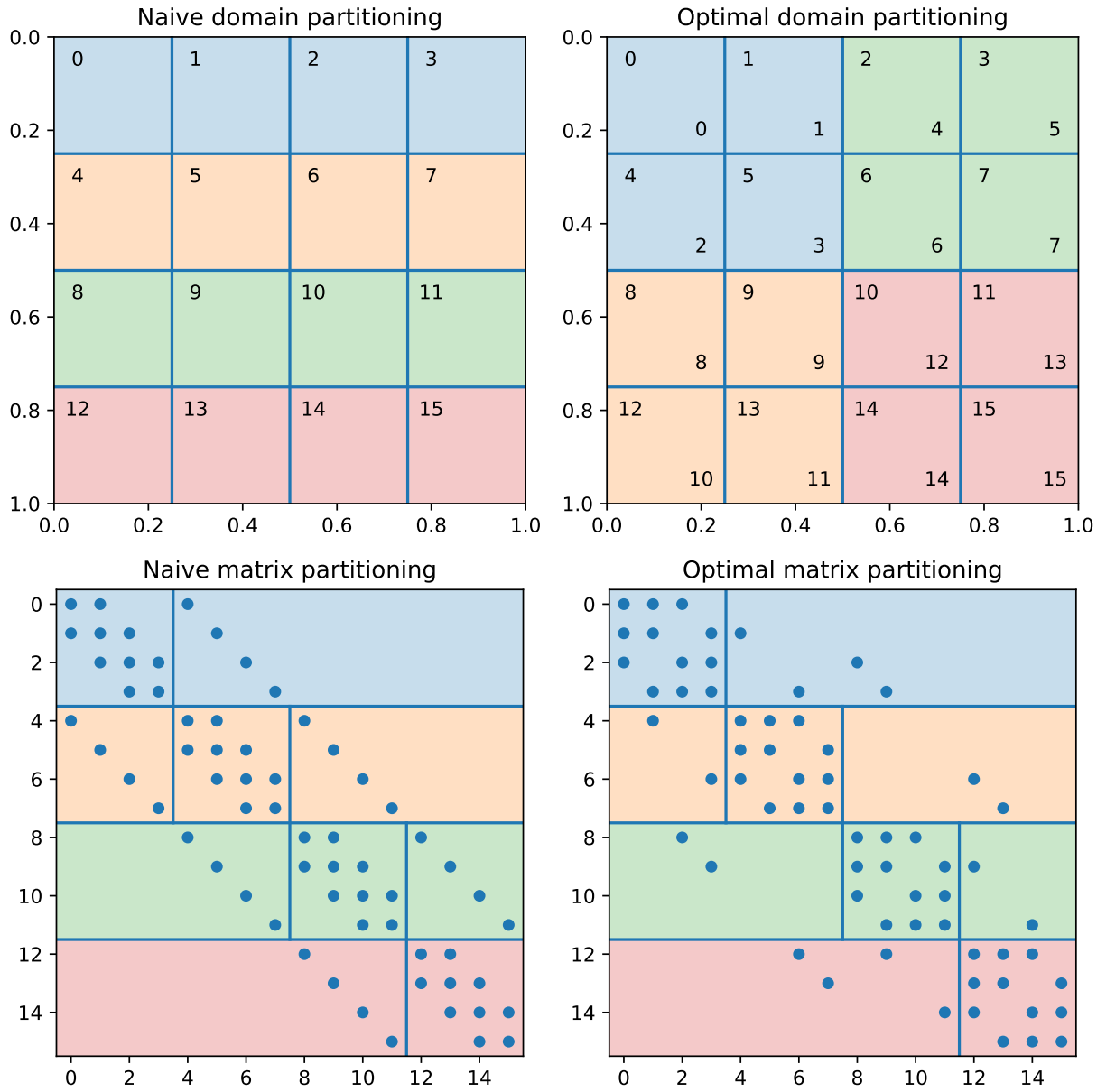

Fig. 2.3: Naive vs optimal partitioning of a 4×4 grid between 4 MPI processes.

The figure shows the finite-diffrence discretization of a 2D Poisson problem on a 4×4 grid in a unit square. The nonzero pattern of the system matrix is presented on the lower left plot. If the grid nodes are numbered row-wise, then the naive partitioning of the system matrix for the 4 MPI processes is shown on the upper left plot. The subdomains belonging to each of the MPI processes correspond to the continuous ranges of grid node indices and are elongated along the X axis. This results in high MPI communication traffic, as the number of the interface nodes is high relative to the number of interior nodes. The upper right plot shows the optimal partitioning of the domain for the 4 MPI

processes. In order to keep the rows owned by a single MPI process adjacent to each other (so that each MPI process owns a continuous range of rows, as required by AMGCL), the grid nodes have to be renumbered. The labels in the top left corner of each grid node show the original numbering, and the lower-rigth labels show the new numbering. The renumbering of the matrix may be expressed as the permutation matrix P, where $P_{ij} = 1$ if the j-th unknown in the original ordering is mapped to the i-th unknown in the new ordering. The reordered system may be written as

$$P^T A P y = P^T f$$

The reordered matrix $P^T A P$ and the corresponding partitioning are shown on the lower right plot. Note that off-diagonal blocks on each MPI process have as much as twice fewer non-zeros compared to the naive partitioning of the matrix. The solution x in the original ordering may be obtained with $x = Py$.

In lines 37–54 we read the system matrix and the RHS vector using the naive ordering (a nicer ordering of the unknowns will be determined later):

```
37      // Read the system matrix and the RHS:
38      prof.tic("read");
39      // Get the global size of the matrix:
40      ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);
41      ptrdiff_t cols;
42
43      // Split the matrix into approximately equal chunks of rows
44      ptrdiff_t chunk = (rows + world.size - 1) / world.size;
45      ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
46      ptrdiff_t row_end = std::min(rows, row_beg + chunk);
47      chunk = row_end - row_beg;
48
49      // Read our part of the system matrix and the RHS.
50      std::vector<ptrdiff_t> ptr, col;
51      std::vector<double> val, rhs;
52      amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);
53      amgcl::io::read_dense(argv[2], rows, cols, rhs, row_beg, row_end);
54      prof.toc("read");
```

First, we read the total (global) number of rows in the matrix from the binary file using the `amgcl::io::crs_size()` function. Next, we divide the global rows between the MPI processes, and read our portions of the matrix and the RHS using `amgcl::io::read_crs()` and `amgcl::io::read_dense()` functions. The `row_beg` and `row_end` parameters to the functions specify the regions (in row numbers) to read. The column indices are kept in global numbering.

In lines 62–72 we define the backend and the solver types:

```
62      // Compose the solver type
63      typedef amgcl::backend::builtin<double> DBackend;
64      typedef amgcl::backend::builtin<float>  FBackend;
65      typedef amgcl::mpi::make_solver<
66          amgcl::mpi::amg<
67              FBackend,
68              amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
69              amgcl::mpi::relaxation::spai0<FBackend>
70              >,
71          amgcl::mpi::solver::bicgstab<DBackend>
72          > Solver;
```

The structure of the solver is the same as in the shared memory case in the *Poisson problem* tutorial, but we are using the components from the `amgcl::mpi` namespace. Again, we are using the mixed-precision approach and the preconditioner backend is defined with a single-precision value type.

In lines 74–76 we create the distributed matrix from the local strips read by each of the MPI processes:

```
74      // Create the distributed matrix from the local parts.
75      auto A = std::make_shared<amgcl::mpi::distributed_matrix<DBackend>>(
76              world, std::tie(chunk, ptr, col, val));
```

We could directly use the tuple of the CRS arrays `std::tie(chunk, ptr, col, val)` to construct the solver (the distributed matrix would be created behind the scenes for us), but here we need to explicitly create the matrix for a couple of reasons. First, since we are using the mixed-precision approach, we need the double-precision distributed matrix for the solution step. And second, the matrix will be used to repartition the system using either ParMETIS or PT-SCOTCH libraries in lines 78–110:

```
78      // Partition the matrix and the RHS vector.
79      // If neither ParMETIS not PT-SCOTCH are not available,
80      // just keep the current naive partitioning.
81  #if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
82  #  if defined(AMGCL_HAVE_PARMETIS)
83      typedef amgcl::mpi::partition::parmetis<DBackend> Partition;
84  #  elif defined(AMGCL_HAVE_SCOTCH)
85      typedef amgcl::mpi::partition::ptscotch<DBackend> Partition;
86  #  endif
87
88      if (world.size > 1) {
89          prof.tic("partition");
90          Partition part;
91
92          // part(A) returns the distributed permutation matrix:
93          auto P = part(*A);
94          auto R = transpose(*P);
95
96          // Reorder the matrix:
97          A = product(*R, *product(*A, *P));
98
99          // and the RHS vector:
100         std::vector<double> new_rhs(R->loc_rows());
101         R->move_to_backend(typename DBackend::params());
102         amgcl::backend::spmv(1, *R, rhs, 0, new_rhs);
103         rhs.swap(new_rhs);
104
105         // Update the number of the local rows
106         // (it may have changed as a result of permutation):
107         chunk = A->loc_rows();
108         prof.toc("partition");
109     }
110 #endif
```

We determine if either ParMETIS or PT-SCOTCH is available in lines 81–86, and use the corresponding wrapper provided by the AMGCL. The wrapper computes the permutation matrix P, which is used to reorder both the system matrix and the RHS vector. Since the reordering may change the number of rows owned by each MPI process, we update the number of local rows stored in the `chunk` variable.

```
112     // Initialize the solver:
113     prof.tic("setup");
114     Solver solve(world, A);
115     prof.toc("setup");
116
117     // Show the mini-report on the constructed solver:
118     if (world.rank == 0)
119         std::cout << solve << std::endl;
```

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```
120
121     // Solve the system with the zero initial approximation:
122     int iters;
123     double error;
124     std::vector<double> x(chunk, 0.0);
125
126     prof.tic("solve");
127     std::tie(iters, error) = solve(*A, rhs, x);
128     prof.toc("solve");
```

At this point we are ready to initialize the solver (line 115), and solve the system (line 128). Here is the output of the compiled program. Note that the environment variable `OMP_NUM_THREADS` is set to 1 in order to not oversubscribe the available CPU cores:

```
$ export OMP_NUM_THREADS=1
$ mpirun -np 4 ./poisson3Db_mpi poisson3Db.bin poisson3Db_b.bin
World size: 4
Matrix poisson3Db.bin: 85623x85623
RHS poisson3Db_b.bin: 85623x1
Partitioning[ParMETIS] 4 -> 4
Type:             BiCGStab
Unknowns:         21671
Memory footprint: 1.16 M

Number of levels:    3
Operator complexity: 1.20
Grid complexity:     1.08

level     unknowns       nonzeros
---------------------------------
    0        85623        2374949 (83.06%) [4]
    1         6377         450473 (15.75%) [4]
    2          401          34039 ( 1.19%) [4]

Iters: 24
Error: 6.09835e-09

[poisson3Db MPI:     1.273 s] (100.00%)
[ self:              0.044 s] (  3.49%)
[  partition:        0.626 s] ( 49.14%)
[  read:             0.012 s] (  0.93%)
[  setup:            0.152 s] ( 11.92%)
[  solve:            0.439 s] ( 34.52%)
```

Similarly to how it was done in the *Poisson problem* section, we can use the GPU backend in order to speed up the solution step. Since the CUDA backend does not support the mixed-precision approach, we will use the VexCL backend, which allows to employ CUDA, OpenCL, or OpenMP compute devices. The source code (tutorial/1.poisson3Db/poisson3Db_mpi_vexcl.cpp) is very similar to the version using the builtin backend and is shown below with the differences highlighted.

```
1  #include <vector>
2  #include <iostream>
3
4  #include <amgcl/backend/vexcl.hpp>
5  #include <amgcl/adapter/crs_tuple.hpp>
6
```

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```
#include <amgcl/mpi/distributed_matrix.hpp>
#include <amgcl/mpi/make_solver.hpp>
#include <amgcl/mpi/amg.hpp>
#include <amgcl/mpi/coarsening/smoothed_aggregation.hpp>
#include <amgcl/mpi/relaxation/spai0.hpp>
#include <amgcl/mpi/solver/bicgstab.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

#if defined(AMGCL_HAVE_PARMETIS)
#  include <amgcl/mpi/partition/parmetis.hpp>
#elif defined(AMGCL_HAVE_SCOTCH)
#  include <amgcl/mpi/partition/ptscotch.hpp>
#endif

//---------------------------------------------------------------------------
int main(int argc, char *argv[]) {
    // The matrix and the RHS file names should be in the command line options:
    if (argc < 3) {
        std::cerr << "Usage: " << argv[0] << " <matrix.bin> <rhs.bin>" << std::endl;
        return 1;
    }

    amgcl::mpi::init mpi(&argc, &argv);
    amgcl::mpi::communicator world(MPI_COMM_WORLD);

    // Create VexCL context. Use vex::Filter::Exclusive so that different MPI
    // processes get different GPUs. Each process gets a single GPU:
    vex::Context ctx(vex::Filter::Exclusive(vex::Filter::Count(1)));
    for(int i = 0; i < world.size; ++i) {
        // unclutter the output:
        if (i == world.rank)
            std::cout << world.rank << ": " << ctx.queue(0) << std::endl;
        MPI_Barrier(world);
    }

    // The profiler:
    amgcl::profiler<> prof("poisson3Db MPI(VexCL)");

    // Read the system matrix and the RHS:
    prof.tic("read");
    // Get the global size of the matrix:
    ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);
    ptrdiff_t cols;

    // Split the matrix into approximately equal chunks of rows
    ptrdiff_t chunk = (rows + world.size - 1) / world.size;
    ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
    ptrdiff_t row_end = std::min(rows, row_beg + chunk);
    chunk = row_end - row_beg;

    // Read our part of the system matrix and the RHS.
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val, rhs;
    amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);
    amgcl::io::read_dense(argv[2], rows, cols, rhs, row_beg, row_end);
```

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```
    prof.toc("read");

    // Copy the RHS vector to the backend:
    vex::vector<double> f(ctx, rhs);

    if (world.rank == 0)
        std::cout
            << "World size: " << world.size << std::endl
            << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl
            << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;

    // Compose the solver type
    typedef amgcl::backend::vexcl<double> DBackend;
    typedef amgcl::backend::vexcl<float>  FBackend;
    typedef amgcl::mpi::make_solver<
        amgcl::mpi::amg<
            FBackend,
            amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
            amgcl::mpi::relaxation::spai0<FBackend>
            >,
        amgcl::mpi::solver::bicgstab<DBackend>
        > Solver;

    // Create the distributed matrix from the local parts.
    auto A = std::make_shared<amgcl::mpi::distributed_matrix<DBackend>>(
            world, std::tie(chunk, ptr, col, val));

    // Partition the matrix and the RHS vector.
    // If neither ParMETIS not PT-SCOTCH are not available,
    // just keep the current naive partitioning.
#if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
#  if defined(AMGCL_HAVE_PARMETIS)
    typedef amgcl::mpi::partition::parmetis<DBackend> Partition;
#  elif defined(AMGCL_HAVE_SCOTCH)
    typedef amgcl::mpi::partition::ptscotch<DBackend> Partition;
#  endif

    if (world.size > 1) {
        prof.tic("partition");
        Partition part;

        // part(A) returns the distributed permutation matrix:
        auto P = part(*A);
        auto R = transpose(*P);

        // Reorder the matrix:
        A = product(*R, *product(*A, *P));

        // and the RHS vector:
        vex::vector<double> new_rhs(ctx, R->loc_rows());
        R->move_to_backend(typename DBackend::params());
        amgcl::backend::spmv(1, *R, f, 0, new_rhs);
        f.swap(new_rhs);

        // Update the number of the local rows
        // (it may have changed as a result of permutation):
        chunk = A->loc_rows();
```

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```
        prof.toc("partition");
    }
#endif

    // Initialize the solver:
    Solver::params prm;
    DBackend::params bprm;
    bprm.q = ctx;

    prof.tic("setup");
    Solver solve(world, A, prm, bprm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    if (world.rank == 0)
        std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    vex::vector<double> x(ctx, chunk);
    x = 0.0;

    prof.tic("solve");
    std::tie(iters, error) = solve(*A, f, x);
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    if (world.rank == 0)
        std::cout
            << "Iters: " << iters << std::endl
            << "Error: " << error << std::endl
            << prof << std::endl;
}
```

Basically, we replace the `builtin` backend with the `vexcl` one, initialize the VexCL context and reference the context in the backend parameters. The RHS and the solution vectors are need to be transfered/allocated on the GPUs. Below is the output of the VexCL version using the OpenCL technology. Note that the system the tests were performed on has only two GPUs, so the test used just two MPI processes. The environment variable `OMP_NUM_THREADS` was set to 2 in order to fully utilize all available CPU cores:

```
$ export OMP_NUM_THREADS=2
$ mpirun -np 2 ./poisson3Db_mpi_vexcl_cl poisson3Db.bin poisson3Db_b.bin
0: GeForce GTX 960 (NVIDIA CUDA)
1: GeForce GTX 1050 Ti (NVIDIA CUDA)
World size: 2
Matrix poisson3Db.bin: 85623x85623
RHS poisson3Db_b.bin: 85623x1
Partitioning[ParMETIS] 2 -> 2
Type:             BiCGStab
Unknowns:         43255
Memory footprint: 2.31 M

Number of levels:    3
Operator complexity: 1.20
```

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```
Grid complexity:     1.08

level     unknowns       nonzeros
---------------------------------
    0        85623        2374949 (83.03%) [2]
    1         6381         451279 (15.78%) [2]
    2          396          34054 ( 1.19%) [2]

Iters: 24
Error: 9.14603e-09

[poisson3Db MPI(VexCL):     1.132 s] (100.00%)
[ self:                     0.040 s] (  3.56%)
[  partition:               0.607 s] ( 53.58%)
[  read:                    0.015 s] (  1.31%)
[  setup:                   0.287 s] ( 25.31%)
[  solve:                   0.184 s] ( 16.24%)
```

2.4.3 Structural problem

This system may be downloaded from the Serena page (use the Matrix Market download option). According to the description, the system represents a 3D gas resevoir simulation for CO2 sequestration, and was obtained from a structural problem discretizing a gas reservoir with tetrahedral Finite Elements. The medium is strongly heterogeneous and characterized by a complex geometry consisting of alternating sequences of thin clay and sand layers. More details available in [FGJT10]. Note that the RHS vector for the Serena problem is not provided, and we use the RHS vector filled with ones.

The system matrix is symmetric, and has 1,391,349 rows and 64,131,971 nonzero values, which corresponds to an average of 46 nonzeros per row. The matrix portrait is shown on the figure below.

As in the case of *Poisson problem* tutorial, we start experimenting with the examples/solver utility provided by AMGCL. The default options do not seem to work this time. The relative error did not reach the required threshold of 1e-8 and the solver exited after the default limit of 100 iterations:

```
$ solver -A Serena.mtx
Solver
======
Type:             BiCGStab
Unknowns:         1391349
Memory footprint: 74.31 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.22
Grid complexity:     1.08
Memory footprint:    1.45 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0      1391349       64531701      1.22 G (82.01%)
    1        98824       13083884    218.40 M (16.63%)
    2         5721        1038749     16.82 M ( 1.32%)
    3          279          29151    490.75 K ( 0.04%)
```

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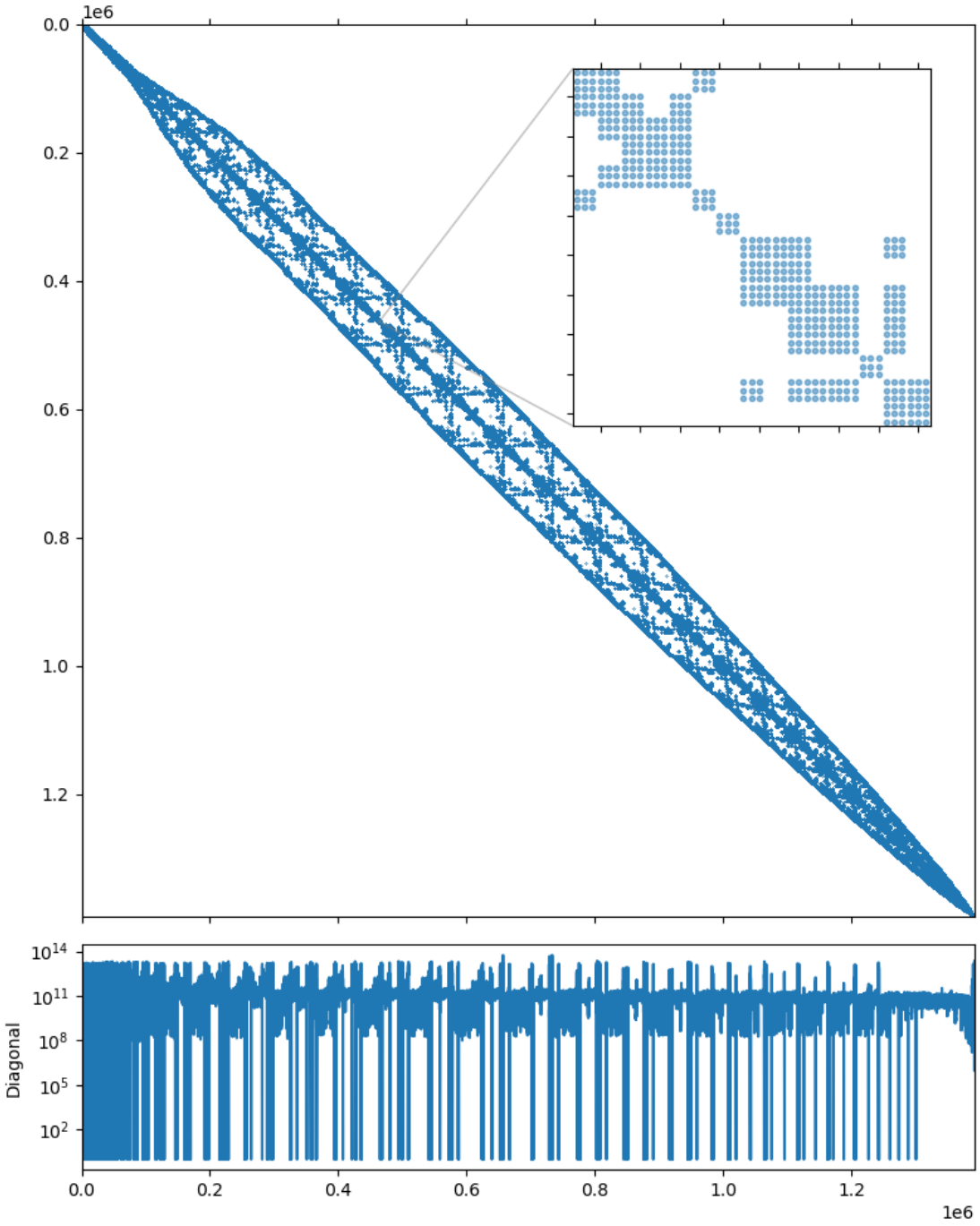

Fig. 2.4: Serena matrix portrait

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```
Iterations: 100
Error:      0.000874761

[Profile:      74.102 s] (100.00%)
[  reading:    18.505 s] ( 24.97%)
[  setup:       2.101 s] (  2.84%)
[  solve:      53.489 s] ( 72.18%)
```

The system is quite large and just reading from the text-based Matrix Market format takes 18.5 seconds. No one has that amount of free time on their hands, so lets convert the matrix into the binary format with the examples/mm2bin utility. This should make the experiments slightly less painful:

```
mm2bin -i Serena.mtx -o Serena.bin
Wrote 1391349 by 1391349 sparse matrix, 64531701 nonzeros
```

The `-B` option tells the solver that the input is in binary format now. Lets also increase the maximum iteration limit this time to see if the solver manages to converge at all:

```
$ solver -B -A Serena.bin solver.maxiter=1000
Solver
======
Type:             BiCGStab
Unknowns:         1391349
Memory footprint: 74.31 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.22
Grid complexity:     1.08
Memory footprint:    1.45 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0      1391349       64531701      1.22 G (82.01%)
    1        98824       13083884    218.40 M (16.63%)
    2         5721        1038749     16.82 M ( 1.32%)
    3          279          29151    490.75 K ( 0.04%)

Iterations: 211
Error:      8.54558e-09

[Profile:     114.703 s] (100.00%)
[  reading:     0.550 s] (  0.48%)
[  setup:       2.114 s] (  1.84%)
[  solve:     112.034 s] ( 97.67%)
```

The input matrix is read much faster now, and the solver does converge, but the convergence rate is not great. Looking closer at the *Serena matrix portrait* figure, the matrix seems to have block structure with 3×3 blocks. This is usually the case when the system has been obtained via discretization of a system of coupled PDEs, or has vector unknowns. We have to guess here, but since the problem is described as "structural", then each block probably corresponds to the 3D displacement vector of a single grid node. We can communicate this piece of information to AMGCL using the `block_size` parameter of the aggregation method:

```
$ solver -B -A Serena.bin solver.maxiter=1000 \
      precond.coarsening.aggr.block_size=3
```

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```
Solver
======
Type:             BiCGStab
Unknowns:         1391349
Memory footprint: 74.31 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.31
Grid complexity:     1.08
Memory footprint:    1.84 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0      1391349       64531701      1.50 G (76.48%)
    1       109764       17969220    316.66 M (21.30%)
    2         6291        1788507     29.51 M ( 2.12%)
    3          429          82719      1.23 M ( 0.10%)

Iterations: 120
Error:      9.73074e-09

[Profile:      73.296 s] (100.00%)
[  reading:     0.587 s] (  0.80%)
[  setup:       2.709 s] (  3.70%)
[  solve:      69.994 s] ( 95.49%)
```

This has definitely improved the convergence! We also know that the matrix is symmetric, so lets switch the solver from the default BiCGStab to the slightly less expensive CG:

```
$ solver -B -A Serena.bin \
      solver.type=cg \
      solver.maxiter=1000 \
      precond.coarsening.aggr.block_size=3
Solver
======
Type:             CG
Unknowns:         1391349
Memory footprint: 42.46 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.31
Grid complexity:     1.08
Memory footprint:    1.84 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0      1391349       64531701      1.50 G (76.48%)
    1       109764       17969220    316.66 M (21.30%)
    2         6291        1788507     29.51 M ( 2.12%)
    3          429          82719      1.23 M ( 0.10%)

Iterations: 177
```

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```
Error:      8.6598e-09

[Profile:      55.250 s] (100.00%)
[  reading:     0.550 s] (  1.00%)
[  setup:       2.801 s] (  5.07%)
[  solve:      51.894 s] ( 93.92%)
```

This reduces the solution time, even though the number of iterations has grown. Each iteration of BiCGStab costs about twice as much as a CG iteration, because BiCGStab does two matrix-vector products and preconditioner applications per iteration, while CG only does one.

The problem description states that *the medium is strongly heterogeneous and characterized by a complex geometry consisting of alternating sequences of thin clay and sand layers*. This may result in high contrast between matrix coefficients in the neighboring rows, which is confirmed by the plot of the matrix diagonal in *Serena matrix portrait*: the diagonal coefficients span more than 10 orders of magnitude! Scaling the matrix (so that it has the unit diagonal) should help with the convergence. The `-s` option tells the solver to do that:

```
$ solver -B -A Serena.bin -s \
      solver.type=cg solver.maxiter=200 \
      precond.coarsening.aggr.block_size=3
Solver
======
Type:             CG
Unknowns:         1391349
Memory footprint: 42.46 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.29
Grid complexity:     1.08
Memory footprint:    1.82 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0      1391349       64531701      1.51 G (77.81%)
    1       100635       16771185    294.81 M (20.22%)
    2         5643        1571157     25.92 M ( 1.89%)
    3          342          60264    802.69 K ( 0.07%)

Iterations: 112
Error:      9.84457e-09

[Profile:      36.021 s] (100.00%)
[ self:         0.204 s] (  0.57%)
[  reading:     0.564 s] (  1.57%)
[  setup:       2.684 s] (  7.45%)
[  solve:      32.568 s] ( 90.42%)
```

And the convergence has indeed been improved! Finally, when the matrix has block structure, as in this case, it often pays to use the block-valued backend, so that the system matrix has three times fewer rows and columns, but each nonzero entry is a statically sized 3×3 matrix. This should be done instead of specifying the `block_size` aggregation parameter, as the aggregation now naturally operates with the 3×3 blocks:

```
$ solver -B -A Serena.bin solver.type=cg solver.maxiter=200 -s -b3
Solver
```

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```
======
Type:             CG
Unknowns:         463783
Memory footprint: 42.46 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.27
Grid complexity:     1.08
Memory footprint:    1.04 G

level     unknowns       nonzeros      memory
---------------------------------------------
    0       463783        7170189    891.53 M (78.80%)
    1        33052        1772434    159.22 M (19.48%)
    2         1722         151034     12.72 M ( 1.66%)
    3           98           5756    612.72 K ( 0.06%)

Iterations: 162
Error:      9.7497e-09

[Profile:      31.122 s] (100.00%)
[ self:         0.204 s] (  0.66%)
[  reading:     0.550 s] (  1.77%)
[  setup:       1.013 s] (  3.26%)
[  solve:      29.354 s] ( 94.32%)
```

Note that the preconditioner now requires 1.04G of memory as opposed to 1.82G in the scalar case. The setup is about 2.5 times faster, and the solution phase performance has been slightly improved, even though the number of iteration has grown. This is explained by the fact that the matrix is now symbolically smaller, and is easier to analyze during setup. The matrix also occupies less memory for the CRS arrays, and is more cache-friendly, which helps to speed up the solution phase. This seems to be the best we can get with this system, so let us implement this version. We will also use the mixed precision approach in order to get as much performance as possible from the solution. The listing below shows the complete solution and is also available in tutorial/2.Serena/serena.cpp.

Listing 2.8: The source code for the solution of the Serena problem.

```
#include <vector>
#include <iostream>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/solver/cg.hpp>
#include <amgcl/value_type/static_matrix.hpp>
#include <amgcl/adapter/block_matrix.hpp>

#include <amgcl/io/mm.hpp>
#include <amgcl/profiler.hpp>

int main(int argc, char *argv[]) {
    // The command line should contain the matrix file name:
```

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```
    if (argc < 2) {
        std::cerr << "Usage: " << argv[0] << " <matrix.mtx>" << std::endl;
        return 1;
    }

    // The profiler:
    amgcl::profiler<> prof("Serena");

    // Read the system matrix:
    ptrdiff_t rows, cols;
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val;

    prof.tic("read");
    std::tie(rows, cols) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // The RHS is filled with ones:
    std::vector<double> f(rows, 1.0);

    // Scale the matrix so that it has the unit diagonal.
    // First, find the diagonal values:
    std::vector<double> D(rows, 1.0);
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            if (col[j] == i) {
                D[i] = 1 / sqrt(val[j]);
                break;
            }
        }
    }

    // Then, apply the scaling in-place:
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            val[j] *= D[i] * D[col[j]];
        }
        f[i] *= D[i];
    }

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::static_matrix<double, 3, 3> dmat_type; // matrix value type in␣
↪double precision
    typedef amgcl::static_matrix<double, 3, 1> dvec_type; // the corresponding vector␣
↪value type
    typedef amgcl::static_matrix<float,  3, 3> smat_type; // matrix value type in␣
↪single precision

    typedef amgcl::backend::builtin<dmat_type> SBackend; // the solver backend
    typedef amgcl::backend::builtin<smat_type> PBackend; // the preconditioner backend

```

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```
73      typedef amgcl::make_solver<
74          amgcl::amg<
75              PBackend,
76              amgcl::coarsening::smoothed_aggregation,
77              amgcl::relaxation::spai0
78              >,
79          amgcl::solver::cg<SBackend>
80          > Solver;
81
82      // Solver parameters
83      Solver::params prm;
84      prm.solver.maxiter = 500;
85
86      // Initialize the solver with the system matrix.
87      // Use the block_matrix adapter to convert the matrix into
88      // the block format on the fly:
89      prof.tic("setup");
90      auto Ab = amgcl::adapter::block_matrix<dmat_type>(A);
91      Solver solve(Ab, prm);
92      prof.toc("setup");
93
94      // Show the mini-report on the constructed solver:
95      std::cout << solve << std::endl;
96
97      // Solve the system with the zero initial approximation:
98      int iters;
99      double error;
100     std::vector<double> x(rows, 0.0);
101
102     // Reinterpret both the RHS and the solution vectors as block-valued:
103     auto f_ptr = reinterpret_cast<dvec_type*>(f.data());
104     auto x_ptr = reinterpret_cast<dvec_type*>(x.data());
105     auto F = amgcl::make_iterator_range(f_ptr, f_ptr + rows / 3);
106     auto X = amgcl::make_iterator_range(x_ptr, x_ptr + rows / 3);
107
108     prof.tic("solve");
109     std::tie(iters, error) = solve(Ab, F, X);
110     prof.toc("solve");
111
112     // Output the number of iterations, the relative error,
113     // and the profiling data:
114     std::cout << "Iters: " << iters << std::endl
115               << "Error: " << error << std::endl
116               << prof << std::endl;
117 }
```

In addition the the includes described in *Poisson problem*, we also include the headers for the `amgcl::static_matrix` value type, and the `amgcl::adapter::block_matrix()` adapter that transparently converts a scalar matrix to the block format. In lines 42–58 we apply the scaling according to the following formula:

$$A_s = D^{-1/2} A D^{-1/2}, \quad f_s = D^{-1/2} f$$

where A_s and f_s are the scaled matrix and the RHS vector, and D is the diagonal of the matrix A. After solving the scaled system $A_s y = f_s$, the solution to the original system may be found as $x = D^{-1/2} y$.

In lines 66–68 we define the block value types for the matrix and the RHS and solution vectors. `dmat_type` and `smat_type` are 3×3 static matrices used as value types with the double precision solver backend and the single

precision preconditioner backend. `dvec_type` is a double precision 3×1 matrix (or a vector) used as a value type for the RHS and the solution.

The solver class definition in lines 73–80 is almost the same as in the *Poisson problem* case, with the exception that we are using the CG iterative solver this time. In lines 83–84 we define the solver parameters. Namely, we increase the maximum iterations limit to 500 iterations.

In lines 90–91 we instantiate the solver, using the `block_matrix` adapter in order to convert the scalar matrix into the block format. The adapter operates on a row-by-row basis and does not create a temporary copy of the matrix.

In lines 103–106 we convert the scalar RHS and solution vectors to the block-valued ones. We use the fact that 3 consecutive elements of a scalar array may be reinterpreted as a single 3×1 static matrix. Using the `reinterpret_cast` trick we can get the block-valued view into the RHS and the solution vectors data without extra memory copies.

Here is the output of the program:

```
$ ./serena Serena.mtx
Matrix Serena.mtx: 1391349x1391349
Solver
======
Type:             CG
Unknowns:         463783
Memory footprint: 42.46 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.27
Grid complexity:     1.08
Memory footprint:    585.33 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       463783        7170189    490.45 M (78.80%)
    1        33052        1772434     87.58 M (19.48%)
    2         1722         151034      7.00 M ( 1.66%)
    3           98           5756    306.75 K ( 0.06%)

Iters: 162
Error: 9.74929e-09

[Serena:     48.427 s] (100.00%)
[ self:       0.166 s] (  0.34%)
[  read:     21.115 s] ( 43.60%)
[  setup:     0.749 s] (  1.55%)
[  solve:    26.397 s] ( 54.51%)
```

Note that due to the use of mixed precision the preconditioner consumes 585.33M of memory as opposed to 1.08G from the example above. The setup and the solution are faster that the full precision version by about 30% and 10% correspondingly.

Let us see if using a GPU backend may further improve the performance. The CUDA backend does not support block value types, so we will use the VexCL backend (which, in turn, may use either OpenCL, CUDA, or OpenMP). The listing below contains the complete source for the solution (available at tutorial/2.Serena/serena_vexcl.cpp). The differences with the builtin backend version are highlighted.

Listing 2.9: The solution of the Serena problem with the VexCL backend.

```
#include <vector>
#include <iostream>

#include <amgcl/backend/vexcl.hpp>
#include <amgcl/backend/vexcl_static_matrix.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/solver/cg.hpp>
#include <amgcl/value_type/static_matrix.hpp>
#include <amgcl/adapter/block_matrix.hpp>

#include <amgcl/io/mm.hpp>
#include <amgcl/profiler.hpp>

int main(int argc, char *argv[]) {
    // The command line should contain the matrix file name:
    if (argc < 2) {
        std::cerr << "Usage: " << argv[0] << " <matrix.mtx>" << std::endl;
        return 1;
    }

    // Create VexCL context. Set the environment variable OCL_DEVICE to
    // control which GPU to use in case multiple are available,
    // and use single device:
    vex::Context ctx(vex::Filter::Env && vex::Filter::Count(1));
    std::cout << ctx << std::endl;

    // Enable support for block-valued matrices in the VexCL kernels:
    vex::scoped_program_header h1(ctx, amgcl::backend::vexcl_static_matrix_declaration
↪<double,3>());
    vex::scoped_program_header h2(ctx, amgcl::backend::vexcl_static_matrix_declaration
↪<float,3>());

    // The profiler:
    amgcl::profiler<> prof("Serena (VexCL)");

    // Read the system matrix:
    ptrdiff_t rows, cols;
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val;

    prof.tic("read");
    std::tie(rows, cols) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // The RHS is filled with ones:
    std::vector<double> f(rows, 1.0);

    // Scale the matrix so that it has the unit diagonal.
    // First, find the diagonal values:
    std::vector<double> D(rows, 1.0);
```

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```
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            if (col[j] == i) {
                D[i] = 1 / sqrt(val[j]);
                break;
            }
        }
    }

    // Then, apply the scaling in-place:
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            val[j] *= D[i] * D[col[j]];
        }
        f[i] *= D[i];
    }

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::static_matrix<double, 3, 3> dmat_type; // matrix value type in␣
↪double precision
    typedef amgcl::static_matrix<double, 3, 1> dvec_type; // the corresponding vector␣
↪value type
    typedef amgcl::static_matrix<float,  3, 3> smat_type; // matrix value type in␣
↪single precision

    typedef amgcl::backend::vexcl<dmat_type> SBackend; // the solver backend
    typedef amgcl::backend::vexcl<smat_type> PBackend; // the preconditioner backend

    typedef amgcl::make_solver<
        amgcl::amg<
            PBackend,
            amgcl::coarsening::smoothed_aggregation,
            amgcl::relaxation::spai0
            >,
        amgcl::solver::cg<SBackend>
        > Solver;

    // Solver parameters
    Solver::params prm;
    prm.solver.maxiter = 500;

    // Set the VexCL context in the backend parameters
    SBackend::params bprm;
    bprm.q = ctx;

    // Initialize the solver with the system matrix.
    // We use the block_matrix adapter to convert the matrix into the block
    // format on the fly:
    prof.tic("setup");
    auto Ab = amgcl::adapter::block_matrix<dmat_type>(A);
    Solver solve(Ab, prm, bprm);
    prof.toc("setup");
```

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```
108
109     // Show the mini-report on the constructed solver:
110     std::cout << solve << std::endl;
111
112     // Solve the system with the zero initial approximation:
113     int iters;
114     double error;
115     std::vector<double> x(rows, 0.0);
116
117     // Since we are using mixed precision, we have to transfer the system matrix to␣
    ↪the GPU:
118     prof.tic("GPU matrix");
119     auto A_gpu = SBackend::copy_matrix(
120             std::make_shared<amgcl::backend::crs<dmat_type>>(Ab), bprm);
121     prof.toc("GPU matrix");
122
123     // We reinterpret both the RHS and the solution vectors as block-valued,
124     // and copy them to the VexCL vectors:
125     auto f_ptr = reinterpret_cast<dvec_type*>(f.data());
126     auto x_ptr = reinterpret_cast<dvec_type*>(x.data());
127     vex::vector<dvec_type> F(ctx, rows / 3, f_ptr);
128     vex::vector<dvec_type> X(ctx, rows / 3, x_ptr);
129
130     prof.tic("solve");
131     std::tie(iters, error) = solve(*A_gpu, F, X);
132     prof.toc("solve");
133
134     // Output the number of iterations, the relative error,
135     // and the profiling data:
136     std::cout << "Iters: " << iters << std::endl
137               << "Error: " << error << std::endl
138               << prof << std::endl;
139 }
```

In the include section, we replace the header for the builtin backend with the one for the VexCL backend, and also include the header with support for block values in VexCL (lines 4–5). In lines 28–29 we initialize the VexCL context, and in lines 32–33 we enable the VexCL support for 3×3 static matrices in both double and single precision.

In lines 81–82 we define the solver and preconditioner backends as VexCL backends with the corresponding matrix value types. In lines 98–99 we reference the VexCL context in the backend parameters.

Since we are using the GPU backend, we have to explicitly form the block valued matrix and transfer it to the GPU. This is done in lines 119–120. In lines 127–128 we copy the RHS and the solution vectors to the GPU, and we solve the system in line 131.

The output of the program is shown below:

```
$ ./serena_vexcl_cuda Serena.mtx
1. GeForce GTX 1050 Ti

Matrix Serena.mtx: 1391349x1391349
Solver
======
Type:             CG
Unknowns:         463783
Memory footprint: 42.46 M
```

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```
Preconditioner
==============
Number of levels:    4
Operator complexity: 1.27
Grid complexity:     1.08
Memory footprint:    585.33 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       463783        7170189    490.45 M (78.80%)
    1        33052        1772434     87.58 M (19.48%)
    2         1722         151034      7.00 M ( 1.66%)
    3           98           5756    309.04 K ( 0.06%)

Iters: 162
Error: 9.74928e-09

[Serena (VexCL):  27.208 s] (100.00%)
[ self:            0.180 s] (  0.66%)
[  GPU matrix:     0.604 s] (  2.22%)
[  read:          18.699 s] ( 68.73%)
[  setup:          1.308 s] (  4.81%)
[  solve:          6.417 s] ( 23.59%)
```

The setup time has increased from 0.7 seconds for the builtin backend to 1.3 seconds, and we also see the additional 0.6 seconds for transferring the matrix to the GPU. But the solution time has decreased from 26.4 to 6.4 seconds, which is about 4 times faster.

2.4.4 Structural problem (MPI version)

In this section we look at how to use the MPI version of the AMGCL solver with the Serena system. We have already determined in the *Structural problem* section that the system is best solved with the block-valued backend, and needs to be scaled so that it has the unit diagonal. The MPI solution will be very closer to the one we have seen in the *Poisson problem (MPI version)* section. The only differences are:

- The system needs to be scaled so that it has the unit diagonal. This is complicated by the fact that the matrix product $D^{-1/2}AD^{-1/2}$ has to done in the distributed memory environment.
- The solution has to use the block-valued backend, and the partitioning needs to take this into account. Namely, the partitioning should not split any of the 3×3 blocks between MPI processes.
- Even though the system is symmetric, the convergence of the CG solver in the distributed case stalls at the relative error of about 10^{-6}. Switching to the BiCGStab solver helps with the convergence.

The next listing is the MPI version of the Serena system solver (tutorial/2.Serena/serena_mpi.cpp). In the following paragraphs we highlight the differences between this version and the code in the *Poisson problem (MPI version)* and *Structural problem* sections.

Listing 2.10: The MPI solution of the Serena problem

```
1 #include <vector>
2 #include <iostream>
3
4 #include <amgcl/backend/builtin.hpp>
5 #include <amgcl/value_type/static_matrix.hpp>
6 #include <amgcl/adapter/crs_tuple.hpp>
```

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```
#include <amgcl/adapter/block_matrix.hpp>

#include <amgcl/mpi/distributed_matrix.hpp>
#include <amgcl/mpi/make_solver.hpp>
#include <amgcl/mpi/amg.hpp>
#include <amgcl/mpi/coarsening/smoothed_aggregation.hpp>
#include <amgcl/mpi/relaxation/spai0.hpp>
#include <amgcl/mpi/solver/bicgstab.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

#if defined(AMGCL_HAVE_PARMETIS)
#  include <amgcl/mpi/partition/parmetis.hpp>
#elif defined(AMGCL_HAVE_SCOTCH)
#  include <amgcl/mpi/partition/ptscotch.hpp>
#endif

// Block size
const int B = 3;

//---------------------------------------------------------------------------
int main(int argc, char *argv[]) {
    // The command line should contain the matrix file name:
    if (argc < 2) {
        std::cerr << "Usage: " << argv[0] << " <matrix.bin>" << std::endl;
        return 1;
    }

    amgcl::mpi::init mpi(&argc, &argv);
    amgcl::mpi::communicator world(MPI_COMM_WORLD);

    // The profiler:
    amgcl::profiler<> prof("Serena MPI");

    prof.tic("read");
    // Get the global size of the matrix:
    ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);

    // Split the matrix into approximately equal chunks of rows, and
    // make sure each chunk size is divisible by the block size.
    ptrdiff_t chunk = (rows + world.size - 1) / world.size;
    if (chunk % B) chunk += B - chunk % B;

    ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
    ptrdiff_t row_end = std::min(rows, row_beg + chunk);
    chunk = row_end - row_beg;

    // Read our part of the system matrix.
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val;
    amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);
    prof.toc("read");

    if (world.rank == 0) std::cout
        << "World size: " << world.size << std::endl
        << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
```

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```
64
65      // Declare the backend and the solver types
66      typedef amgcl::static_matrix<double, B, B> dmat_type;
67      typedef amgcl::static_matrix<double, B, 1> dvec_type;
68      typedef amgcl::static_matrix<float,  B, B> fmat_type;
69      typedef amgcl::backend::builtin<dmat_type> DBackend;
70      typedef amgcl::backend::builtin<fmat_type> FBackend;
71
72      typedef amgcl::mpi::make_solver<
73          amgcl::mpi::amg<
74              FBackend,
75              amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
76              amgcl::mpi::relaxation::spai0<FBackend>
77              >,
78          amgcl::mpi::solver::bicgstab<DBackend>
79          > Solver;
80
81      // Solver parameters
82      Solver::params prm;
83      prm.solver.maxiter = 200;
84
85      // We need to scale the matrix, so that it has the unit diagonal.
86      // Since we only have the local rows for the matrix, and we may need the
87      // remote diagonal values, it is more convenient to represent the scaling
88      // with the matrix-matrix product (As = D^-1/2 A D^-1/2).
89      prof.tic("scale");
90      // Find the local diagonal values,
91      // and form the CRS arrays for a diagonal matrix.
92      std::vector<double> dia(chunk, 1.0);
93      std::vector<ptrdiff_t> d_ptr(chunk + 1), d_col(chunk);
94      for(ptrdiff_t i = 0, I = row_beg; i < chunk; ++i, ++I) {
95          d_ptr[i] = i;
96          d_col[i] = I;
97          for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
98              if (col[j] == I) {
99                  dia[i] = 1 / sqrt(val[j]);
100                 break;
101             }
102         }
103     }
104     d_ptr.back() = chunk;
105
106     // Create the distributed diagonal matrix:
107     amgcl::mpi::distributed_matrix<DBackend> D(world,
108             amgcl::adapter::block_matrix<dmat_type>(
109                 std::tie(chunk, d_ptr, d_col, dia)));
110
111     // The scaled matrix is formed as product D * A * D,
112     // where A is the local chunk of the matrix
113     // converted to the block format on the fly.
114     auto A = product(D, *product(
115                 amgcl::mpi::distributed_matrix<DBackend>(world,
116                     amgcl::adapter::block_matrix<dmat_type>(
117                         std::tie(chunk, ptr, col, val))),
118                 D));
119     prof.toc("scale");
120
```

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```
    // Since the RHS in this case is filled with ones,
    // the scaled RHS is equal to dia.
    // Reinterpret the pointer to dia data to get the RHS in the block format:
    auto f_ptr = reinterpret_cast<dvec_type*>(dia.data());
    std::vector<dvec_type> rhs(f_ptr, f_ptr + chunk / B);

    // Partition the matrix and the RHS vector.
    // If neither ParMETIS not PT-SCOTCH are not available,
    // just keep the current naive partitioning.
#if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
#  if defined(AMGCL_HAVE_PARMETIS)
    typedef amgcl::mpi::partition::parmetis<DBackend> Partition;
#  elif defined(AMGCL_HAVE_SCOTCH)
    typedef amgcl::mpi::partition::ptscotch<DBackend> Partition;
#  endif

    if (world.size > 1) {
        prof.tic("partition");
        Partition part;

        // part(A) returns the distributed permutation matrix:
        auto P = part(*A);
        auto R = transpose(*P);

        // Reorder the matrix:
        A = product(*R, *product(*A, *P));

        // and the RHS vector:
        std::vector<dvec_type> new_rhs(R->loc_rows());
        R->move_to_backend();
        amgcl::backend::spmv(1, *R, rhs, 0, new_rhs);
        rhs.swap(new_rhs);

        // Update the number of the local rows
        // (it may have changed as a result of permutation).
        // Note that A->loc_rows() returns the number of blocks,
        // as the matrix uses block values.
        chunk = A->loc_rows();
        prof.toc("partition");
    }
#endif

    // Initialize the solver:
    prof.tic("setup");
    Solver solve(world, A, prm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    if (world.rank == 0) std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    std::vector<dvec_type> x(chunk, amgcl::math::zero<dvec_type>());

    prof.tic("solve");
    std::tie(iters, error) = solve(*A, rhs, x);
```

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```
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    if (world.rank == 0) std::cout
        << "Iterations: " << iters << std::endl
        << "Error:      " << error << std::endl
        << prof << std::endl;
}
```

We make sure that the paritioning takes the block structure of the matrix into account by keeping the number of rows in the initial naive partitioning divisible by 3 (here the constant `B` is equal to 3):

```
    // Split the matrix into approximately equal chunks of rows, and
    // make sure each chunk size is divisible by the block size.
    ptrdiff_t chunk = (rows + world.size - 1) / world.size;
    if (chunk % B) chunk += B - chunk % B;

    ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
    ptrdiff_t row_end = std::min(rows, row_beg + chunk);
    chunk = row_end - row_beg;
```

We also create all the distributed matrices using the block values, so the partitioning naturally is block-aware. We are using the mixed precision approach, so the preconditioner backend is defined with the single precision:

```
    // Declare the backend and the solver types
    typedef amgcl::static_matrix<double, B, B> dmat_type;
    typedef amgcl::static_matrix<double, B, 1> dvec_type;
    typedef amgcl::static_matrix<float,  B, B> fmat_type;
    typedef amgcl::backend::builtin<dmat_type> DBackend;
    typedef amgcl::backend::builtin<fmat_type> FBackend;

    typedef amgcl::mpi::make_solver<
        amgcl::mpi::amg<
            FBackend,
            amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
            amgcl::mpi::relaxation::spai0<FBackend>
            >,
        amgcl::mpi::solver::bicgstab<DBackend>
        > Solver;
```

The scaling is done similarly to how we apply the reordering: first, we find the diagonal of the local diagonal block on each of the MPI processes, and then we create the distributed diagonal matrix with the inverted square root of the system matrix diagonal. After that, the scaled matrix $A_s = D^{-1/2}AD^{-1/2}$ is computed using the `amgcl::mpi::product()` function. The scaled RHS vector $f_s = D^{-1/2}f$ in principle may be found using the `amgcl::backend::spmv()` primitive, but, since the RHS vector in this case is simply filled with ones, the scaled RHS $f_s = D^{-1/2}$.

```
    // We need to scale the matrix, so that it has the unit diagonal.
    // Since we only have the local rows for the matrix, and we may need the
    // remote diagonal values, it is more convenient to represent the scaling
    // with the matrix-matrix product (As = D^-1/2 A D^-1/2).
    prof.tic("scale");
    // Find the local diagonal values,
    // and form the CRS arrays for a diagonal matrix.
    std::vector<double> dia(chunk, 1.0);
```

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```
    std::vector<ptrdiff_t> d_ptr(chunk + 1), d_col(chunk);
    for(ptrdiff_t i = 0, I = row_beg; i < chunk; ++i, ++I) {
        d_ptr[i] = i;
        d_col[i] = I;
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            if (col[j] == I) {
                dia[i] = 1 / sqrt(val[j]);
                break;
            }
        }
    }
    d_ptr.back() = chunk;

    // Create the distributed diagonal matrix:
    amgcl::mpi::distributed_matrix<DBackend> D(world,
            amgcl::adapter::block_matrix<dmat_type>(
                std::tie(chunk, d_ptr, d_col, dia)));

    // The scaled matrix is formed as product D * A * D,
    // where A is the local chunk of the matrix
    // converted to the block format on the fly.
    auto A = product(D, *product(
                amgcl::mpi::distributed_matrix<DBackend>(world,
                    amgcl::adapter::block_matrix<dmat_type>(
                        std::tie(chunk, ptr, col, val))),
                D));
    prof.toc("scale");

    // Since the RHS in this case is filled with ones,
    // the scaled RHS is equal to dia.
    // Reinterpret the pointer to dia data to get the RHS in the block format:
    auto f_ptr = reinterpret_cast<dvec_type*>(dia.data());
    std::vector<dvec_type> rhs(f_ptr, f_ptr + chunk / B);
```

Here is the output from the compiled program:

```
$ export OMP_NUM_THREADS=1
$ mpirun -np 4 ./serena_mpi Serena.bin
World size: 4
Matrix Serena.bin: 1391349x1391349
Partitioning[ParMETIS] 4 -> 4
Type:             BiCGStab
Unknowns:         118533
Memory footprint: 18.99 M

Number of levels:    4
Operator complexity: 1.27
Grid complexity:     1.07

level     unknowns       nonzeros
---------------------------------
    0       463783         7170189 (79.04%) [4]
    1        32896         1752778 (19.32%) [4]
    2         1698          144308 ( 1.59%) [4]
    3           95            4833 ( 0.05%) [4]

Iterations: 80
```

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```
Error:      9.34355e-09

[Serena MPI:     24.840 s] (100.00%)
[  partition:     1.159 s] (  4.67%)
[  read:          0.265 s] (  1.07%)
[  scale:         0.583 s] (  2.35%)
[  setup:         0.811 s] (  3.26%)
[  solve:        22.017 s] ( 88.64%)
```

The version that uses the VexCL backend should be familiar at this point. Below is the source code (tutorial/2.Serena/serena_mpi_vexcl.cpp) where the differences with the builtin backend version are highlighted:

Listing 2.11: The MPI solution of the Serena problem using the VexCL backend

```
#include <vector>
#include <iostream>

#include <amgcl/backend/vexcl.hpp>
#include <amgcl/backend/vexcl_static_matrix.hpp>
#include <amgcl/value_type/static_matrix.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/adapter/block_matrix.hpp>

#include <amgcl/mpi/distributed_matrix.hpp>
#include <amgcl/mpi/make_solver.hpp>
#include <amgcl/mpi/amg.hpp>
#include <amgcl/mpi/coarsening/smoothed_aggregation.hpp>
#include <amgcl/mpi/relaxation/spai0.hpp>
#include <amgcl/mpi/solver/bicgstab.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

#if defined(AMGCL_HAVE_PARMETIS)
#  include <amgcl/mpi/partition/parmetis.hpp>
#elif defined(AMGCL_HAVE_SCOTCH)
#  include <amgcl/mpi/partition/ptscotch.hpp>
#endif

// Block size
const int B = 3;

//---------------------------------------------------------------------------
int main(int argc, char *argv[]) {
    // The command line should contain the matrix file name:
    if (argc < 2) {
        std::cerr << "Usage: " << argv[0] << " <matrix.bin>" << std::endl;
        return 1;
    }

    amgcl::mpi::init mpi(&argc, &argv);
    amgcl::mpi::communicator world(MPI_COMM_WORLD);

    // Create VexCL context. Use vex::Filter::Exclusive so that different MPI
    // processes get different GPUs. Each process gets a single GPU:
```

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```
    vex::Context ctx(vex::Filter::Exclusive(vex::Filter::Env &&␣
↪vex::Filter::Count(1)));
    for(int i = 0; i < world.size; ++i) {
        // unclutter the output:
        if (i == world.rank)
            std::cout << world.rank << ": " << ctx.queue(0) << std::endl;
        MPI_Barrier(world);
    }

    // Enable support for block-valued matrices in the VexCL kernels:
    vex::scoped_program_header h1(ctx, amgcl::backend::vexcl_static_matrix_declaration
↪<double,B>());
    vex::scoped_program_header h2(ctx, amgcl::backend::vexcl_static_matrix_declaration
↪<float,B>());

    // The profiler:
    amgcl::profiler<> prof("Serena MPI(VexCL)");

    prof.tic("read");
    // Get the global size of the matrix:
    ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);

    // Split the matrix into approximately equal chunks of rows, and
    // make sure each chunk size is divisible by the block size.
    ptrdiff_t chunk = (rows + world.size - 1) / world.size;
    if (chunk % B) chunk += B - chunk % B;

    ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
    ptrdiff_t row_end = std::min(rows, row_beg + chunk);
    chunk = row_end - row_beg;

    // Read our part of the system matrix.
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val;
    amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);
    prof.toc("read");

    if (world.rank == 0) std::cout
        << "World size: " << world.size << std::endl
        << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;

    // Declare the backend and the solver types
    typedef amgcl::static_matrix<double, B, B> dmat_type;
    typedef amgcl::static_matrix<double, B, 1> dvec_type;
    typedef amgcl::static_matrix<float,  B, B> fmat_type;
    typedef amgcl::backend::vexcl<dmat_type> DBackend;
    typedef amgcl::backend::vexcl<fmat_type> FBackend;

    typedef amgcl::mpi::make_solver<
        amgcl::mpi::amg<
            FBackend,
            amgcl::mpi::coarsening::smoothed_aggregation<FBackend>,
            amgcl::mpi::relaxation::spai0<FBackend>
            >,
        amgcl::mpi::solver::bicgstab<DBackend>
        > Solver;

```

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```
96      // Solver parameters
97      Solver::params prm;
98      prm.solver.maxiter = 200;
99
100     // Set the VexCL context in the backend parameters
101     DBackend::params bprm;
102     bprm.q = ctx;
103
104     // We need to scale the matrix, so that it has the unit diagonal.
105     // Since we only have the local rows for the matrix, and we may need the
106     // remote diagonal values, it is more convenient to represent the scaling
107     // with the matrix-matrix product (As = D^-1/2 A D^-1/2).
108     prof.tic("scale");
109     // Find the local diagonal values,
110     // and form the CRS arrays for a diagonal matrix.
111     std::vector<double> dia(chunk, 1.0);
112     std::vector<ptrdiff_t> d_ptr(chunk + 1), d_col(chunk);
113     for(ptrdiff_t i = 0, I = row_beg; i < chunk; ++i, ++I) {
114         d_ptr[i] = i;
115         d_col[i] = I;
116         for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
117             if (col[j] == I) {
118                 dia[i] = 1 / sqrt(val[j]);
119                 break;
120             }
121         }
122     }
123     d_ptr.back() = chunk;
124
125     // Create the distributed diagonal matrix:
126     amgcl::mpi::distributed_matrix<DBackend> D(world,
127             amgcl::adapter::block_matrix<dmat_type>(
128                 std::tie(chunk, d_ptr, d_col, dia)));
129
130     // The scaled matrix is formed as product D * A * D,
131     // where A is the local chunk of the matrix
132     // converted to the block format on the fly.
133     auto A = product(D, *product(
134                 amgcl::mpi::distributed_matrix<DBackend>(world,
135                     amgcl::adapter::block_matrix<dmat_type>(
136                         std::tie(chunk, ptr, col, val))),
137                 D));
138     prof.toc("scale");
139
140     // Since the RHS in this case is filled with ones,
141     // the scaled RHS is equal to dia.
142     // Reinterpret the pointer to dia data to get the RHS in the block format:
143     auto f_ptr = reinterpret_cast<dvec_type*>(dia.data());
144     vex::vector<dvec_type> rhs(ctx, chunk / B, f_ptr);
145
146     // Partition the matrix and the RHS vector.
147     // If neither ParMETIS not PT-SCOTCH are not available,
148     // just keep the current naive partitioning.
149 #if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
150 #  if defined(AMGCL_HAVE_PARMETIS)
151     typedef amgcl::mpi::partition::parmetis<DBackend> Partition;
152 #  elif defined(AMGCL_HAVE_SCOTCH)
```

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```
153     typedef amgcl::mpi::partition::ptscotch<DBackend> Partition;
154 #   endif
155
156     if (world.size > 1) {
157         prof.tic("partition");
158         Partition part;
159
160         // part(A) returns the distributed permutation matrix:
161         auto P = part(*A);
162         auto R = transpose(*P);
163
164         // Reorder the matrix:
165         A = product(*R, *product(*A, *P));
166
167         // and the RHS vector:
168         vex::vector<dvec_type> new_rhs(ctx, R->loc_rows());
169         R->move_to_backend(bprm);
170         amgcl::backend::spmv(1, *R, rhs, 0, new_rhs);
171         rhs.swap(new_rhs);
172
173         // Update the number of the local rows
174         // (it may have changed as a result of permutation).
175         // Note that A->loc_rows() returns the number of blocks,
176         // as the matrix uses block values.
177         chunk = A->loc_rows();
178         prof.toc("partition");
179     }
180 #endif
181
182     // Initialize the solver:
183     prof.tic("setup");
184     Solver solve(world, A, prm, bprm);
185     prof.toc("setup");
186
187     // Show the mini-report on the constructed solver:
188     if (world.rank == 0) std::cout << solve << std::endl;
189
190     // Solve the system with the zero initial approximation:
191     int iters;
192     double error;
193     vex::vector<dvec_type> x(ctx, chunk);
194     x = amgcl::math::zero<dvec_type>();
195
196     prof.tic("solve");
197     std::tie(iters, error) = solve(*A, rhs, x);
198     prof.toc("solve");
199
200     // Output the number of iterations, the relative error,
201     // and the profiling data:
202     if (world.rank == 0) std::cout
203         << "Iterations: " << iters << std::endl
204         << "Error:      " << error << std::endl
205         << prof << std::endl;
206 }
```

Here is the output of the MPI version with the VexCL backend:

```
$ export OMP_NUM_THREADS=1
$ mpirun -np 2 ./serena_mpi_vexcl_cl Serena.bin
0: GeForce GTX 960 (NVIDIA CUDA)
1: GeForce GTX 1050 Ti (NVIDIA CUDA)
World size: 2
Matrix Serena.bin: 1391349x1391349
Partitioning[ParMETIS] 2 -> 2
Type:             BiCGStab
Unknowns:         231112
Memory footprint: 37.03 M

Number of levels:    4
Operator complexity: 1.27
Grid complexity:     1.07

level     unknowns       nonzeros
---------------------------------
    0       463783        7170189 (79.01%) [2]
    1        32887        1754795 (19.34%) [2]
    2         1708         146064 ( 1.61%) [2]
    3           85           4059 ( 0.04%) [2]

Iterations: 83
Error:      9.80582e-09

[Serena MPI(VexCL):    10.943 s] (100.00%)
[  partition:           1.357 s] ( 12.40%)
[  read:                0.370 s] (  3.38%)
[  scale:               0.729 s] (  6.66%)
[  setup:               1.966 s] ( 17.97%)
[  solve:               6.512 s] ( 59.51%)
```

2.4.5 Fully coupled poroelastic problem

This system may be downloaded from the CoupCons3D page (use the Matrix Market download option). According to the description, the system has been obtained through a Finite Element transient simulation of a fully coupled consolidation problem on a three-dimensional domain using Finite Differences for the discretization in time. More details available in [FePG09] and [FeJP12]. The RHS vector for the CoupCons3D problem is not provided, and we use the RHS vector filled with ones.

The system matrix is non-symmetric and has 416,800 rows and 17,277,420 nonzero values, which corresponds to an average of 41 nonzeros per row. The matrix portrait is shown on the figure below.

Once again, lets start our experiments with the examples/solver utility after converting the matrix into binary format with examples/mm2bin. The default options do not seem to work for this problem:

```
$ solver -B -A CoupCons3D.bin
Solver
======
Type:             BiCGStab
Unknowns:         416800
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    4
```

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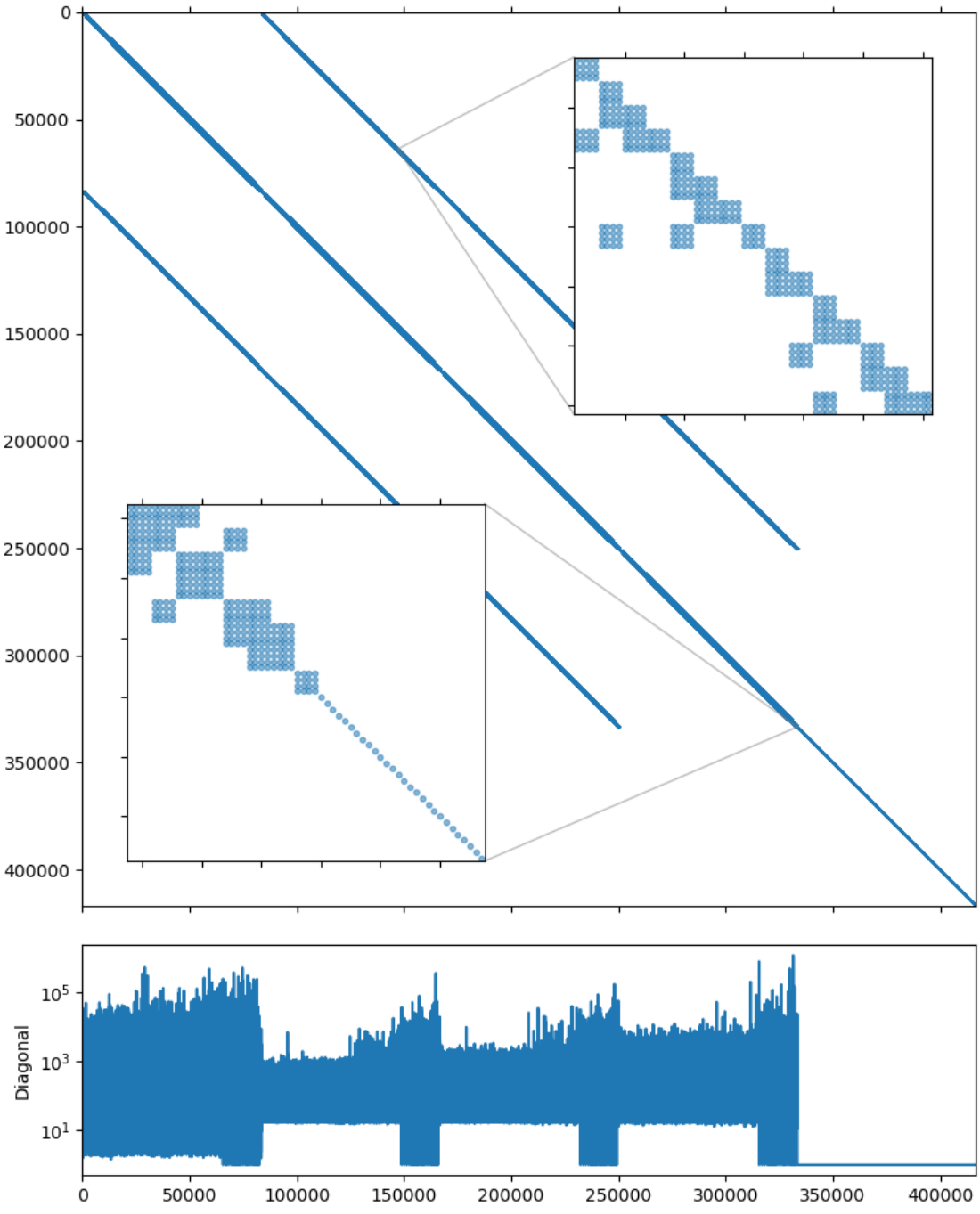

Fig. 2.5: CoupCons3D matrix portrait

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```
Operator complexity: 1.11
Grid complexity:     1.09
Memory footprint:    447.17 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       416800       22322336    404.08 M (90.13%)
    1        32140        2214998     38.49 M ( 8.94%)
    2         3762         206242      3.58 M ( 0.83%)
    3          522          22424      1.03 M ( 0.09%)

Iterations: 100
Error:      0.705403

[Profile:      16.981 s] (100.00%)
[  reading:     0.187 s] (  1.10%)
[  setup:       0.584 s] (  3.44%)
[  solve:      16.209 s] ( 95.45%)
```

What seems to works is using the higher quality relaxation (incomplete LU decomposition with zero fill-in):

```
$ solver -B -A CoupCons3D.bin precond.relax.type=ilu0
Solver
======
Type:             BiCGStab
Unknowns:         416800
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.11
Grid complexity:     1.09
Memory footprint:    832.12 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       416800       22322336    751.33 M (90.13%)
    1        32140        2214998     72.91 M ( 8.94%)
    2         3762         206242      6.85 M ( 0.83%)
    3          522          22424      1.03 M ( 0.09%)

Iterations: 47
Error:      4.8263e-09

[Profile:      13.664 s] (100.00%)
[  reading:     0.188 s] (  1.38%)
[  setup:       1.708 s] ( 12.50%)
[  solve:      11.765 s] ( 86.11%)
```

From the matrix diagonal plot in *CoupCons3D matrix portrait* it is clear that the system, as in *Structural problem* case, has high contrast coefficients. Scaling the matrix so it has the unit diagonal should help here as well:

```
$ solver -B -A CoupCons3D.bin precond.relax.type=ilu0 -s
Solver
======
```

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```
Type:             BiCGStab
Unknowns:         416800
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.10
Grid complexity:     1.08
Memory footprint:    834.51 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       416800       22322336    751.33 M (90.54%)
    1        32140        2214998     73.06 M ( 8.98%)
    2         2221         116339     10.12 M ( 0.47%)

Iterations: 11
Error:      9.79966e-09

[Profile:       4.826 s] (100.00%)
[ self:         0.064 s] (  1.34%)
[  reading:     0.188 s] (  3.90%)
[  setup:       1.885 s] ( 39.06%)
[  solve:       2.689 s] ( 55.71%)
```

Another thing to note from the *CoupCons3D matrix portrait* is that the system matrix has block structure, with two diagonal subblocks. The upper left subblock contains 333,440 unknowns and seems to have a block structure of its own with small 4×4 blocks, and the lower right subblock is a simple diagonal matrix with 83,360 unknowns. Fortunately, 83,360 is divisible by 4, so we should be able to treat the whole system as if it had 4×4 block structure:

```
$ solver -B -A CoupCons3D.bin precond.relax.type=ilu0 -s -b4
Solver
======
Type:             BiCGStab
Unknowns:         104200
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.18
Grid complexity:     1.11
Memory footprint:    525.68 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       104200        1395146    445.04 M (84.98%)
    1        10365         235821     70.07 M (14.36%)
    2          600          10792     10.57 M ( 0.66%)

Iterations: 4
Error:      2.90461e-09

[Profile:       1.356 s] (100.00%)
[ self:         0.063 s] (  4.62%)
```

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```
[  reading:     0.188 s] ( 13.84%)
[  setup:       0.478 s] ( 35.23%)
[  solve:       0.628 s] ( 46.30%)
```

This is much better! Looks like switching to the block-valued backend not only improved the setup and solution performance, but also increased the convergence speed. This version is about 12 times faster than the first working approach. Lets see how this translates to the code, with the added bonus of using the mixed precision solution. The source below shows the complete solution and is also available in tutorial/3.CoupCons3D/coupcons3d.cpp. The only differences (highlighted in the listing) with the solution from *Structural problem* are the choices of the iterative solver and the smoother, and the block size.

Listing 2.12: The source code for the solution of the CoupCons3D problem.

```
#include <vector>
#include <iostream>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/ilu0.hpp>
#include <amgcl/solver/bicgstab.hpp>
#include <amgcl/value_type/static_matrix.hpp>
#include <amgcl/adapter/block_matrix.hpp>

#include <amgcl/io/mm.hpp>
#include <amgcl/profiler.hpp>

int main(int argc, char *argv[]) {
    // The command line should contain the matrix file name:
    if (argc < 2) {
        std::cerr << "Usage: " << argv[0] << " <matrix.mtx>" << std::endl;
        return 1;
    }

    // The profiler:
    amgcl::profiler<> prof("Serena");

    // Read the system matrix:
    ptrdiff_t rows, cols;
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val;

    prof.tic("read");
    std::tie(rows, cols) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // The RHS is filled with ones:
    std::vector<double> f(rows, 1.0);

    // Scale the matrix so that it has the unit diagonal.
    // First, find the diagonal values:
    std::vector<double> D(rows, 1.0);
```

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```
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            if (col[j] == i) {
                D[i] = 1 / sqrt(val[j]);
                break;
            }
        }
    }

    // Then, apply the scaling in-place:
    for(ptrdiff_t i = 0; i < rows; ++i) {
        for(ptrdiff_t j = ptr[i], e = ptr[i+1]; j < e; ++j) {
            val[j] *= D[i] * D[col[j]];
        }
        f[i] *= D[i];
    }

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::static_matrix<double, 4, 4> dmat_type; // matrix value type in␣
↪double precision
    typedef amgcl::static_matrix<double, 4, 1> dvec_type; // the corresponding vector␣
↪value type
    typedef amgcl::static_matrix<float,  4, 4> smat_type; // matrix value type in␣
↪single precision

    typedef amgcl::backend::builtin<dmat_type> SBackend; // the solver backend
    typedef amgcl::backend::builtin<smat_type> PBackend; // the preconditioner backend

    typedef amgcl::make_solver<
        amgcl::amg<
            PBackend,
            amgcl::coarsening::smoothed_aggregation,
            amgcl::relaxation::ilu0
            >,
        amgcl::solver::bicgstab<SBackend>
        > Solver;

    // Initialize the solver with the system matrix.
    // Use the block_matrix adapter to convert the matrix into
    // the block format on the fly:
    prof.tic("setup");
    auto Ab = amgcl::adapter::block_matrix<dmat_type>(A);
    Solver solve(Ab);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    std::vector<double> x(rows, 0.0);
```

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```
97
98      // Reinterpret both the RHS and the solution vectors as block-valued:
99      auto f_ptr = reinterpret_cast<dvec_type*>(f.data());
100     auto x_ptr = reinterpret_cast<dvec_type*>(x.data());
101     auto F = amgcl::make_iterator_range(f_ptr, f_ptr + rows / 4);
102     auto X = amgcl::make_iterator_range(x_ptr, x_ptr + rows / 4);
103
104     prof.tic("solve");
105     std::tie(iters, error) = solve(Ab, F, X);
106     prof.toc("solve");
107
108     // Output the number of iterations, the relative error,
109     // and the profiling data:
110     std::cout << "Iters: " << iters << std::endl
111               << "Error: " << error << std::endl
112               << prof << std::endl;
113 }
```

The output from the compiled program is given below. The main improvement here is the reduced memory footprint of the single-precision preconditioner: it takes 279.83M as opposed to 525.68M in the full precision case. The setup and the solution are slightly faster as well:

```
$ ./coupcons3d CoupCons3D.mtx
Matrix CoupCons3D.mtx: 416800x416800
Solver
======
Type:             BiCGStab
Unknowns:         104200
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.18
Grid complexity:     1.11
Memory footprint:    279.83 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       104200        1395146    237.27 M (84.98%)
    1        10365         235821     37.27 M (14.36%)
    2          600          10792      5.29 M ( 0.66%)

Iters: 4
Error: 2.90462e-09

[Serena:     14.415 s] (100.00%)
[ self:       0.057 s] (  0.39%)
[  read:     13.426 s] ( 93.14%)
[  setup:     0.345 s] (  2.39%)
[  solve:     0.588 s] (  4.08%)
```

We can also use the VexCL backend to accelerate the solution using the GPU. Again, this is very close to the approach described in *Structural problem* (see tutorial/3.CoupCons3D/coupcons3d_vexcl.cpp). However, the ILU(0) relaxation is an intrinsically serial algorithm, and is not effective with the fine grained parallelism of the GPU. Instead, the solutions of the lower and upper parts of the incomplete LU decomposition in AMGCL are approximated with several Jacobi iterations [ChPa15]. This makes the relaxation relatively more expensive than on the CPU, and the speedup

from using the GPU backend is not as prominent:

```
$ ./coupcons3d_vexcl_cuda CoupCons3D.mtx
1. GeForce GTX 1050 Ti

Matrix CoupCons3D.mtx: 416800x416800
Solver
======
Type:             BiCGStab
Unknowns:         104200
Memory footprint: 22.26 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.18
Grid complexity:     1.11
Memory footprint:    281.49 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       104200        1395146    238.79 M (84.98%)
    1        10365         235821     37.40 M (14.36%)
    2          600          10792      5.31 M ( 0.66%)

Iters: 5
Error: 6.30647e-09

[Serena:          14.432 s] (100.00%)
[ self:            0.060 s] (  0.41%)
[  GPU matrix:     0.213 s] (  1.47%)
[  read:          13.381 s] ( 92.72%)
[  setup:          0.549 s] (  3.81%)
[  solve:          0.229 s] (  1.59%)
```

Note: We used the fact that the matrix size is divisible by 4 in order to use the block-valued backend. If it was not the case, we could use the Schur pressure correction preconditioner to split the matrix into two large subsystems, and use the block-valued solver for the upper left subsystem. See an example of such a solution in tutorial/3.CoupCons3D/coupcons3d_spc.cpp. The performance is worse than what we were able to achive above, but still is better than the first working version:

```
$ ./coupcons3d_spc CoupCons3D.mtx 333440
Matrix CoupCons3D.mtx: 416800x416800
Solver
======
Type:             BiCGStab
Unknowns:         416800
Memory footprint: 22.26 M

Preconditioner
==============
Schur complement (two-stage preconditioner)
  Unknowns: 416800(83360)
  Nonzeros: 22322336
  Memory:  549.90 M

[ U ]
```

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```
Solver
======
Type:             PreOnly
Unknowns:         83360
Memory footprint: 0.00 B

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.21
Grid complexity:     1.23
Memory footprint:    206.09 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        83360        1082798    167.26 M (82.53%)
    1        14473         184035     28.49 M (14.03%)
    2         4105          39433      6.04 M ( 3.01%)
    3          605           5761      4.30 M ( 0.44%)


[ P ]
Solver
======
Type:             PreOnly
Unknowns:         83360
Memory footprint: 0.00 B

Preconditioner
==============
Relaxation as preconditioner
  Unknowns: 83360
  Nonzeros: 2332064
  Memory:   27.64 M


Iters: 7
Error: 5.0602e-09

[CoupCons3D:    14.427 s] (100.00%)
[  read:        13.010 s] ( 90.18%)
[  setup:        0.336 s] (  2.33%)
[  solve:        1.079 s] (  7.48%)
```

2.4.6 Stokes-like problem

In this section we consider a saddle point system which was obtained by discretization of the steady incompressible Stokes flow equations in a unit cube with a locally divergence-free weak Galerkin finite element method. The UCube(4) system studied here may be downloaded from the the dataset accompanying the paper [DeMW20]. We will use the UCube(4) system from the dataset. The system matrix is symmetric and has 554,496 rows and 14,292,884 nonzero values, which corresponds to an average of 26 nonzero entries per row. The matrix sparsity portrait is shown on the figure below.

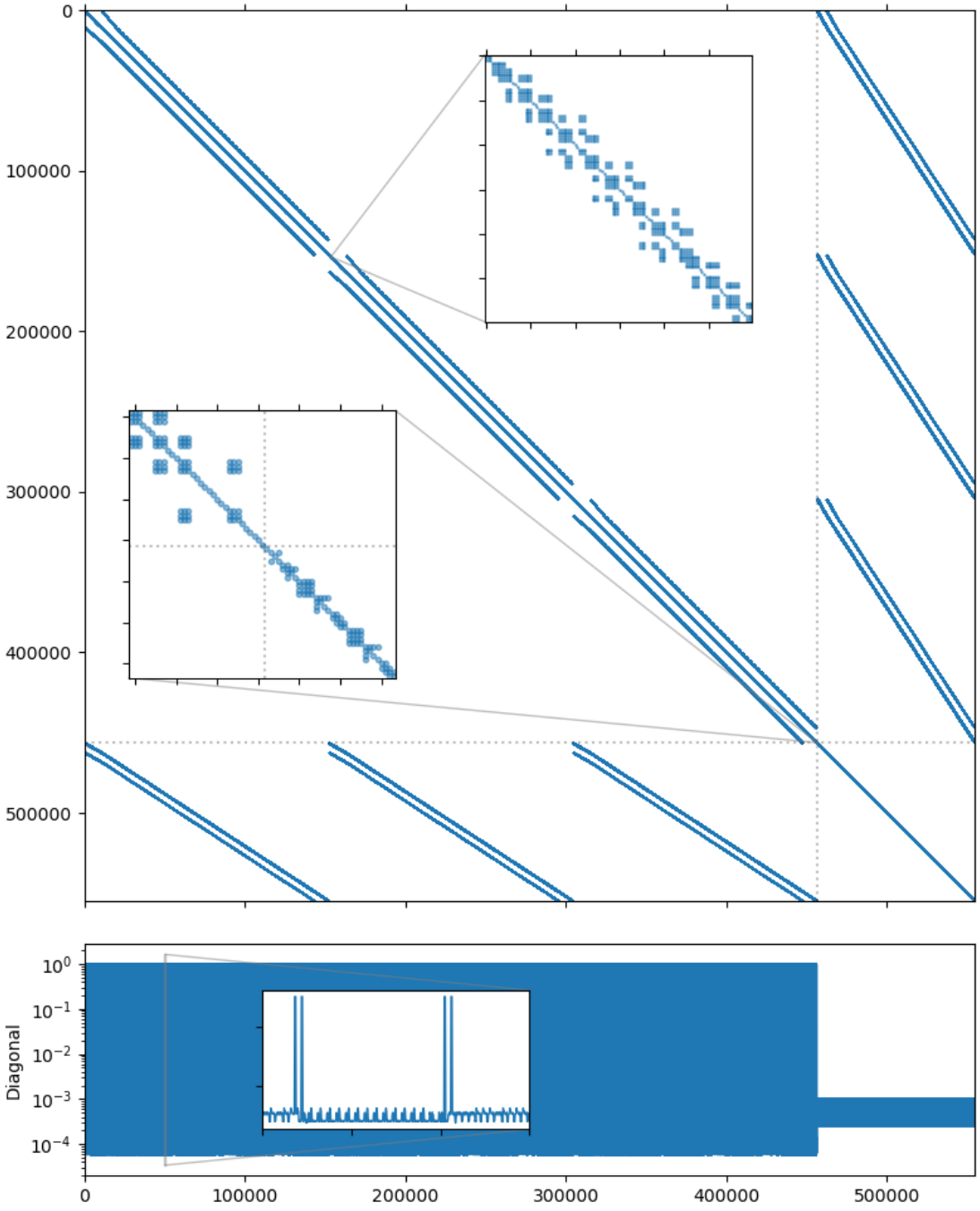

Fig. 2.6: UCube(4) matrix portrait

As with any Stokes-like problem, the system has a general block-wise structure:

$$\begin{bmatrix} A & B_1^T \\ B_2 & C \end{bmatrix} \begin{bmatrix} \mathbf{x}_u \\ \mathbf{x}_p \end{bmatrix} = \begin{bmatrix} \mathbf{b}_u \\ \mathbf{b}_p \end{bmatrix}$$

In this case, the upper left subblock A corresponds the the flow unknowns, and itself has block-wise structure with small 3×3 blocks. The lower right subblock C corresponds to the pressure unknowns. There is a lot of research dedicated to the efficient solution of such systems, see [BeGL05] for an extensive overview. The direct approach of using a monolithic preconditioner usually does not work very well, but we may try it to have a reference point. The AMG preconditioning does not yield a converging solution, but a single level ILU(0) relaxation seems to work with a CG iterative solver:

```
$ solver -B -A ucube_4_A.bin -f ucube_4_b.bin \
      solver.type=cg solver.maxiter=500 \
      precond.class=relaxation precond.type=ilu0
Solver
======
Type:             CG
Unknowns:         554496
Memory footprint: 16.92 M

Preconditioner
==============
Relaxation as preconditioner
  Unknowns: 554496
  Nonzeros: 14292884
  Memory:   453.23 M

Iterations: 270
Error:      6.84763e-09

[Profile:       9.300 s] (100.00%)
[  reading:     0.133 s] (  1.43%)
[  setup:       0.561 s] (  6.03%)
[  solve:       8.599 s] ( 92.46%)
```

A preconditioner that takes the structure of the system into account should be a better choice performance-wise. AMGCL provides an implementation of the Schur complement pressure correction preconditioner. The preconditioning step consists of solving two linear systems:

$$\begin{aligned} S\mathbf{x}_p &= \mathbf{b}_p - B_2 A^{-1} \mathbf{b}_u, \\ A\mathbf{x}_u &= \mathbf{b}_u - B_1^T \mathbf{b}_p. \end{aligned} \tag{2.2}$$

Here S is the Schur complement $S = C - B_2 A^{-1} B_1^T$. Note that forming the Schur complement matrix explicitly is prohibitively expensive, and the following approximation is used to create the preconditioner for the first equation in (2.2):

$$\hat{S} = C - \operatorname{diag}\left(B_2 \operatorname{diag}(A)^{-1} B_1^T\right).$$

There is no need to solve the equations (2.2) exactly. It is enough to perform a single application of the corresponding preconditioner as an approximation to S^{-1} and A^{-1}. This means that the overall preconditioner is linear, and we may use a non-flexible iterative solver with it. The approximation matrix $\hat{S}$ has a simple band diagonal structure, and a diagonal SPAI(0) preconditioner should have reasonable performance.

Similar to the examples/solver, the examples/schur_pressure_correction utility allows to play with the Schur pressure correction preconditioner options before trying to write any code. We found that using the non-smoothed aggregation with ILU(0) smoothing on each level for the flow subsystem (`usolver`) and single-level SPAI(0) relaxation for the Schur complement subsystem (`psolver`) works best. We also disable lumping of the diagonal of the A matrix in

the Schur complement approximation with the `precond.simplec_dia=false` option, and enable block-valued backend for the flow susbsystem with the `--ub 3` option. The `-m '>456192'` option sets the pressure mask pattern. It tells the solver that all unknowns starting with the 456192-th belong to the pressure subsystem:

```
$ schur_pressure_correction -B -A ucube_4_A.bin -f ucube_4_b.bin -m '>456192' \
    -p solver.type=cg solver.maxiter=200 \
       precond.simplec_dia=false \
       precond.usolver.solver.type=preonly \
       precond.usolver.precond.coarsening.type=aggregation \
       precond.usolver.precond.relax.type=ilu0 \
       precond.psolver.solver.type=preonly \
       precond.psolver.precond.class=relaxation \
       --ub 3
Solver
======
Type:             CG
Unknowns:         554496
Memory footprint: 16.92 M

Preconditioner
==============
Schur complement (two-stage preconditioner)
  Unknowns: 554496(98304)
  Nonzeros: 14292884
  Memory:  587.45 M

[ U ]
Solver
======
Type:             PreOnly
Unknowns:         152064
Memory footprint: 0.00 B

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.25
Grid complexity:     1.14
Memory footprint:    233.07 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       152064         982416    188.13 M (80.25%)
    1        18654         197826     35.07 M (16.16%)
    2         2619          35991      6.18 M ( 2.94%)
    3          591           7953      3.69 M ( 0.65%)


[ P ]
Solver
======
Type:             PreOnly
Unknowns:         98304
Memory footprint: 0.00 B

Preconditioner
==============
Relaxation as preconditioner
```

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```
  Unknowns: 98304
  Nonzeros: 274472
  Memory:   5.69 M


Iterations: 35
Error:      8.57921e-09

[Profile:                3.872 s] (100.00%)
[  reading:              0.131 s] (  3.38%)
[  schur_complement:     3.741 s] ( 96.62%)
[   self:                0.031 s] (  0.79%)
[    setup:              0.301 s] (  7.78%)
[    solve:              3.409 s] ( 88.05%)
```

Lets see how this translates to the code. Below is the complete listing of the solver (tutorial/4.Stokes/stokes_ucube.cpp) which uses the mixed precision approach.

Listing 2.13: The source code for the solution of the UCube(4) problem.

```
#include <iostream>
#include <string>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/value_type/static_matrix.hpp>
#include <amgcl/adapter/block_matrix.hpp>
#include <amgcl/preconditioner/schur_pressure_correction.hpp>
#include <amgcl/make_solver.hpp>
#include <amgcl/make_block_solver.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/solver/cg.hpp>
#include <amgcl/solver/preonly.hpp>
#include <amgcl/coarsening/aggregation.hpp>
#include <amgcl/relaxation/ilu0.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/relaxation/as_preconditioner.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

//---------------------------------------------------------------------------
int main(int argc, char *argv[]) {
    // The command line should contain the matrix and the RHS file names,
    // and the number of unknowns in the flow subsytem:
    if (argc < 4) {
        std::cerr << "Usage: " << argv[0] << " <matrix.bin> <rhs.bin> <nu>" <<␣
↪std::endl;
        return 1;
    }

    // The profiler:
    amgcl::profiler<> prof("UCube4");

    // Read the system matrix:
    ptrdiff_t rows, cols;
```

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```
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val, rhs;

    prof.tic("read");
    amgcl::io::read_crs(argv[1], rows, ptr, col, val);
    amgcl::io::read_dense(argv[2], rows, cols, rhs);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
    std::cout << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // The number of unknowns in the U subsystem
    ptrdiff_t nu = std::stoi(argv[3]);

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::backend::builtin<double> SBackend; // the outer iterative solver␣
↪backend
    typedef amgcl::backend::builtin<float> PBackend;  // the PSolver backend
    typedef amgcl::backend::builtin<
        amgcl::static_matrix<float,3,3>> UBackend;    // the USolver backend

    typedef amgcl::make_solver<
        amgcl::preconditioner::schur_pressure_correction<
            amgcl::make_block_solver<
                amgcl::amg<
                    UBackend,
                    amgcl::coarsening::aggregation,
                    amgcl::relaxation::ilu0
                    >,
                amgcl::solver::preonly<UBackend>
                >,
            amgcl::make_solver<
                amgcl::relaxation::as_preconditioner<
                    PBackend,
                    amgcl::relaxation::spai0
                    >,
                amgcl::solver::preonly<PBackend>
                >
            >,
        amgcl::solver::cg<SBackend>
        > Solver;

    // Solver parameters
    Solver::params prm;
    prm.precond.simplec_dia = false;
    prm.precond.pmask.resize(rows);
    for(ptrdiff_t i = 0; i < rows; ++i) prm.precond.pmask[i] = (i >= nu);

    // Initialize the solver with the system matrix.
    prof.tic("setup");
    Solver solve(A, prm);
    prof.toc("setup");

```

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```
92      // Show the mini-report on the constructed solver:
93      std::cout << solve << std::endl;
94
95      // Solve the system with the zero initial approximation:
96      int iters;
97      double error;
98      std::vector<double> x(rows, 0.0);
99      prof.tic("solve");
100     std::tie(iters, error) = solve(A, rhs, x);
101     prof.toc("solve");
102
103     // Output the number of iterations, the relative error,
104     // and the profiling data:
105     std::cout << "Iters: " << iters << std::endl
106               << "Error: " << error << std::endl
107               << prof << std::endl;
108 }
```

Schur pressure correction is composite preconditioner. Its definition includes definition of two nested iterative solvers, one for the "flow" (U) subsystem, and the other for the "pressure" (P) subsystem. In lines 55–58 we define the backends used in the outer iterative solver, and in the two nested solvers. Note that both backends for nested solvers use single precision values, and the flow subsystem backend has block value type:

```
55      typedef amgcl::backend::builtin<double> SBackend; // the outer iterative solver␣
↪backend
56      typedef amgcl::backend::builtin<float> PBackend;  // the PSolver backend
57      typedef amgcl::backend::builtin<
58          amgcl::static_matrix<float,3,3>> UBackend;    // the USolver backend
```

In lines 60-79 we define the solver type. The flow solver is defined in lines 62-69, and the pressure solver – in lines 70–77. Both are using *amgcl::solver::preonly* as "iterative" solver, which in fact only applies the specified preconditioner once. The flow solver is defined with *amgcl::make_block_solver*, which automatically converts its input matrix A to the block format during the setup and reinterprets the scalar RHS and solution vectors as having block values during solution:

```
60      typedef amgcl::make_solver<
61          amgcl::preconditioner::schur_pressure_correction<
62              amgcl::make_block_solver<
63                  amgcl::amg<
64                      UBackend,
65                      amgcl::coarsening::aggregation,
66                      amgcl::relaxation::ilu0
67                      >,
68                  amgcl::solver::preonly<UBackend>
69                  >,
70              amgcl::make_solver<
71                  amgcl::relaxation::as_preconditioner<
72                      PBackend,
73                      amgcl::relaxation::spai0
74                      >,
75                  amgcl::solver::preonly<PBackend>
76                  >
77              >,
78          amgcl::solver::cg<SBackend>
79          > Solver;
```

In the solver parameters we disable lumping of the matrix A diagonal for the Schur complement approimation (line

83) and fill the pressure mask to indicate which unknowns correspond to the pressure subsystem (lines 84–85):

```
81      // Solver parameters
82      Solver::params prm;
83      prm.precond.simplec_dia = false;
84      prm.precond.pmask.resize(rows);
85      for(ptrdiff_t i = 0; i < rows; ++i) prm.precond.pmask[i] = (i >= nu);
```

Here is the output from the compiled program. The preconditioner uses 398M or memory, as opposed to 587M in the case of the full precision preconditioner used in the examples/schur_pressure_correction, and both the setup and the solution are about 50% faster due to the use of the mixed precision approach:

```
$ ./stokes_ucube ucube_4_A.bin ucube_4_b.bin 456192
Matrix ucube_4_A.bin: 554496x554496
RHS ucube_4_b.bin: 554496x1
Solver
======
Type:             CG
Unknowns:         554496
Memory footprint: 16.92 M

Preconditioner
==============
Schur complement (two-stage preconditioner)
  Unknowns: 554496(98304)
  Nonzeros: 14292884
  Memory:  398.39 M

[ U ]
Solver
======
Type:             PreOnly
Unknowns:         152064
Memory footprint: 0.00 B

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.25
Grid complexity:     1.14
Memory footprint:    130.49 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       152064         982416    105.64 M (80.25%)
    1        18654         197826     19.56 M (16.16%)
    2         2619          35991      3.44 M ( 2.94%)
    3          591           7953      1.85 M ( 0.65%)


[ P ]
Solver
======
Type:             PreOnly
Unknowns:         98304
Memory footprint: 0.00 B

Preconditioner
```

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```
==============
Relaxation as preconditioner
  Unknowns: 98304
  Nonzeros: 274472
  Memory:   4.27 M


Iters: 35
Error: 8.57996e-09

[UCube4:      2.502 s] (100.00%)
[  read:      0.129 s] (  5.16%)
[  setup:     0.240 s] (  9.57%)
[  solve:     2.132 s] ( 85.19%)
```

Converting the solver to the VexCL backend in order to accelerate the solution with GPGPU is straightforward. Below is the complete source code of the solver (tutorial/4.Stokes/stokes_ucube_vexcl.cpp), with the differences between the OpenMP and the VexCL versions highlighted. Note that the GPU version of the ILU(0) smoother approximates the lower and upper triangular solves in the incomplete LU decomposition with a couple of Jacobi iterations [ChPa15]. Here we set the number of iterations to 4 (line 94).

Listing 2.14: The source code for the solution of the UCube(4) problem with the VexCL backend.

```
1  #include <iostream>
2  #include <string>
3
4  #include <amgcl/backend/vexcl.hpp>
5  #include <amgcl/backend/vexcl_static_matrix.hpp>
6  #include <amgcl/adapter/crs_tuple.hpp>
7  #include <amgcl/value_type/static_matrix.hpp>
8  #include <amgcl/adapter/block_matrix.hpp>
9  #include <amgcl/preconditioner/schur_pressure_correction.hpp>
10 #include <amgcl/make_solver.hpp>
11 #include <amgcl/make_block_solver.hpp>
12 #include <amgcl/amg.hpp>
13 #include <amgcl/solver/cg.hpp>
14 #include <amgcl/solver/preonly.hpp>
15 #include <amgcl/coarsening/aggregation.hpp>
16 #include <amgcl/relaxation/ilu0.hpp>
17 #include <amgcl/relaxation/spai0.hpp>
18 #include <amgcl/relaxation/as_preconditioner.hpp>
19
20 #include <amgcl/io/binary.hpp>
21 #include <amgcl/profiler.hpp>
22
23 //---------------------------------------------------------------------------
24 int main(int argc, char *argv[]) {
25     // The command line should contain the matrix and the RHS file names,
26     // and the number of unknowns in the flow subsytem:
27     if (argc < 4) {
28         std::cerr << "Usage: " << argv[0] << " <matrix.bin> <rhs.bin> <nu>" <<␣
   ↪std::endl;
29         return 1;
30     }
31
```

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```
    // Create VexCL context. Set the environment variable OCL_DEVICE to
    // control which GPU to use in case multiple are available,
    // and use single device:
    vex::Context ctx(vex::Filter::Env && vex::Filter::Count(1));
    std::cout << ctx << std::endl;

    // Enable support for block-valued matrices in the VexCL kernels:
    vex::scoped_program_header header(ctx, amgcl::backend::vexcl_static_matrix_
↪declaration<float,3>());

    // The profiler:
    amgcl::profiler<> prof("UCube4 (VexCL)");

    // Read the system matrix:
    ptrdiff_t rows, cols;
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val, rhs;

    prof.tic("read");
    amgcl::io::read_crs(argv[1], rows, ptr, col, val);
    amgcl::io::read_dense(argv[2], rows, cols, rhs);
    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
    std::cout << "RHS " << argv[2] << ": " << rows << "x" << cols << std::endl;
    prof.toc("read");

    // The number of unknowns in the U subsystem
    ptrdiff_t nu = std::stoi(argv[3]);

    // We use the tuple of CRS arrays to represent the system matrix.
    // Note that std::tie creates a tuple of references, so no data is actually
    // copied here:
    auto A = std::tie(rows, ptr, col, val);

    // Compose the solver type
    typedef amgcl::backend::vexcl<double> SBackend; // the outer iterative solver␣
↪backend
    typedef amgcl::backend::vexcl<float>  PBackend; // the PSolver backend
    typedef amgcl::backend::vexcl<
        amgcl::static_matrix<float,3,3>> UBackend;    // the USolver backend

    typedef amgcl::make_solver<
        amgcl::preconditioner::schur_pressure_correction<
            amgcl::make_block_solver<
                amgcl::amg<
                    UBackend,
                    amgcl::coarsening::aggregation,
                    amgcl::relaxation::ilu0
                    >,
                amgcl::solver::preonly<UBackend>
                >,
            amgcl::make_solver<
                amgcl::relaxation::as_preconditioner<
                    PBackend,
                    amgcl::relaxation::spai0
                    >,
                amgcl::solver::preonly<PBackend>
                >
```

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```
            >,
        amgcl::solver::cg<SBackend>
        > Solver;

    // Solver parameters
    Solver::params prm;
    prm.precond.simplec_dia = false;
    prm.precond.usolver.precond.relax.solve.iters = 4;
    prm.precond.pmask.resize(rows);
    for(ptrdiff_t i = 0; i < rows; ++i) prm.precond.pmask[i] = (i >= nu);

    // Set the VexCL context in the backend parameters
    SBackend::params bprm;
    bprm.q = ctx;

    // Initialize the solver with the system matrix.
    prof.tic("setup");
    Solver solve(A, prm, bprm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    std::cout << solve << std::endl;

    // Since we are using mixed precision, we have to transfer the system matrix to the GPU:
    prof.tic("GPU matrix");
    auto A_gpu = SBackend::copy_matrix(std::make_shared<amgcl::backend::crs<double>>(A), bprm);
    prof.toc("GPU matrix");

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    vex::vector<double> f(ctx, rhs);
    vex::vector<double> x(ctx, rows);
    x = 0.0;

    prof.tic("solve");
    std::tie(iters, error) = solve(*A_gpu, f, x);
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    std::cout << "Iters: " << iters << std::endl
              << "Error: " << error << std::endl
              << prof << std::endl;
}
```

The output of the VexCL version is shown below. The solution phase is about twice as fast as the OpenMP version:

```
$ ./stokes_ucube_vexcl_cuda ucube_4_A.bin ucube_4_b.bin 456192
1. GeForce GTX 1050 Ti

Matrix ucube_4_A.bin: 554496x554496
RHS ucube_4_b.bin: 554496x1
Solver
======
```

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```
Type:             CG
Unknowns:         554496
Memory footprint: 16.92 M

Preconditioner
==============
Schur complement (two-stage preconditioner)
  Unknowns: 554496(98304)
  Nonzeros: 14292884
  Memory:  399.66 M

[ U ]
Solver
======
Type:             PreOnly
Unknowns:         152064
Memory footprint: 0.00 B

Preconditioner
==============
Number of levels:    4
Operator complexity: 1.25
Grid complexity:     1.14
Memory footprint:    131.76 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0       152064         982416    106.76 M (80.25%)
    1        18654         197826     19.68 M (16.16%)
    2         2619          35991      3.45 M ( 2.94%)
    3          591           7953      1.86 M ( 0.65%)


[ P ]
Solver
======
Type:             PreOnly
Unknowns:         98304
Memory footprint: 0.00 B

Preconditioner
==============
Relaxation as preconditioner
  Unknowns: 98304
  Nonzeros: 274472
  Memory:   4.27 M


Iters: 36
Error: 7.26253e-09

[UCube4 (VexCL):   1.858 s] (100.00%)
[ self:            0.004 s] (  0.20%)
[  GPU matrix:     0.213 s] ( 11.46%)
[  read:           0.128 s] (  6.87%)
[  setup:          0.519 s] ( 27.96%)
[  solve:          0.994 s] ( 53.52%)
```

2.4.7 Using near null-space vectors

Using near null-space vectors may greately improve the quality of the aggregation AMG preconditioner. For the elasticity or structural problems the near-null space vectors may be computed as rigid body modes from the coordinates of the discretization grid nodes. In this tutorial we will use the system obtained by discretization of a 3D elasticity problem modeling a connecting rod:

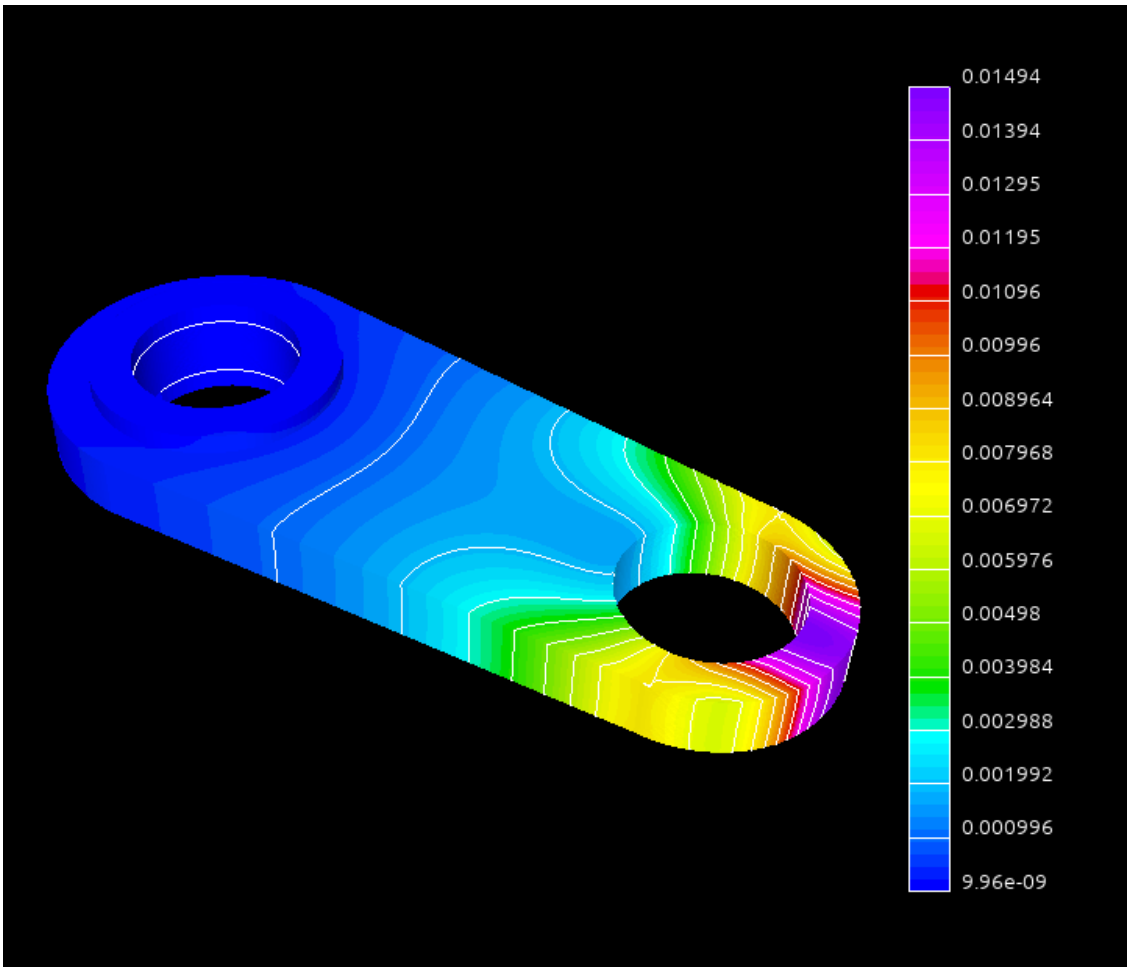

Fig. 2.7: The connecting rod geometry with the computed displacements

The dataset was kindly provided by David Herrero Pérez (@davidherreroperez) in the issue #135 on Github and is available for download at doi:10.5281/zenodo.4299865. The system matrix is symmetric, has block structure with small 3×3 blocks, and has 81,657 rows and 3,171,111 nonzero values (about 39 nonzero entries per row on average). The matrix portrait is shown on the figure below:

It is possible to solve the system using the CG iterative solver preconditioned with the smoothed aggregation AMG, but the convergence is not that great:

```
$ solver -A A.mtx -f b.mtx solver.type=cg solver.maxiter=1000
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M
```

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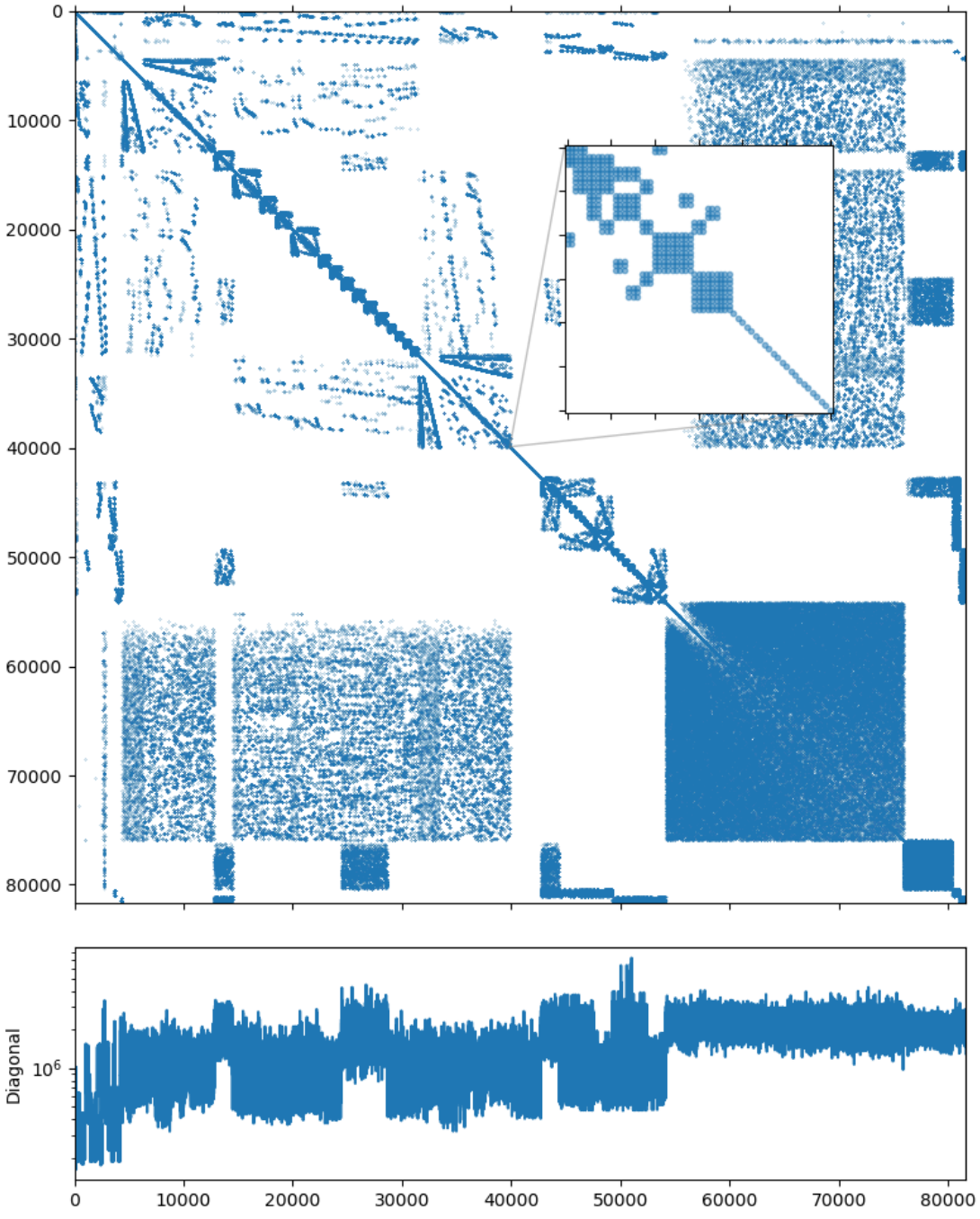

Fig. 2.8: The nonzero portrait of the connecting rod system.

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```
Preconditioner
==============
Number of levels:    3
Operator complexity: 1.14
Grid complexity:     1.07
Memory footprint:    70.09 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     62.49 M (87.98%)
    1         5067         417837      7.16 M (11.59%)
    2          305          15291    450.07 K ( 0.42%)

Iterations: 698
Error:      8.96391e-09

[Profile:      11.717 s] (100.00%)
[  reading:     2.123 s] ( 18.12%)
[  setup:       0.122 s] (  1.04%)
[  solve:       9.472 s] ( 80.84%)
```

We can improve the solution time by taking the block structure of the system into account in the aggregation algorithm:

```
$ solver -A A.mtx -f b.mtx solver.type=cg solver.maxiter=1000 \
      precond.coarsening.aggr.block_size=3
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.29
Grid complexity:     1.10
Memory footprint:    92.40 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     75.83 M (77.71%)
    1         7773         858051     15.70 M (21.03%)
    2          555          51327    890.16 K ( 1.26%)

Iterations: 197
Error:      8.76043e-09

[Profile:       5.525 s] (100.00%)
[  reading:     2.170 s] ( 39.28%)
[  setup:       0.173 s] (  3.14%)
[  solve:       3.180 s] ( 57.56%)
```

However, since this is an elasticity problem and we know the coordinates for the discretization mesh, we can compute the rigid body modes and provide them as the near null-space vectors for the smoothed aggregation AMG method. AMGCL has a convenience function `amgcl::coarsening::rigid_body_modes()` that takes the 2D or 3D coordinates and converts them into the rigid body modes. The examples/solver utility allows to specify the file con-

taining the coordinates on the command line:

```
$ solver -A A.mtx -f b.mtx solver.type=cg \
      precond.coarsening.aggr.eps_strong=0 -C C.mtx
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    132.15 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111    102.70 M (65.77%)
    1         7704        1640736     29.33 M (34.03%)
    2          144           9576    122.07 K ( 0.20%)

Iterations: 63
Error:      8.4604e-09

[Profile:       3.764 s] (100.00%)
[  reading:     2.217 s] ( 58.89%)
[  setup:       0.350 s] (  9.30%)
[  solve:       1.196 s] ( 31.78%)
```

In the 3D case we get 6 near null-space vectors corresponding to the rigid body modes. Note that this makes the preconditioner more expensive memory-wise: the memory footprint of the preconditioner has increased to 132M from 70M in the simplest case and 92M in the case using the block structure of the matrix. But this pays up in terms of performance: the number of iterations dropped from 197 to 63 and the solution time decreased from 3.2 seconds to 1.2 seconds.

In principle, it is also possible to approximate the near null-space vectors by solving the homogeneous system $Ax = 0$, starting with a random initial solution x. We may use the computed x as a near-null space vector, solve the homogeneous system again from a different random start, and do this until we have enough near null-space vectors. The examples/ns_search.cpp example shows how to do this. However, this process is quite expensive, because we need to solve the system multiple times, starting with a badly tuned solver at that. It is probably only worth the time in case one needs to solve the same system efficiently for multiple right-hand side vectors. Below is an example of searching for the 6 near null-space vectors:

```
$ ns_search -A A.mtx -f b.mtx solver.type=cg solver.maxiter=1000 \
      precond.coarsening.aggr.eps_strong=0 -n6 -o N6.mtx

-------------------------
-- Searching for vector 0
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M
```

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```
Preconditioner
==============
Number of levels:    2
Operator complexity: 1.01
Grid complexity:     1.02
Memory footprint:    62.79 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     60.56 M (98.58%)
    1         1284          45576      2.24 M ( 1.42%)

Iterations: 932
Error:      8.66233e-09

-------------------------
-- Searching for vector 1
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    2
Operator complexity: 1.01
Grid complexity:     1.02
Memory footprint:    62.79 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     60.56 M (98.58%)
    1         1284          45576      2.24 M ( 1.42%)

Iterations: 750
Error:      9.83476e-09

-------------------------
-- Searching for vector 2
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    2
Operator complexity: 1.06
Grid complexity:     1.03
Memory footprint:    76.72 M

level     unknowns       nonzeros      memory
---------------------------------------------
```

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```
    0        81657        3171111     68.98 M (94.56%)
    1         2568         182304      7.74 M ( 5.44%)

Iterations: 528
Error:      8.74633e-09

-------------------------
-- Searching for vector 3
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.13
Grid complexity:     1.05
Memory footprint:    84.87 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     77.41 M (88.49%)
    1         3852         410184      7.42 M (11.45%)
    2           72           2394     31.36 K ( 0.07%)

Iterations: 391
Error:      9.04425e-09

-------------------------
-- Searching for vector 4
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.23
Grid complexity:     1.06
Memory footprint:    99.01 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     85.84 M (81.22%)
    1         5136         729216     13.11 M (18.68%)
    2           96           4256     55.00 K ( 0.11%)

Iterations: 238
Error:      9.51092e-09

-------------------------
```

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```
-- Searching for vector 5
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.36
Grid complexity:     1.08
Memory footprint:    114.78 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     94.27 M (73.45%)
    1         6420        1139400     20.42 M (26.39%)
    2          120           6650     85.24 K ( 0.15%)

Iterations: 175
Error:      9.43207e-09

-------------------------
-- Solving the system
-------------------------
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    132.15 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111    102.70 M (65.77%)
    1         7704        1640736     29.33 M (34.03%)
    2          144           9576    122.07 K ( 0.20%)

Iterations: 100
Error:      8.14427e-09

[Profile:         48.503 s] (100.00%)
[  apply:          2.373 s] (  4.89%)
[    setup:        0.422 s] (  0.87%)
[    solve:        1.949 s] (  4.02%)
[  read:           2.113 s] (  4.36%)
[  search:        43.713 s] ( 90.12%)
[    vector 0:    12.437 s] ( 25.64%)
[      setup:      0.101 s] (  0.21%)
```

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```
[      solve:     12.335 s] ( 25.43%)
[    vector 1:     9.661 s] ( 19.92%)
[      setup:      0.115 s] (  0.24%)
[      solve:      9.545 s] ( 19.68%)
[    vector 2:     7.584 s] ( 15.64%)
[      setup:      0.217 s] (  0.45%)
[      solve:      7.365 s] ( 15.18%)
[    vector 3:     6.137 s] ( 12.65%)
[      setup:      0.180 s] (  0.37%)
[      solve:      5.954 s] ( 12.28%)
[    vector 4:     4.353 s] (  8.97%)
[      setup:      0.246 s] (  0.51%)
[      solve:      4.100 s] (  8.45%)
[    vector 5:     3.541 s] (  7.30%)
[      setup:      0.337 s] (  0.69%)
[      solve:      3.200 s] (  6.60%)
[  write:          0.303 s] (  0.63%)
```

Note that the number of iterations required to find the next vector is gradually decreasing, as the quality of the solver increases. The 6 orthogonalized vectors are saved to the output file `N6.mtx` and are also used to solve the original system. We can also use the file with the examples/solver:

```
$ solver -A A.mtx -f b.mtx solver.type=cg \
      precond.coarsening.aggr.eps_strong=0 -N N6.mtx
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    132.15 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111    102.70 M (65.77%)
    1         7704        1640736     29.33 M (34.03%)
    2          144           9576    122.07 K ( 0.20%)

Iterations: 100
Error:      8.14427e-09

[Profile:       4.736 s] (100.00%)
[  reading:     2.407 s] ( 50.83%)
[  setup:       0.354 s] (  7.47%)
[  solve:       1.974 s] ( 41.69%)
```

This is an improvement with respect to the version that only uses the blockwize structure of the matrix, but is about 50% less effective than the version using the grid coordinates in order to compute the rigid body modes.

The listing below shows the complete source code computing the near null-space vectors from the mesh coordinates and using the vectors in order to improve the quality of the preconditioner. We include the `<amgcl/coarsening/rigid_body_modes.hpp>` header to bring the definition of the

`amgcl::coarsening::rigid_body_modes()` function in line 9, and use the function to convert the 3D coordinates into the 6 near null-space vectors (rigid body modes) in lines 65–66. In lines 37–38 we check that the coordinate file has the correct dimensions (since each grid node has three displacement components associated with the node, the coordinate file should have three times less rows than the system matrix). The rest of the code should be quite familiar.

Listing 2.15: The solution of the connecting rod problem using the near null-space vectors.

```
1  #include <vector>
2  #include <iostream>
3
4  #include <amgcl/backend/builtin.hpp>
5  #include <amgcl/adapter/crs_tuple.hpp>
6  #include <amgcl/make_solver.hpp>
7  #include <amgcl/amg.hpp>
8  #include <amgcl/coarsening/smoothed_aggregation.hpp>
9  #include <amgcl/coarsening/rigid_body_modes.hpp>
10 #include <amgcl/relaxation/spai0.hpp>
11 #include <amgcl/solver/cg.hpp>
12
13 #include <amgcl/io/mm.hpp>
14 #include <amgcl/profiler.hpp>
15
16 int main(int argc, char *argv[]) {
17     // The command line should contain the matrix, the RHS, and the coordinate files:
18     if (argc < 4) {
19         std::cerr << "Usage: " << argv[0] << " <A.mtx> <b.mtx> <coo.mtx>" <<␣
   ↪std::endl;
20         return 1;
21     }
22
23     // The profiler:
24     amgcl::profiler<> prof("Nullspace");
25
26     // Read the system matrix, the RHS, and the coordinates:
27     ptrdiff_t rows, cols, ndim, ncoo;
28     std::vector<ptrdiff_t> ptr, col;
29     std::vector<double> val, rhs, coo;
30
31     prof.tic("read");
32     std::tie(rows, rows) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
33     std::tie(rows, cols) = amgcl::io::mm_reader(argv[2])(rhs);
34     std::tie(ncoo, ndim) = amgcl::io::mm_reader(argv[3])(coo);
35     prof.toc("read");
36
37     amgcl::precondition(ncoo * ndim == rows && (ndim == 2 || ndim == 3),
38             "The coordinate file has wrong dimensions");
39
40     std::cout << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
41     std::cout << "RHS "    << argv[2] << ": " << rows << "x" << cols << std::endl;
42     std::cout << "Coords " << argv[3] << ": " << ncoo << "x" << ndim << std::endl;
43
44     // Declare the solver type
45     typedef amgcl::backend::builtin<double> SBackend; // the solver backend
46     typedef amgcl::backend::builtin<float>  PBackend; // the preconditioner backend
47
48     typedef amgcl::make_solver<
```

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```
        amgcl::amg<
            PBackend,
            amgcl::coarsening::smoothed_aggregation,
            amgcl::relaxation::spai0
            >,
        amgcl::solver::cg<SBackend>
        > Solver;

    // Solver parameters:
    Solver::params prm;
    prm.precond.coarsening.aggr.eps_strong = 0;

    // Convert the coordinates to the rigid body modes.
    // The function returns the number of near null-space vectors
    // (3 in 2D case, 6 in 3D case) and writes the vectors to the
    // std::vector<double> specified as the last argument:
    prm.precond.coarsening.nullspace.cols = amgcl::coarsening::rigid_body_modes(
            ndim, coo, prm.precond.coarsening.nullspace.B);

    // We use the tuple of CRS arrays to represent the system matrix.
    auto A = std::tie(rows, ptr, col, val);

    // Initialize the solver with the system matrix.
    prof.tic("setup");
    Solver solve(A, prm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    std::vector<double> x(rows, 0.0);

    prof.tic("solve");
    std::tie(iters, error) = solve(A, rhs, x);
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    std::cout << "Iters: " << iters << std::endl
              << "Error: " << error << std::endl
              << prof << std::endl;
}
```

The output of the compiled program is shown below:

```
$ ./nullspace A.mtx b.mtx C.mtx
Matrix A.mtx: 81657x81657
RHS b.mtx: 81657x1
Coords C.mtx: 27219x3
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M
```

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```
Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    98.76 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     76.73 M (65.77%)
    1         7704        1640736     21.97 M (34.03%)
    2          144           9576     61.60 K ( 0.20%)

Iters: 63
Error: 8.46024e-09

[Nullspace:     3.653 s] (100.00%)
[  read:        2.173 s] ( 59.48%)
[  setup:       0.326 s] (  8.94%)
[  solve:       1.150 s] ( 31.48%)
```

As was noted above, using the near null-space vectors makes the preconditioner less memory-efficient: since the 6 rigid-body modes are used as null-space vectors, every fine-grid aggregate is converted to 6 unknowns on the coarser level. The following figure shows the structure of the system matrix on the second level of the hierarchy, and it is obvious that the matrix has 6×6 block structure:

It should be possible to represent both the initial matrix and the matrices on each level of the hiearachy using the 3×3 block value type, as we did in the *Structural problem* example. Unfortunaltely, AMGCL is not yet able to utilize near null-space vectors with block-valued backends.

One possible solution to this problem, suggested by Piotr Hellstein (@dokotor) in GitHub issue #215, is to convert the matrices to the block-wise storage format after the hiearchy has been constructed. This has been implemented in form of the *hybrid OpenMP and VexCL backends*.

The listing below shows an example of using the hybrid OpenMP backend (tutorial/5.Nullspace/nullspace_hybrid.cpp). The only difference with the *scalar* code is the definition of the block value type and the use of the hybrid backend (lines 46–49).

Listing 2.16: Using hybrid OpenMP backend while providing near null-space vectors.

```
1  #include <vector>
2  #include <iostream>
3
4  #include <amgcl/backend/builtin_hybrid.hpp>
5  #include <amgcl/value_type/static_matrix.hpp>
6  #include <amgcl/adapter/crs_tuple.hpp>
7  #include <amgcl/make_solver.hpp>
8  #include <amgcl/amg.hpp>
9  #include <amgcl/coarsening/smoothed_aggregation.hpp>
10 #include <amgcl/coarsening/rigid_body_modes.hpp>
11 #include <amgcl/relaxation/spai0.hpp>
12 #include <amgcl/solver/cg.hpp>
13
14 #include <amgcl/io/mm.hpp>
15 #include <amgcl/profiler.hpp>
```

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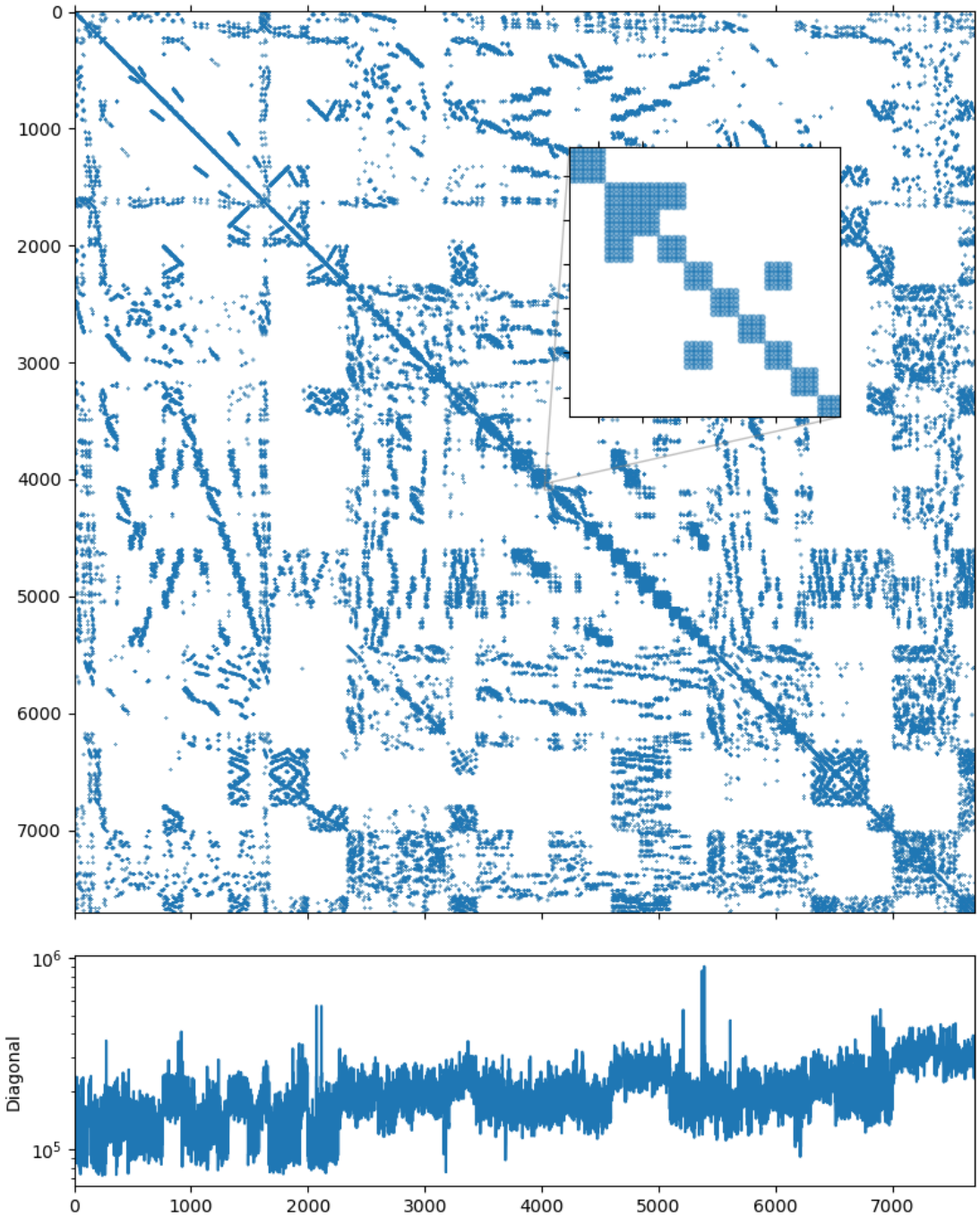

Fig. 2.9: The nonzero portrait of the system matrix on the second level of the AMG hierarchy.

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```
16
17  int main(int argc, char *argv[]) {
18      // The command line should contain the matrix, the RHS, and the coordinate files:
19      if (argc < 4) {
20          std::cerr << "Usage: " << argv[0] << " <A.mtx> <b.mtx> <coo.mtx>" <<␣
    ↪std::endl;
21          return 1;
22      }
23
24      // The profiler:
25      amgcl::profiler<> prof("Nullspace");
26
27      // Read the system matrix, the RHS, and the coordinates:
28      ptrdiff_t rows, cols, ndim, ncoo;
29      std::vector<ptrdiff_t> ptr, col;
30      std::vector<double> val, rhs, coo;
31
32      prof.tic("read");
33      std::tie(rows, rows) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
34      std::tie(rows, cols) = amgcl::io::mm_reader(argv[2])(rhs);
35      std::tie(ncoo, ndim) = amgcl::io::mm_reader(argv[3])(coo);
36      prof.toc("read");
37
38      amgcl::precondition(ncoo * ndim == rows && (ndim == 2 || ndim == 3),
39              "The coordinate file has wrong dimensions");
40
41      std::cout << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
42      std::cout << "RHS "    << argv[2] << ": " << rows << "x" << cols << std::endl;
43      std::cout << "Coords " << argv[3] << ": " << ncoo << "x" << ndim << std::endl;
44
45      // Declare the solver type
46      typedef amgcl::static_matrix<double, 3, 3> DBlock;
47      typedef amgcl::static_matrix<float, 3, 3> FBlock;
48      typedef amgcl::backend::builtin_hybrid<DBlock> SBackend; // the solver backend
49      typedef amgcl::backend::builtin_hybrid<FBlock> PBackend; // the preconditioner␣
    ↪backend
50
51      typedef amgcl::make_solver<
52          amgcl::amg<
53              PBackend,
54              amgcl::coarsening::smoothed_aggregation,
55              amgcl::relaxation::spai0
56              >,
57          amgcl::solver::cg<SBackend>
58          > Solver;
59
60      // Solver parameters:
61      Solver::params prm;
62      prm.precond.coarsening.aggr.eps_strong = 0;
63
64      // Convert the coordinates to the rigid body modes.
65      // The function returns the number of near null-space vectors
66      // (3 in 2D case, 6 in 3D case) and writes the vectors to the
67      // std::vector<double> specified as the last argument:
68      prm.precond.coarsening.nullspace.cols = amgcl::coarsening::rigid_body_modes(
69              ndim, coo, prm.precond.coarsening.nullspace.B);
70
```

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```
    // We use the tuple of CRS arrays to represent the system matrix.
    auto A = std::tie(rows, ptr, col, val);

    // Initialize the solver with the system matrix.
    prof.tic("setup");
    Solver solve(A, prm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
    std::vector<double> x(rows, 0.0);

    prof.tic("solve");
    std::tie(iters, error) = solve(A, rhs, x);
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    std::cout << "Iters: " << iters << std::endl
              << "Error: " << error << std::endl
              << prof << std::endl;
}
```

This results in the following output. Note that the memory footprint of the preconditioner dropped from 98M to 41M (by 58%), and the solution time dropped from 1.150s to 0.707s (by 38%):

```
$ ./nullspace_hybrid A.mtx b.mtx C.mtx
Matrix A.mtx: 81657x81657
RHS b.mtx: 81657x1
Coords C.mtx: 27219x3
Solver
======
Type:             CG
Unknowns:         81657
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    40.98 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        81657        3171111     31.90 M (65.77%)
    1         7704        1640736      9.01 M (34.03%)
    2          144           9576     61.60 K ( 0.20%)

Iters: 63
Error: 8.4562e-09
```

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```
[Nullspace:     3.304 s] (100.00%)
[ self:         0.003 s] (  0.10%)
[  read:        2.245 s] ( 67.94%)
[  setup:       0.349 s] ( 10.57%)
[  solve:       0.707 s] ( 21.38%)
```

Another possible solution is to use a block-valued backend both for constructing the hierarchy and for the solution phase. In order to allow for the coarsening scheme to use the near null-space vectors, the *amgcl::coarsening::as_scalar* coarsening wrapper may be used. The wrapper converts the input matrix to scalar format, applies the base coarsening strategy to the scalar matrix, and converts the computed transfer operators back to block format. This approach results in faster setup times, since every other operation besides coarsening is performed using block arithmetics.

The listing below shows an example of using the *amgcl::coarsening::as_scalar* wrapper (tutorial/5.Nullspace/nullspace_block.cpp). The system matrix is converted to block format in line 78 in the same way it was done in the *Structural problem* tutorial. The RHS and the solution vectors are reinterpreted to contain block values in lines 94-95. The SPAI0 relaxation here resulted in the increased number of interations, so we used the ILU(0) relaxaion.

Listing 2.17: Using *amgcl::coarsening::as_scalar* coarsening wrapper with a block-valued backend.

```
1  #include <vector>
2  #include <iostream>
3
4  #include <amgcl/backend/builtin.hpp>
5  #include <amgcl/value_type/static_matrix.hpp>
6  #include <amgcl/adapter/crs_tuple.hpp>
7  #include <amgcl/adapter/block_matrix.hpp>
8  #include <amgcl/make_solver.hpp>
9  #include <amgcl/amg.hpp>
10 #include <amgcl/coarsening/smoothed_aggregation.hpp>
11 #include <amgcl/coarsening/rigid_body_modes.hpp>
12 #include <amgcl/coarsening/as_scalar.hpp>
13 #include <amgcl/relaxation/ilu0.hpp>
14 #include <amgcl/solver/cg.hpp>
15
16 #include <amgcl/io/mm.hpp>
17 #include <amgcl/profiler.hpp>
18
19 int main(int argc, char *argv[]) {
20     // The command line should contain the matrix, the RHS, and the coordinate files:
21     if (argc < 4) {
22         std::cerr << "Usage: " << argv[0] << " <A.mtx> <b.mtx> <coo.mtx>" <<␣
   ↪std::endl;
23         return 1;
24     }
25
26     // The profiler:
27     amgcl::profiler<> prof("Nullspace");
28
29     // Read the system matrix, the RHS, and the coordinates:
30     ptrdiff_t rows, cols, ndim, ncoo;
31     std::vector<ptrdiff_t> ptr, col;
32     std::vector<double> val, rhs, coo;
33
```

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```
    prof.tic("read");
    std::tie(rows, rows) = amgcl::io::mm_reader(argv[1])(ptr, col, val);
    std::tie(rows, cols) = amgcl::io::mm_reader(argv[2])(rhs);
    std::tie(ncoo, ndim) = amgcl::io::mm_reader(argv[3])(coo);
    prof.toc("read");

    amgcl::precondition(ncoo * ndim == rows && (ndim == 2 || ndim == 3),
            "The coordinate file has wrong dimensions");

    std::cout << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl;
    std::cout << "RHS "    << argv[2] << ": " << rows << "x" << cols << std::endl;
    std::cout << "Coords " << argv[3] << ": " << ncoo << "x" << ndim << std::endl;

    // Declare the solver type
    typedef amgcl::static_matrix<double, 3, 3> DBlock;
    typedef amgcl::static_matrix<float, 3, 3> FBlock;
    typedef amgcl::backend::builtin<DBlock> SBackend; // the solver backend
    typedef amgcl::backend::builtin<FBlock> PBackend; // the preconditioner backend

    typedef amgcl::make_solver<
        amgcl::amg<
            PBackend,
            amgcl::coarsening::as_scalar<
                amgcl::coarsening::smoothed_aggregation
                >::type,
            amgcl::relaxation::ilu0
            >,
        amgcl::solver::cg<SBackend>
        > Solver;

    // Solver parameters:
    Solver::params prm;
    prm.solver.maxiter = 500;
    prm.precond.coarsening.aggr.eps_strong = 0;

    // Convert the coordinates to the rigid body modes.
    // The function returns the number of near null-space vectors
    // (3 in 2D case, 6 in 3D case) and writes the vectors to the
    // std::vector<double> specified as the last argument:
    prm.precond.coarsening.nullspace.cols = amgcl::coarsening::rigid_body_modes(
            ndim, coo, prm.precond.coarsening.nullspace.B);

    // We use the tuple of CRS arrays to represent the system matrix.
    auto A = std::tie(rows, ptr, col, val);
    auto Ab = amgcl::adapter::block_matrix<DBlock>(A);

    // Initialize the solver with the system matrix.
    prof.tic("setup");
    Solver solve(Ab, prm);
    prof.toc("setup");

    // Show the mini-report on the constructed solver:
    std::cout << solve << std::endl;

    // Solve the system with the zero initial approximation:
    int iters;
    double error;
```

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```
    std::vector<double> x(rows, 0.0);

    // Reinterpret both the RHS and the solution vectors as block-valued:
    auto F = amgcl::backend::reinterpret_as_rhs<DBlock>(rhs);
    auto X = amgcl::backend::reinterpret_as_rhs<DBlock>(x);

    prof.tic("solve");
    std::tie(iters, error) = solve(Ab, F, X);
    prof.toc("solve");

    // Output the number of iterations, the relative error,
    // and the profiling data:
    std::cout << "Iters: " << iters << std::endl
              << "Error: " << error << std::endl
              << prof << std::endl;
}
```

This results are presented below. Note that even though the more advanced ILU(0) smoother was used, the setup time has been reduced, since ILU(0) was constructed using block arithmetics.:

```
$ ./nullspace_block A.mtx b.mtx C.mtx
Matrix A.mtx: 81657x81657
RHS b.mtx: 81657x1
Coords C.mtx: 27219x3
Solver
======
Type:             CG
Unknowns:         27219
Memory footprint: 2.49 M

Preconditioner
==============
Number of levels:    3
Operator complexity: 1.52
Grid complexity:     1.10
Memory footprint:    63.24 M

level     unknowns       nonzeros      memory
---------------------------------------------
    0        27219         352371     46.45 M (65.77%)
    1         2568         182304     16.73 M (34.03%)
    2           48           1064     60.85 K ( 0.20%)

Iters: 32
Error: 7.96226e-09

[Nullspace:     2.885 s] (100.00%)
[  read:        2.160 s] ( 74.87%)
[  setup:       0.249 s] (  8.64%)
[  solve:       0.473 s] ( 16.39%)
```

2.4.8 Using near null-space vectors (MPI version)

Let us look at how to use the near null-space vectors in the MPI version of the solver for the elasticity problem (see *Using near null-space vectors*). The following points need to be kept in mind:

- The near null-space vectors need to be partitioned (and reordered) similar to the RHS vector.
- Since we are using coordinates of the discretization grid nodes for the computation of the rigid body modes, in order to be able to do this locally we need to partition the system in such a way that DOFs from a single grid node are owned by the same MPI process. In this case this means we need to do a block-wise partitioning with a 3×3 blocks.
- It is more convenient to partition the coordinate matrix and then to compute the rigid body modes.

The listing below shows the complete source code for the MPI elasticity solver (tutorial/5.Nullspace/nullspace_mpi.cpp)

Listing 2.18: The MPI solution of the elasticity problem

```
#include <vector>
#include <iostream>

#include <amgcl/backend/builtin.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
#include <amgcl/coarsening/rigid_body_modes.hpp>

#include <amgcl/mpi/distributed_matrix.hpp>
#include <amgcl/mpi/make_solver.hpp>
#include <amgcl/mpi/amg.hpp>
#include <amgcl/mpi/coarsening/smoothed_aggregation.hpp>
#include <amgcl/mpi/relaxation/spai0.hpp>
#include <amgcl/mpi/solver/cg.hpp>

#include <amgcl/io/binary.hpp>
#include <amgcl/profiler.hpp>

#if defined(AMGCL_HAVE_PARMETIS)
#  include <amgcl/mpi/partition/parmetis.hpp>
#elif defined(AMGCL_HAVE_SCOTCH)
#  include <amgcl/mpi/partition/ptscotch.hpp>
#endif

int main(int argc, char *argv[]) {
    // The command line should contain the matrix, the RHS, and the coordinate files:
    if (argc < 4) {
        std::cerr << "Usage: " << argv[0] << " <A.bin> <b.bin> <coo.bin>" <<␣
↪std::endl;
        return 1;
    }

    amgcl::mpi::init mpi(&argc, &argv);
    amgcl::mpi::communicator world(MPI_COMM_WORLD);

    // The profiler:
    amgcl::profiler<> prof("Nullspace");

    // Read the system matrix, the RHS, and the coordinates:
    prof.tic("read");
    // Get the global size of the matrix:
    ptrdiff_t rows = amgcl::io::crs_size<ptrdiff_t>(argv[1]);

    // Split the matrix into approximately equal chunks of rows, and
    // make sure each chunk size is divisible by 3.
    ptrdiff_t chunk = (rows + world.size - 1) / world.size;
```

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```
    if (chunk % 3) chunk += 3 - chunk % 3;

    ptrdiff_t row_beg = std::min(rows, chunk * world.rank);
    ptrdiff_t row_end = std::min(rows, row_beg + chunk);
    chunk = row_end - row_beg;

    // Read our part of the system matrix, the RHS and the coordinates.
    std::vector<ptrdiff_t> ptr, col;
    std::vector<double> val, rhs, coo;
    amgcl::io::read_crs(argv[1], rows, ptr, col, val, row_beg, row_end);

    ptrdiff_t n, m;
    amgcl::io::read_dense(argv[2], n, m, rhs, row_beg, row_end);
    amgcl::precondition(n == rows && m == 1, "The RHS file has wrong dimensions");

    amgcl::io::read_dense(argv[3], n, m, coo, row_beg / 3, row_end / 3);
    amgcl::precondition(n * 3 == rows && m == 3, "The coordinate file has wrong␣
↪dimensions");
    prof.toc("read");

    if (world.rank == 0) {
        std::cout
            << "Matrix " << argv[1] << ": " << rows << "x" << rows << std::endl
            << "RHS "    << argv[2] << ": " << rows << "x1" << std::endl
            << "Coords " << argv[3] << ": " << rows / 3 << "x3" << std::endl;
    }

    // Declare the backends and the solver type
    typedef amgcl::backend::builtin<double> SBackend; // the solver backend
    typedef amgcl::backend::builtin<float>  PBackend; // the preconditioner backend

    typedef amgcl::mpi::make_solver<
        amgcl::mpi::amg<
            PBackend,
            amgcl::mpi::coarsening::smoothed_aggregation<PBackend>,
            amgcl::mpi::relaxation::spai0<PBackend>
            >,
        amgcl::mpi::solver::cg<PBackend>
        > Solver;

    // The distributed matrix
    auto A = std::make_shared<amgcl::mpi::distributed_matrix<SBackend>>(
            world, std::tie(chunk, ptr, col, val));

    // Partition the matrix, the RHS vector, and the coordinates.
    // If neither ParMETIS not PT-SCOTCH are not available,
    // just keep the current naive partitioning.
#if defined(AMGCL_HAVE_PARMETIS) || defined(AMGCL_HAVE_SCOTCH)
#  if defined(AMGCL_HAVE_PARMETIS)
    typedef amgcl::mpi::partition::parmetis<SBackend> Partition;
#  elif defined(AMGCL_HAVE_SCOTCH)
    typedef amgcl::mpi::partition::ptscotch<SBackend> Partition;
#  endif

    if (world.size > 1) {
        auto t = prof.scoped_tic("partition");
        Partition part;
```

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```
101
102         // part(A) returns the distributed permutation matrix.
103         // Keep the DOFs belonging to the same grid nodes together
104         // (use block-wise partitioning with block size 3).
105         auto P = part(*A, 3);
106         auto R = transpose(*P);
107
108         // Reorder the matrix:
109         A = product(*R, *product(*A, *P));
110
111         // Reorder the RHS vector and the coordinates:
112         R->move_to_backend();
113         std::vector<double> new_rhs(R->loc_rows());
114         std::vector<double> new_coo(R->loc_rows());
115         amgcl::backend::spmv(1, *R, rhs, 0, new_rhs);
116         amgcl::backend::spmv(1, *R, coo, 0, new_coo);
117         rhs.swap(new_rhs);
118         coo.swap(new_coo);
119
120         // Update the number of the local rows
121         // (it may have changed as a result of permutation).
122         chunk = A->loc_rows();
123     }
124 #endif
125
126     // Solver parameters:
127     Solver::params prm;
128     prm.solver.maxiter = 500;
129     prm.precond.coarsening.aggr.eps_strong = 0;
130
131     // Convert the coordinates to the rigid body modes.
132     // The function returns the number of near null-space vectors
133     // (3 in 2D case, 6 in 3D case) and writes the vectors to the
134     // std::vector<double> specified as the last argument:
135     prm.precond.coarsening.aggr.nullspace.cols = amgcl::coarsening::rigid_body_modes(
136             3, coo, prm.precond.coarsening.aggr.nullspace.B);
137
138     // Initialize the solver with the system matrix.
139     prof.tic("setup");
140     Solver solve(world, A, prm);
141     prof.toc("setup");
142
143     // Show the mini-report on the constructed solver:
144     if (world.rank == 0) std::cout << solve << std::endl;
145
146     // Solve the system with the zero initial approximation:
147     int iters;
148     double error;
149     std::vector<double> x(chunk, 0.0);
150
151     prof.tic("solve");
152     std::tie(iters, error) = solve(*A, rhs, x);
153     prof.toc("solve");
154
155     // Output the number of iterations, the relative error,
156     // and the profiling data:
157     if (world.rank == 0) {
```

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```
158         std::cout
159             << "Iters: " << iters << std::endl
160             << "Error: " << error << std::endl
161             << prof << std::endl;
162     }
163 }
```

In lines 44–49 we split the system into approximately equal chunks of rows, while making sure the chunk sizes are divisible by 3 (the number of DOFs per grid node). This is a naive paritioning that will be improved a bit later:

We read the parts of the system matrix, the RHS vector, and the grid node coordinates that belong to the current MPI process in lines 52–61. The backends for the iterative solver and the preconditioner and the solver type are declared in lines 72–82. In lines 85–86 we create the distributed version of the matrix from the local CRS arrays. After that, we are ready to partition the system using AMGCL wrapper for either ParMETIS or PT-SCOTCH libraries (lines 91–123). Note that we are reordering the coordinate matrix `coo` in the same way the RHS vector is reordered, even though the coordinate matrix has three times less rows than the system matrix. We can do this because the coordinate matrix is stored in the row-major order, and each row of the matrix has three coordinates, which means the total number of elements in the matrix is equal to the number of elements in the RHS vector, and we can apply our block-wise partitioning to the coordinate matrix.

The coordinates for the current MPI domain are converted into the rigid body modes in lines 135–136, after which we are ready to setup the solver (line 140) and solve the system (line 152). Below is the output of the compiled program:

```
$ export OMP_NUM_THREADS=1
$ mpirun -np 4 nullspace_mpi A.bin b.bin C.bin
Matrix A.bin: 81657x81657
RHS b.bin: 81657x1
Coords C.bin: 27219x3
Partitioning[ParMETIS] 4 -> 4
Type:             CG
Unknowns:         19965
Memory footprint: 311.95 K

Number of levels:    3
Operator complexity: 1.53
Grid complexity:     1.10

level     unknowns       nonzeros
---------------------------------
    0        81657        3171111 (65.31%) [4]
    1         7824        1674144 (34.48%) [4]
    2          144          10224 ( 0.21%) [4]

Iters: 104
Error: 9.26388e-09

[Nullspace:       2.833 s] (100.00%)
[ self:           0.070 s] (  2.48%)
[  partition:     0.230 s] (  8.10%)
[  read:          0.009 s] (  0.32%)
[  setup:         1.081 s] ( 38.15%)
[  solve:         1.443 s] ( 50.94%)
```

2.5 Examples

2.5.1 Solving Poisson's equation

The easiest way to solve a problem with AMGCL is to use the *amgcl::make_solver* class. It has two template parameters: the first one specifies a *preconditioner* to use, and the second chooses an *iterative solver*. The class constructor takes the system matrix in one of supported *formats* and parameters for the chosen algorithms and for the *backend*.

Let us consider a simple example of Poisson's equation in a unit square. Here is how the problem may be solved with AMGCL. We will use BiCGStab solver preconditioned with smoothed aggregation multigrid with SPAI(0) for relaxation (smoothing). First, we include the necessary headers. Each of those brings in the corresponding component of the method:

```
#include <amgcl/make_solver.hpp>
#include <amgcl/solver/bicgstab.hpp>
#include <amgcl/amg.hpp>
#include <amgcl/coarsening/smoothed_aggregation.hpp>
#include <amgcl/relaxation/spai0.hpp>
#include <amgcl/adapter/crs_tuple.hpp>
```

Next, we assemble sparse matrix for the Poisson's equation on a uniform 1000x1000 grid. See below for the definition of the `poisson()` function:

```
std::vector<int>    ptr, col;
std::vector<double> val, rhs;
int n = poisson(1000, ptr, col, val, rhs);
```

For this example, we select the *builtin* backend with double precision numbers as value type:

```
typedef amgcl::backend::builtin<double> Backend;
```

Now we can construct the solver for our system matrix. We use the convenient adapter for `std::tuple` here and just tie together the matrix size and its CRS components:

```
typedef amgcl::make_solver<
    // Use AMG as preconditioner:
    amgcl::amg<
        Backend,
        amgcl::coarsening::smoothed_aggregation,
        amgcl::relaxation::spai0
        >,
    // And BiCGStab as iterative solver:
    amgcl::solver::bicgstab<Backend>
    > Solver;

Solver solve( std::tie(n, ptr, col, val) );
```

Once the solver is constructed, we can apply it to the right-hand side to obtain the solution. This may be repeated multiple times for different right-hand sides. Here we start with a zero initial approximation. The solver returns a boost tuple with number of iterations and norm of the achieved residual:

```
std::vector<double> x(n, 0.0);
int    iters;
double error;
std::tie(iters, error) = solve(rhs, x);
```

That's it! Vector `x` contains the solution of our problem now.

2.5.2 Input formats

We used STL vectors to store the matrix components in the above axample. This may seem too restrictive if you want to use AMGCL with your own types. But the *crs_tuple* adapter will take anything that the Boost.Range library recognizes as a random access range. For example, you can wrap raw pointers to your data into a boost::iterator_range:

```
Solver solve( boost::make_tuple(
    n,
    boost::make_iterator_range(ptr.data(), ptr.data() + ptr.size()),
    boost::make_iterator_range(col.data(), col.data() + col.size()),
    boost::make_iterator_range(val.data(), val.data() + val.size())
    ) );
```

Same applies to the right-hand side and the solution vectors. And if that is still not general enough, you can provide your own adapter for your matrix type. See *Matrix Adapters* for further information on this.

2.5.3 Setting parameters

Any component in AMGCL defines its own parameters by declaring a `param` subtype. When a class wraps several subclasses, it includes parameters of its children into its own `param`. For example, parameters for the *amgcl::make_solver<Precond, Solver>* are declared as

```
struct params {
    typename Precond::params precond;
    typename Solver::params solver;
};
```

Knowing that, we can easily set the parameters for individual components. For example, we can set the desired tolerance for the iterative solver in the above example like this:

```
Solver::params prm;
prm.solver.tol = 1e-3;
Solver solve( std::tie(n, ptr, col, val), prm );
```

Parameters may also be initialized with a boost::property_tree::ptree. This is especially convenient when the runtime interface is used, and the exact structure of the parameters is not known at compile time:

```
boost::property_tree::ptree prm;
prm.put("solver.tol", 1e-3);
Solver solve( std::tie(n, ptr, col, val), prm );
```

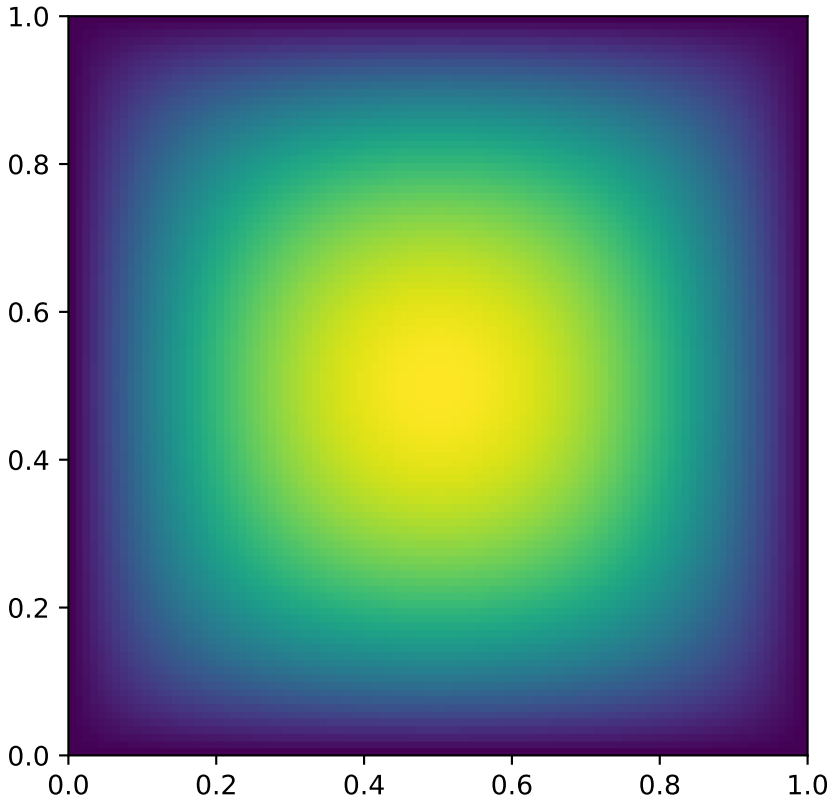
2.5.4 Assembling matrix for Poisson's equation

The section provides an example of assembling the system matrix and the right-hand side for a Poisson's equation in a unit square $\Omega = [0, 1] \times [0, 1]$:

$$-\Delta u = 1,\ u \in \Omega \quad u = 0,\ u \in \partial\Omega$$

The solution to the problem looks like this:

Here is how the problem may be discretized on a uniform $n \times n$ grid:


1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0

```
#include <vector>

// Assembles matrix for Poisson's equation with homogeneous
// boundary conditions on a n x n grid.
// Returns number of rows in the assembled matrix.
// The matrix is returned in the CRS components ptr, col, and val.
// The right-hand side is returned in rhs.
int poisson(
    int n,
    std::vector<int>    &ptr,
    std::vector<int>    &col,
    std::vector<double> &val,
    std::vector<double> &rhs
    )
{
    int    n2 = n * n;         // Number of points in the grid.
    double h = 1.0 / (n - 1); // Grid spacing.

    ptr.clear(); ptr.reserve(n2 + 1); ptr.push_back(0);
    col.clear(); col.reserve(n2 * 5); // We use 5-point stencil, so the matrix
    val.clear(); val.reserve(n2 * 5); // will have at most n2 * 5 nonzero elements.

    rhs.resize(n2);

    for(int j = 0, k = 0; j < n; ++j) {
        for(int i = 0; i < n; ++i, ++k) {
            if (i == 0 || i == n - 1 || j == 0 || j == n - 1) {
                // Boundary point. Use Dirichlet condition.
                col.push_back(k);
                val.push_back(1.0);

                rhs[k] = 0.0;
            } else {
                // Interior point. Use 5-point finite difference stencil.
                col.push_back(k - n);
                val.push_back(-1.0 / (h * h));

                col.push_back(k - 1);
                val.push_back(-1.0 / (h * h));

                col.push_back(k);
                val.push_back(4.0 / (h * h));

                col.push_back(k + 1);
                val.push_back(-1.0 / (h * h));

                col.push_back(k + n);
                val.push_back(-1.0 / (h * h));

                rhs[k] = 1.0;
            }

            ptr.push_back(col.size());
        }
    }

    return n2;
}
```

2.6 Benchmarks

The performance of the shared memory and the distributed memory versions of AMGCL algorithms was tested on two example problems in a three dimensional space. The source code for the benchmarks is available at https://github.com/ddemidov/amgcl_benchmarks.

The first example is the classical 3D Poisson problem. Namely, we look for the solution of the problem

$$-\Delta u = 1,$$

in the unit cube $\Omega = [0, 1]^3$ with homogeneous Dirichlet boundary conditions. The problem is discretized with the finite difference method on a uniform mesh.

The second test problem is an incompressible 3D Navier-Stokes problem discretized on a non uniform 3D mesh with a finite element method:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{b},$$
$$\nabla \cdot \mathbf{u} = 0.$$

The discretization uses an equal-order tetrahedral Finite Elements stabilized with an ASGS-type (algebraic subgrid-scale) approach. This results in a linear system of equations with a block structure of the type

$$\begin{pmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{D} & \mathbf{S} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_u \\ \mathbf{b}_p \end{pmatrix}$$

where each of the matrix subblocks is a large sparse matrix, and the blocks $\mathbf{G}$ and $\mathbf{D}$ are non-square. The overall system matrix for the problem was assembled in the Kratos multi-physics package developed in CIMNE, Barcelona.

2.6.1 Shared Memory Benchmarks

In this section we test performance of the library on a shared memory system. We also compare the results with PETSC and Trilinos ML distributed memory libraries and CUSP GPGPU library. The tests were performed on a dual socket system with two Intel Xeon E5-2640 v3 CPUs. The system also had an NVIDIA Tesla K80 GPU installed, which was used for testing the GPU based versions.

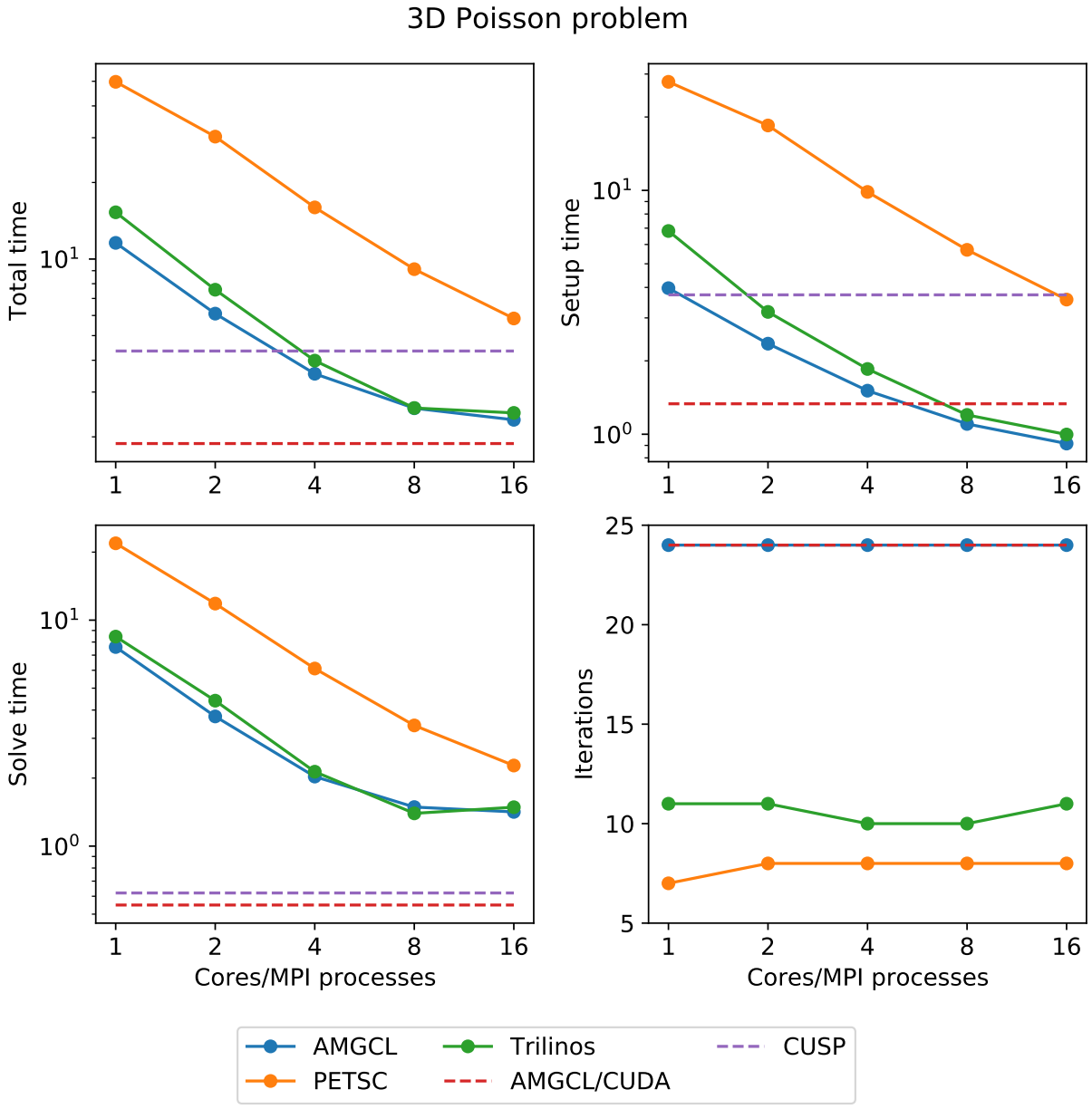
3D Poisson problem

The Poisson problem is discretized with the finite difference method on a uniform mesh, and the resulting linear system contained 3375000 unknowns and 23490000 nonzeros.

The figure below presents the multicore scalability of the problem. Here AMGCL uses the `builtin` OpenMP backend, while PETSC and Trilinos use MPI for parallelization. We also show results for the CUDA backend of AMGCL library compared with the CUSP library. All libraries use the Conjugate Gradient iterative solver preconditioned with a smoothed aggregation AMG. Trilinos and PETSC use default options for smoothers (symmetric Gauss-Seidel and damped Jacobi accordingly) on each level of the hierarchy, AMGCL uses SPAI0, and CUSP uses Gauss-Seidel smoother.

The CPU-based results show that AMGCL performs on par with Trilinos, and both of the libraries outperform PETSC by a large margin. Also, AMGCL is able to setup the solver about 20–100% faster than Trilinos, and 4–7 times faster than PETSC. This is probably due to the fact that both Trilinos and PETSC target distributed memory machines and hence need to do some complicated bookkeeping under the hood. PETSC shows better scalability than both Trilinos and AMGCL, which scale in a similar fashion.

On the GPU, AMGCL performs slightly better than CUSP. If we consider the solution time (without setup), then both libraries are able to outperform CPU-based versions by a factor of 3-4. The total solution time of AMGCL with CUDA


3D Poisson problem
Total time
Setup time
Solve time
Iterations
Cores/MPI processes
Cores/MPI processes
AMGCL
PETSC
Trilinos
AMGCL/CUDA
CUSP

backend is only 30% better than that of either AMGCL with OpenMP backend or Trilinos ML. This is due to the fact that the setup step in AMGCL is always performed on the CPU and in case of the CUDA backend has an additional overhead of moving the constructed hierarchy into the GPU memory.

3D Navier-Stokes problem

The system matrix resulting from the problem discretization has block structure with blocks of 4-by-4 elements, and contains 713456 unknowns and 41277920 nonzeros. The assembled problem is available to download at https://doi.org/10.5281/zenodo.1231818.

There are at least two ways to solve the system. First, one can treat the system as a monolithic one, and provide some minimal help to the preconditioner in form of near null space vectors. Second option is to employ the knowledge about the problem structure, and to combine separate preconditioners for individual fields (in this particular case, for pressure and velocity). In case of AMGCL both options were tested, where the monolithic system was solved with static 4x4 matrices as value type, and the field-split approach was implemented using the `schur_pressure_correction` preconditioner. Trilinos ML only provides the first option; PETSC implement both options, but we only show results for the second, superior option here. CUSP library does not provide field-split preconditioner and does not allow to specify near null space vectors, so it was not tested for this problem.

The figure below shows multicore scalability results for the Navier-Stokes problem. Lines labelled with 'block' correspond to the cases when the problem is treated as a monolithic system, and 'split' results correspond to the field-split approach.

2.6.2 Distributed Memory Benchmarks

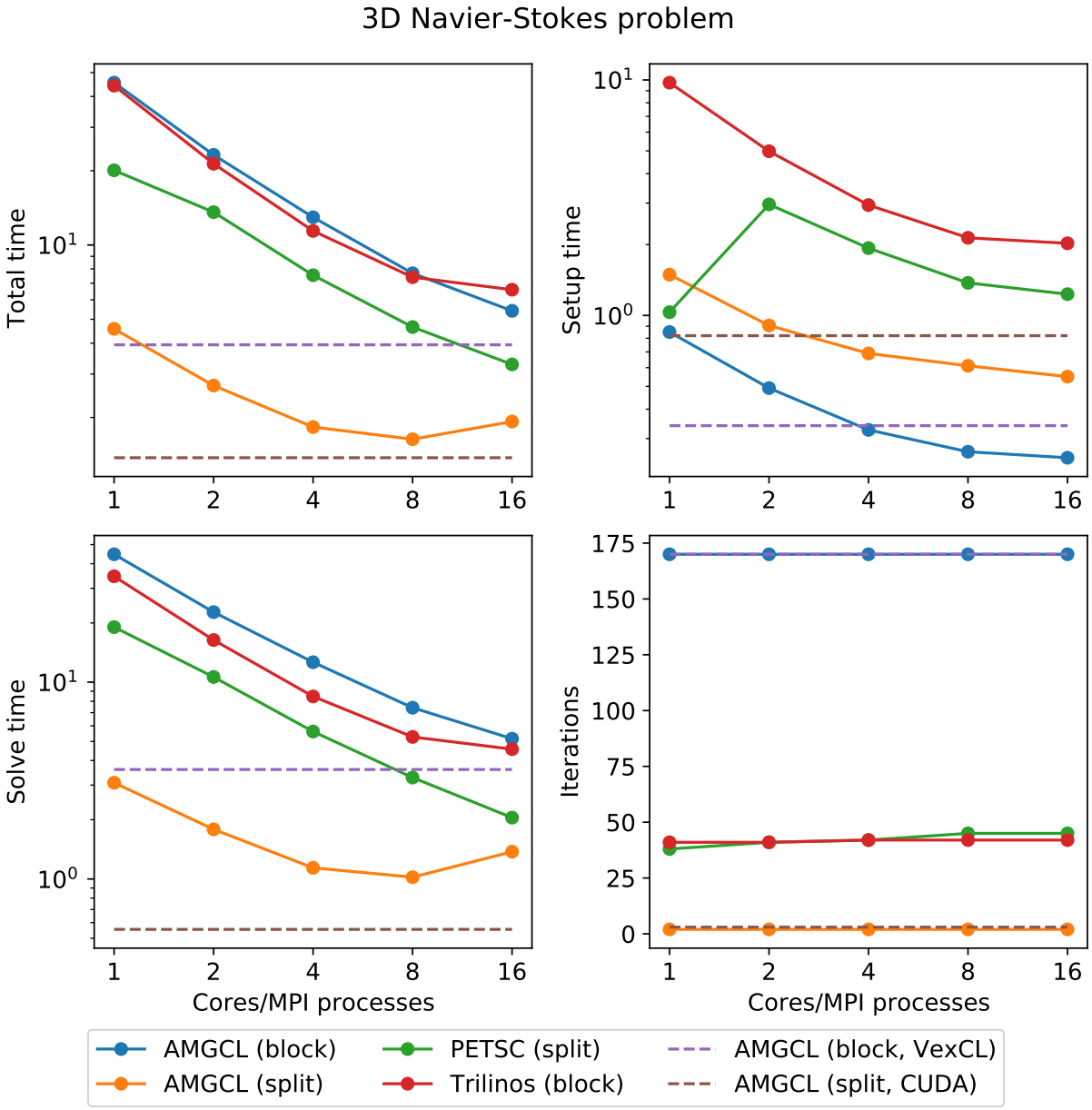
Here we demonstrate performance and scalability of the distributed memory algorithms provided by AMGCL on the example of a Poisson problem and a Navier-Stokes problem in a three dimensional space. To provide a reference, we compare performance of the AMGCL library with that of the well-established Trilinos ML package. The benchmarks were run on MareNostrum 4, PizDaint, and SuperMUC clusters which we gained access to via PRACE program (project 2010PA4058). The MareNostrum 4 cluster has 3456 compute nodes, each equipped with two 24 core Intel Xeon Platinum 8160 CPUs, and 96 GB of RAM. The peak performance of the cluster is 6.2 Petaflops. The PizDaint cluster has 5320 hybrid compute nodes, where each node has one 12 core Intel Xeon E5-2690 v3 CPU with 64 GB RAM and one NVIDIA Tesla P100 GPU with 16 GB RAM. The peak performance of the PizDaint cluster is 25.3 Petaflops. The SuperMUC cluster allowed us to use 512 compute nodes, each equipped with two 14 core Intel Haswell Xeon E5-2697 v3 CPUs, and 64 GB of RAM.

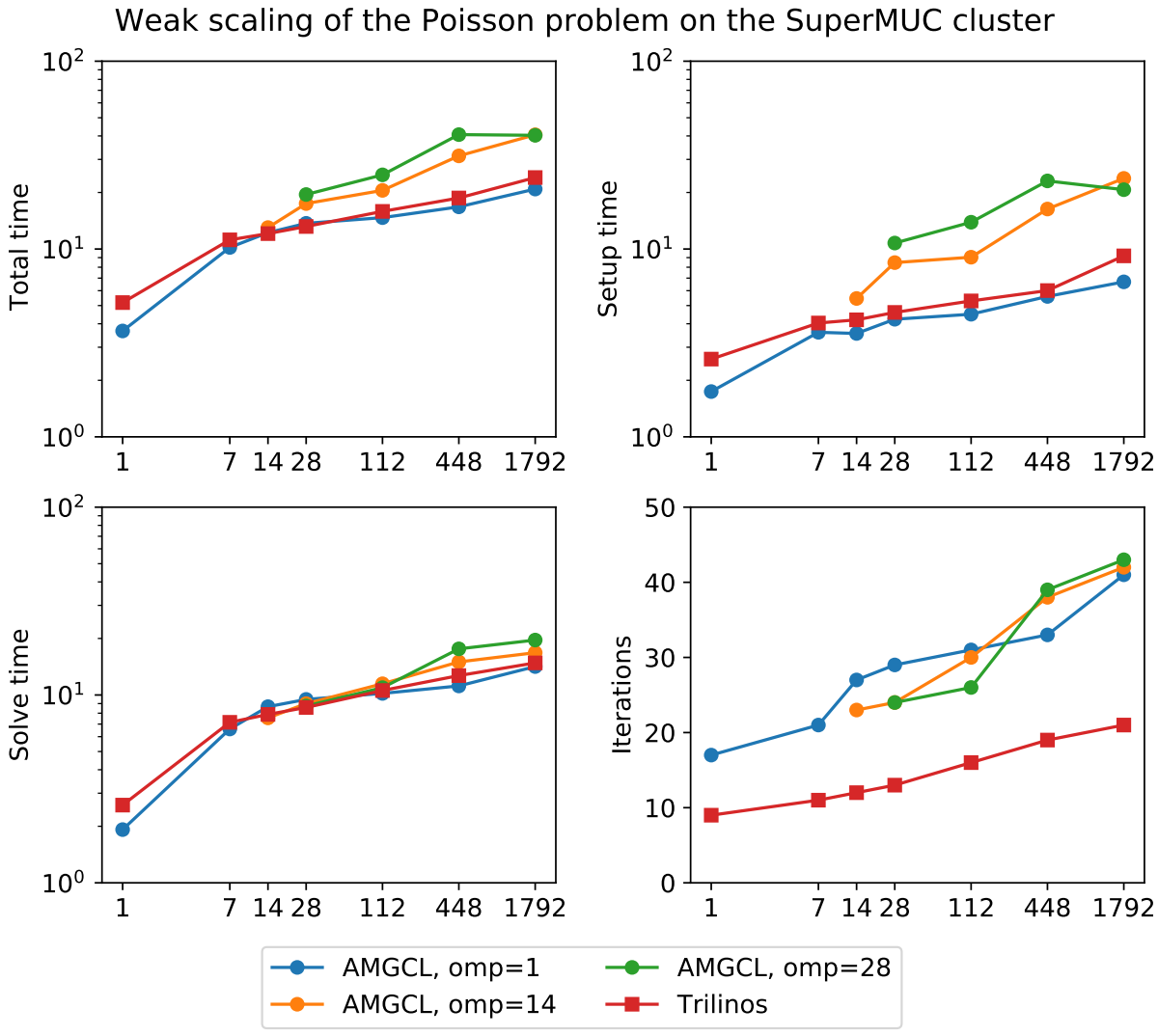
3D Poisson problem

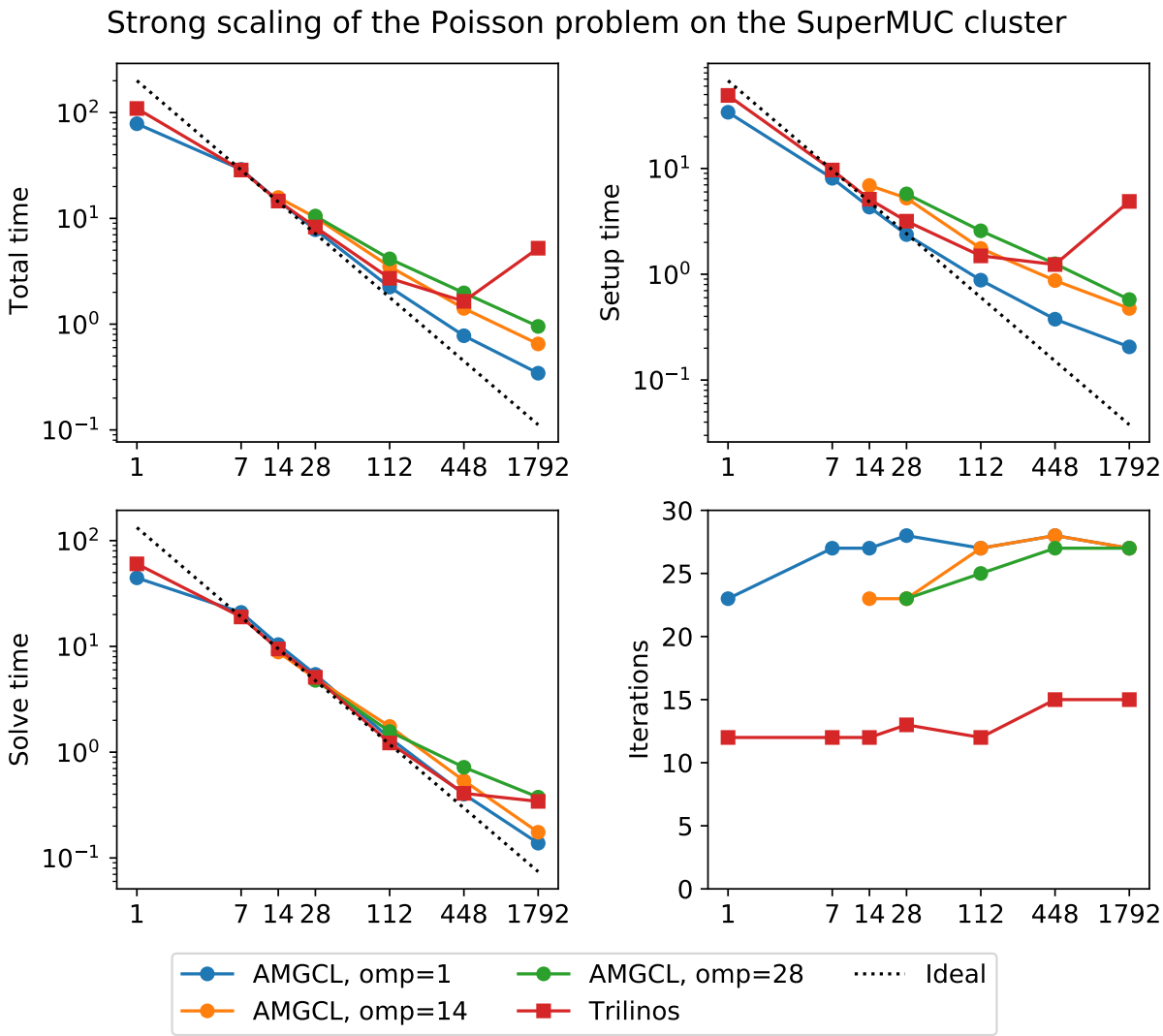
The figure below shows weak scaling of the solution on the SuperMUC cluster. Here the problem size is chosen to be proportional to the number of CPU cores with about 100^3 unknowns per core. Both AMGCL and Trilinos implementations use a CG iterative solver preconditioned with smoothed aggregation AMG. AMGCL uses SPAI(0) for the smoother, and Trilinos uses ILU(0), which are the corresponding defaults for the libraries. The plots in the figure show total computation time, time spent on constructing the preconditioner, solution time, and the number of iterations. The AMGCL library results are labelled 'OMP=n', where n=1,14,28 corresponds to the number of OpenMP threads controlled by each MPI process. The Trilinos library uses single-threaded MPI processes.

Next figure shows strong scaling results for smoothed aggregation AMG preconditioned on the SuperMUC cluster. The problem size is fixed to 256^3 unknowns and ideally the compute time should decrease as we increase the number of CPU cores. The case of ideal scaling is depicted for reference on the plots with thin gray dotted lines.

The AMGCL implementation uses a BiCGStab(2) iterative solver preconditioned with subdomain deflation, as it showed the best behaviour in our tests. Smoothed aggregation AMG is used as the local preconditioner. The Trilinos implementation uses a CG solver preconditioned with smoothed aggregation AMG with default 'SA' settings, or domain decomposition method with default 'DD-ML' settings.


3D Navier-Stokes problem
Total time
Setup time
Solve time
Iterations
Cores/MPI processes
Cores/MPI processes
AMGCL (block)
AMGCL (split)
PETSC (split)
Trilinos (block)
AMGCL (block, VexCL)
AMGCL (split, CUDA)


Weak scaling of the Poisson problem on the SuperMUC cluster
Total time
Setup time
Solve time
Iterations
1
7
14
28
112
448
1792
AMGCL, omp=1
AMGCL, omp=14
AMGCL, omp=28
Trilinos


Strong scaling of the Poisson problem on the SuperMUC cluster
Total time
Setup time
Solve time
Iterations
1
7
14
28
112
448
1792
AMGCL, omp=1
AMGCL, omp=14
AMGCL, omp=28
Trilinos
Ideal

The figure below shows weak scaling of the solution on the MareNostrum 4 cluster. Here the problem size is chosen to be proportional to the number of CPU cores with about 100^3 unknowns per core. The rows in the figure from top to bottom show total computation time, time spent on constructing the preconditioner, solution time, and the number of iterations. The AMGCL library results are labelled 'OMP=n', where n=1,4,12,24 corresponds to the number of OpenMP threads controlled by each MPI process. The Trilinos library uses single-threaded MPI processes. The Trilinos data is only available for up to 1536 MPI processes, which is due to the fact that only 32-bit version of the library was available on the cluster. The AMGCL data points for 19200 cores with 'OMP=1' are missing because factorization of the deflated matrix becomes too expensive for this configuration. AMGCL plots in the left and the right columns correspond to the linear deflation and the constant deflation correspondingly. The Trilinos and Trilinos/DD-ML lines correspond to the smoothed AMG and domain decomposition variants accordingly and are depicted both in the left and the right columns for convenience.

In the case of ideal scaling the timing plots on this figure would be strictly horizontal. This is not the case here: instead, we see that both AMGCL and Trilinos loose about 6-8% efficiency whenever the number of cores doubles. The AMGCL algorithm performs about three times worse that the AMG-based Trilinos version, and about 2.5 times better than the domain decomposition based Trilinos version. This is mostly governed by the number of iterations each version needs to converge.

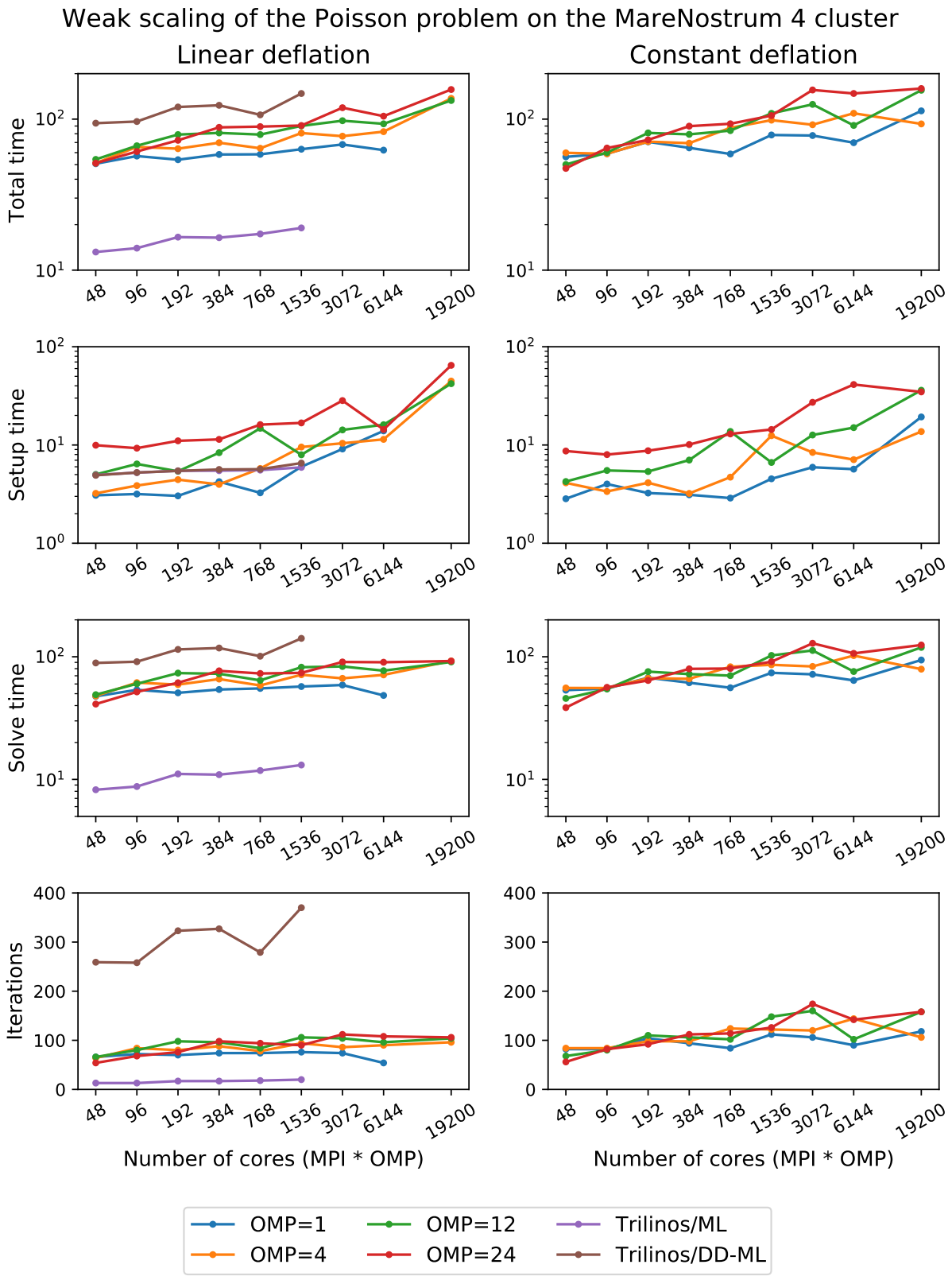
We observe that AMGCL scalability becomes worse at the higher number of cores. We refer to the following table for the explanation:

Cores	Setup		Solve	Iterations
	Total	Factorize E		
Linear deflation, OMP=1				
384	4.23	0.02	54.08	74
1536	6.01	0.64	57.19	76
6144	13.92	8.41	48.40	54
Constant deflation, OMP=1				
384	3.11	0.00	61.41	94
1536	4.52	0.01	73.98	112
6144	5.67	0.16	64.13	90
Linear deflation, OMP=12				
384	8.35	0.00	72.68	96
1536	7.95	0.00	82.22	106
6144	16.08	0.03	77.00	96
19200	42.09	1.76	90.74	104
Constant deflation, OMP=12				
384	7.02	0.00	72.25	106
1536	6.64	0.00	102.53	148
6144	15.02	0.00	75.82	102
19200	36.08	0.03	119.25	158

The table presents the profiling data for the solution of the Poisson problem on the MareNostrum 4 cluster. The first two columns show time spent on the setup of the preconditioner and the solution of the problem; the third column shows the number of iterations required for convergence. The 'Setup' column is further split into subcolumns detailing the total setup time and the time required for factorization of the coarse system. It is apparent from the table that factorization of the coarse (deflated) matrix starts to dominate the setup phase as the number of subdomains (or MPI processes) grows, since we use a sparse direct solver for the coarse problem. This explains the fact that the constant deflation scales better, since the deflation matrix is four times smaller than for a corresponding linear deflation case.

The advantage of the linear deflation is that it results in a better approximation of the problem on a coarse scale and hence needs less iterations for convergence and performs slightly better within its scalability limits, but the constant deflation eventually outperforms linear deflation as the scale grows.

Next figure shows weak scaling of the Poisson problem on the PizDaint cluster. The problem size here is chosen


Weak scaling of the Poisson problem on the MareNostrum 4 cluster
Linear deflation
Constant deflation
Total time
Setup time
Solve time
Iterations
48
96
192
384
768
1536
3072
6144
19200
Number of cores (MPI * OMP)
OMP=1
OMP=4
OMP=12
OMP=24
Trilinos/ML
Trilinos/DD-ML

so that each node owns about 200^3 unknowns. On this cluster we are able to compare performance of the OpenMP and CUDA backends of the AMGCL library. Intel Xeon E5-2690 v3 CPU is used with the OpenMP backend, and NVIDIA Tesla P100 GPU is used with the CUDA backend on each compute node. The scaling behavior is similar to the MareNostrum 4 cluster. We can see that the CUDA backend is about 9 times faster than OpenMP during solution phase and 4 times faster overall. The discrepancy is explained by the fact that the setup phase in AMGCL is always performed on the CPU, and in the case of CUDA backend it has the additional overhead of moving the generated hierarchy into the GPU memory. It should be noted that this additional cost of setup on a GPU (and the cost of setup in general) often can amortized by reusing the preconditioner for different right-hand sides. This is often possible for non-linear or time dependent problems. The performance of the solution step of the AMGCL version with the CUDA backend here is on par with the Trilinos ML package. Of course, this comparison is not entirely fair to Trilinos, but it shows the advantages of using CUDA technology.

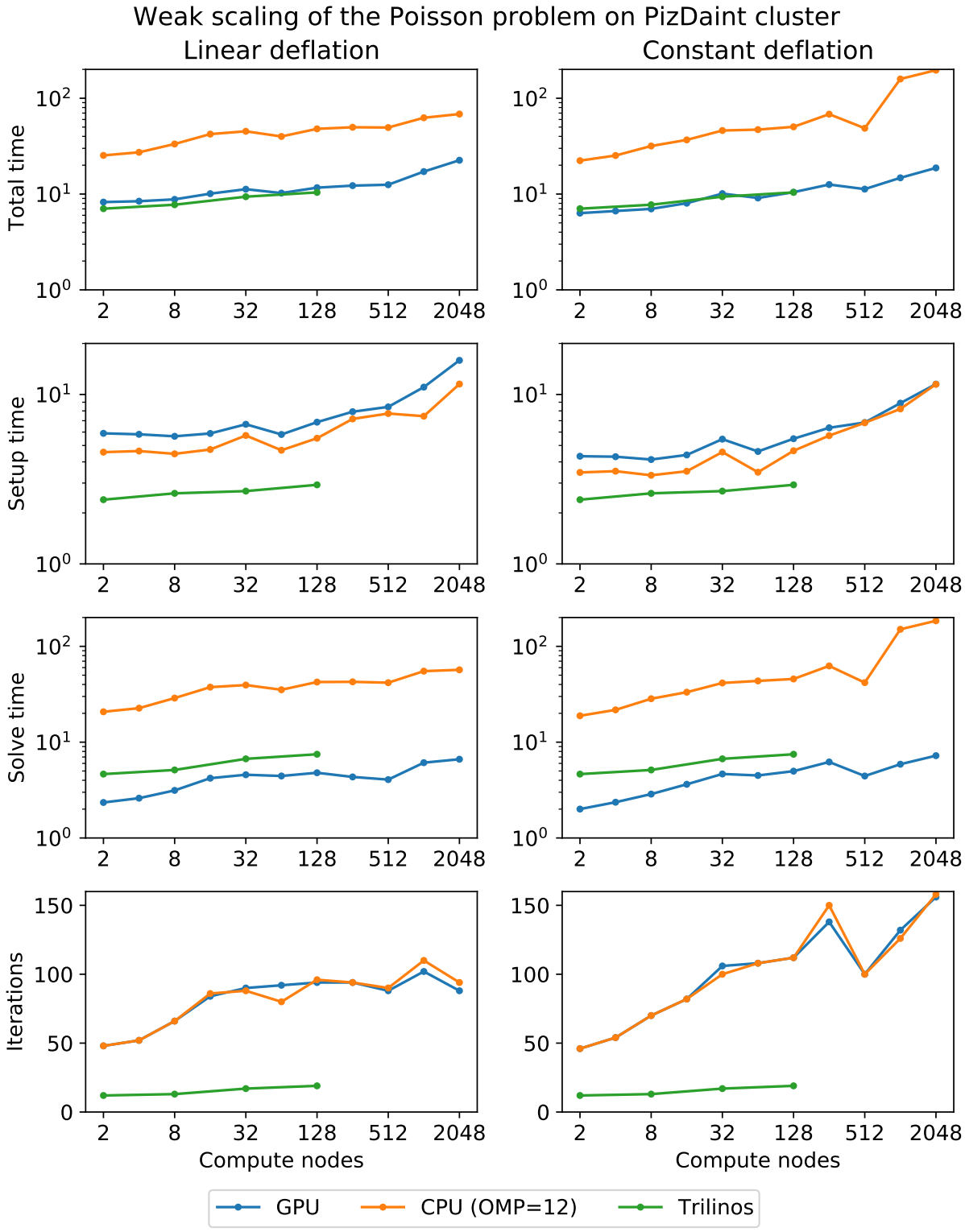
The following figure shows strong scaling results for the MareNostrum 4 cluster. The problem size is fixed to 512^3 unknowns and ideally the compute time should decrease as we increase the number of CPU cores. The case of ideal scaling is depicted for reference on the plots with thin gray dotted lines.

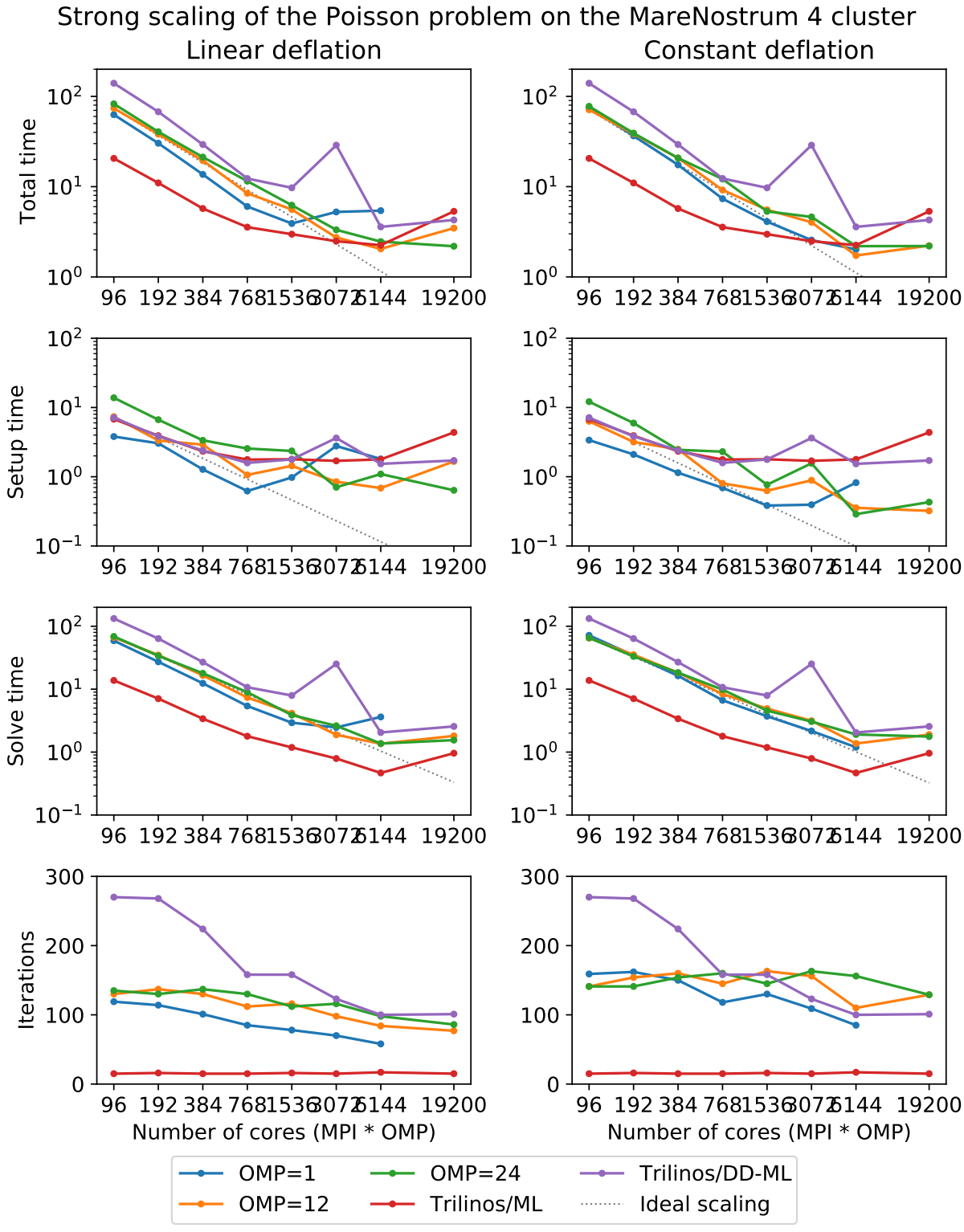
Here, AMGCL demonstrates scalability slightly better than that of the Trilinos ML package. At 384 cores the AMGCL solution for OMP=1 is about 2.5 times slower than Trilinos/AMG, and 2 times faster than Trilinos/DD-ML. As is expected for a strong scalability benchmark, the drop in scalability at higher number of cores for all versions of the tests is explained by the fact that work size per each subdomain becomes too small to cover both setup and communication costs.

The profiling data for the strong scaling case is shown in the table below, and it is apparent that, as in the weak scaling scenario, the deflated matrix factorization becomes the bottleneck for the setup phase performance.

Cores	Setup		Solve	Iterations
	Total	Factorize E		
Linear deflation, OMP=1				
384	1.27	0.02	12.39	101
1536	0.97	0.45	2.93	78
6144	9.09	8.44	3.61	58
Constant deflation, OMP=1				
384	1.14	0.00	16.30	150
1536	0.38	0.01	3.71	130
6144	0.82	0.16	1.19	85
Linear deflation, OMP=12				
384	2.90	0.00	16.57	130
1536	1.43	0.00	4.15	116
6144	0.68	0.03	1.35	84
19200	1.66	1.29	1.80	77
Constant deflation, OMP=12				
384	2.49	0.00	18.25	160
1536	0.62	0.00	4.91	163
6144	0.35	0.00	1.37	110
19200	0.32	0.02	1.89	129

An interesting observation is that convergence of the method improves with growing number of MPI processes. In other words, the number of iterations required to reach the desired tolerance decreases with as the number of subdomains grows, since the deflated system is able to describe the main problem better and better. This is especially apparent from the strong scalability results, where the problem size remains fixed, but is also observable in the weak scaling case for 'OMP=1'.

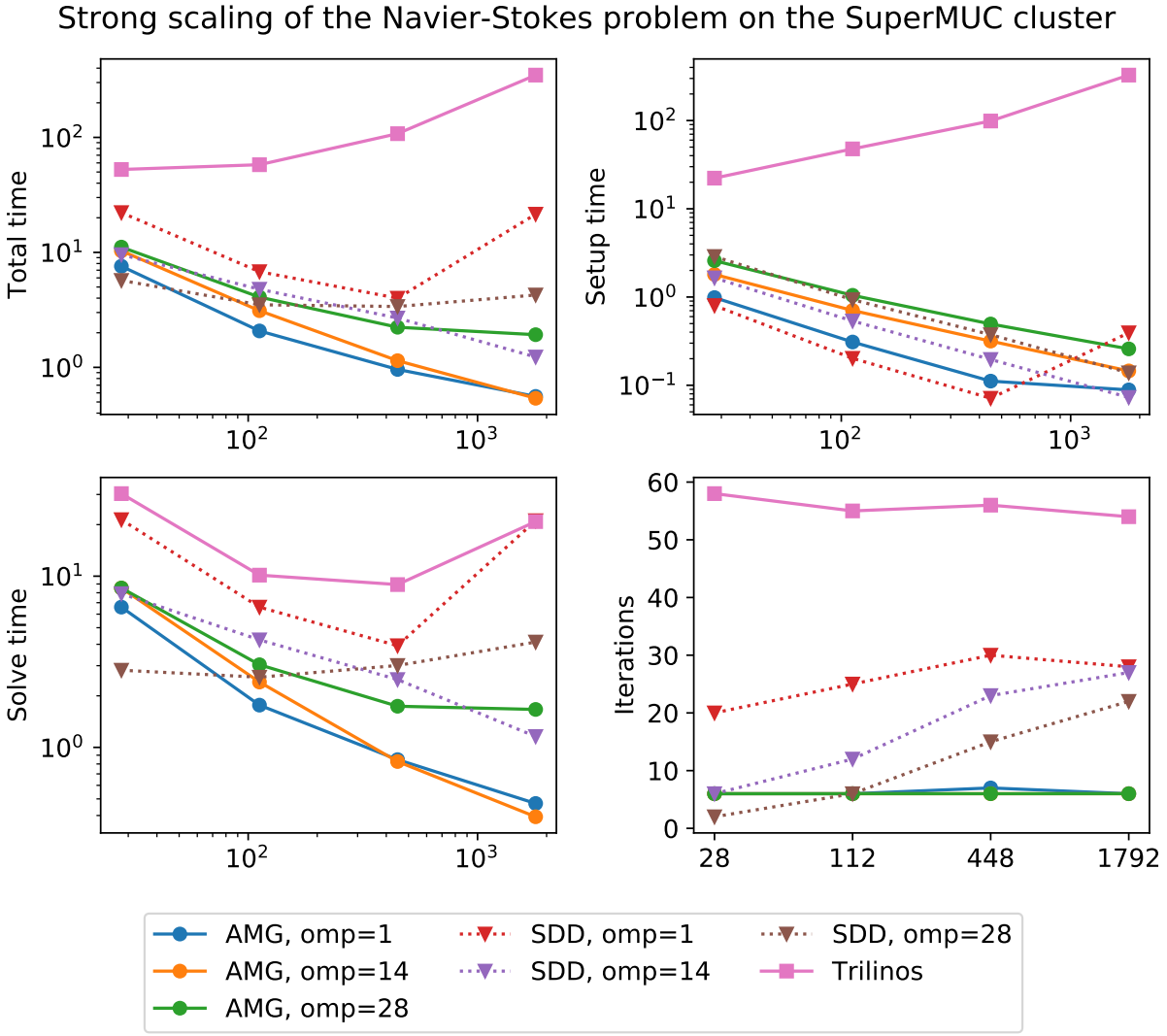

Weak scaling of the Poisson problem on PizDaint cluster
Linear deflation
Constant deflation
Total time
Setup time
Solve time
Iterations
Compute nodes
Compute nodes
GPU
CPU (OMP=12)
Trilinos


Strong scaling of the Poisson problem on the MareNostrum 4 cluster
Linear deflation
Constant deflation
Total time
Setup time
Solve time
Iterations
96 192 384 768 1536 3072 6144 19200
Number of cores (MPI * OMP)
OMP=1
OMP=12
OMP=24
Trilinos/ML
Trilinos/DD-ML
Ideal scaling

3D Navier-Stokes problem

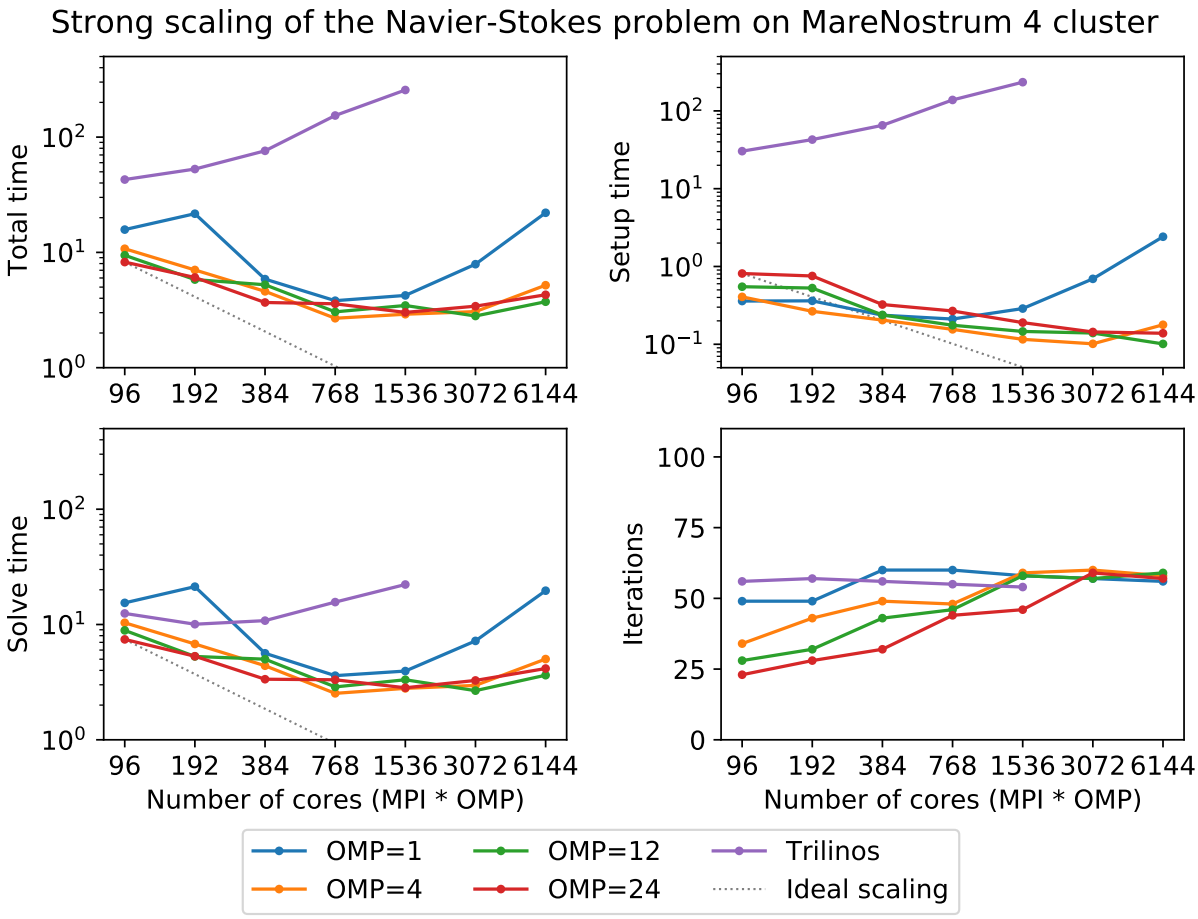
The system matrix in these tests contains 4773588 unknowns and 281089456 nonzeros. The assembled system is available to download at https://doi.org/10.5281/zenodo.1231961. AMGCL library uses field-split approach with the `mpi::schur_pressure_correction` preconditioner. Trilinos ML does not provide field-split type preconditioners, and uses the nonsymmetric smoothed aggregation variant (NSSA) applied to the monolithic problem. Default NSSA parameters were employed in the tests.

The figure below shows scalability results for the Navier-Stokes problem on the SuperMUC cluster. In case of AMGCL, the pressure part of the system is preconditioned with a smoothed aggregation AMG. Since we are solving a fixed-size problem, this is essentially a strong scalability test.



The next figure shows scalability results for the Navier-Stokes problem on the MareNostrum 4 cluster. Since we are solving a fixed-size problem, this is essentially a strong scalability test.

Both AMGCL and ML preconditioners deliver a very flat number of iterations with growing number of MPI processes. As expected, the field-split preconditioner pays off and performs better than the monolithic approach in the solution of the problem. Overall the AMGCL implementation shows a decent, although less than optimal parallel scalability. This is not unexpected since the problem size quickly becomes too little to justify the use of more parallel resources (note that at 192 processes, less than 25000 unknowns are assigned to each MPI subdomain). Unsurprisingly, in this


Strong scaling of the Navier-Stokes problem on MareNostrum 4 cluster
Total time
Setup time
Solve time
Iterations
96 192 384 768 1536 3072 6144
Number of cores (MPI * OMP)
OMP=1
OMP=4
OMP=12
OMP=24
Trilinos
Ideal scaling

context the use of OpenMP within each domain pays off and allows delivering a greater level of scalability.

2.7 Compilation issues

AMGCL is a header-only library, so one does not need to compile it in order to use the library. However, there are some dependencies coming with the library:

1. The runtime interface of AMGCL depends on the header-only Boost.property_tree library that allows the solvers and preconditioners to accept dynamically formed parameters. When the runtime interface is not used, it is possible to get rid of the Boost.property_tree dependency by defining the preprocessor macro `AMGCL_NO_BOOST`.
2. AMGCL uses OpenMP during the setup of the provided solvers and preconditioners, and also for the *amgcl::backend::builtin* backend. OpenMP is supported by most, if not all, of the relatively modern C++ compilers, so that should not be a problem. One just has to remember to enable the OpenMP support during the compilation of the project that uses AMGCL.
3. Each of the AMGCL backends brings its own set of dependencies. For example, the *amgcl::backend::vexcl* backend depends on the header-only VexCL library, which in turn depends on some Boost libraries and either on CUDA or OpenCL support. The *amgcl::backend::cuda* backend depends on the CUDA support and the CUSPARSE and Thrust libraries.

If your project already uses CMake as the build system, then using AMGCL should be easy. Here is a concise example that shows how to compile a project using AMGCL with the builtin backend:

```
cmake_minimum_required(VERSION 3.1)
project(example)

find_package(amgcl)

add_executable(example example.cpp)
target_link_libraries(example amgcl::amgcl)
```

And here is an example of adding the support for the VexCL backend:

```
cmake_minimum_required(VERSION 3.1)
project(example)

find_package(amgcl)
find_package(VexCL)

add_executable(example example.cpp)
target_link_libraries(example amgcl::amgcl VexCL::OpenCL)
```

`find_package(amgcl)` may be used when the cmake support for AMGCL was installed either system-wide, or in the current user home directory. If that is not the case, one can simply copy the amgcl folder into a subdirectory of the main project and replace the `find_package(amgcl)` line with `add_subdirectory(amgcl)`.

Finally, in order to compile the AMGCL tests and examples, the following script may be used:

```
git clone https://github.com/ddemidov/amgcl
cd ./amgcl
cmake -Bbuild -DAMGCL_BUILD_TESTS=ON -DAMGCL_BUILD_EXAMPLES=ON .
cmake --build build
```

After this, the compiled tests and examples may be found in the `build` folder.

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