
AMGCL Documentation

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Contents

1	Contents:	3
1.1	Getting started	3
1.2	Components	6
1.3	Runtime interface	14
1.4	Examples	17
1.5	Benchmarks	22
1.6	Bibliography	33
1.7	Indices and tables	33
	Bibliography	35

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 [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).

AMGCL builds the AMG hierarchy on a CPU and then transfers it to 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 library source code is available under MIT license at <https://github.com/ddemidov/amgcl>.

1.1 Getting started

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*.

1.1.1 Solving Poisson's equation

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 *Assembling matrix for Poisson's equation* for the source code 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 boost tuples 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( boost::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;
boost::tie(iters, error) = solve(rhs, x);
```

That's it! Vector `x` contains the solution of our problem now.

1.1.2 Input formats

We used STL vectors to store the matrix components in the above example. 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.

1.1.3 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 precondition;
    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( boost::tie(n, ptr, col, val), prm );
```

Parameters may also be initialized with a `boost::property_tree::ptree`. This is especially convenient when *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( boost::tie(n, ptr, col, val), prm );
```

1.1.4 The `make_solver` class

template <class Precond, class IterativeSolver>

class `amgcl::make_solver`

Convenience class that bundles together a preconditioner and an iterative solver.

Public Functions

template <class Matrix>

make_solver (const Matrix &A, const *params* &prm = params (), const backend_params &bprm = backend_params())

Sets up the preconditioner and creates the iterative solver.

template <class Matrix, class Vec1, class Vec2>

boost::tuple<size_t, scalar_type> **operator** () (Matrix const &A, Vec1 const &rhs, Vec2 &&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 `boost::tuple`. The solution vector `x` provides initial approximation in 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 Vec1, class Vec2>

boost::tuple<size_t, scalar_type> **operator** () (Vec1 const &rhs, Vec2 &&x) **const**

Computes the solution for the given right-hand side rhs. Returns the number of iterations made and the achieved residual as a `boost::tuple`. The solution vector `x` provides initial approximation in input and holds the computed solution on output.

template <class Vec1, class Vec2>

void **apply** (const Vec1 &rhs, Vec2 &&x) **const**

Acts as a preconditioner. That is, applies the solver to the right-hand side rhs to get the solution `x` with zero initial approximation. Iterative methods usually use estimated residual for exit condition. For some problems the value of the estimated residual can get too far from the true residual due to round-off errors. Nesting iterative solvers in this way may allow to shave the last bits off the error. The method should not be used directly but rather allows nesting `make_solver` classes as in the following example:

```
typedef amgcl::make_solver<
    amgcl::make_solver<
        amgcl::amg<
            Backend, amgcl::coarsening::smoothed_aggregation,
            ↪amgcl::relaxation::spai0
```

```
    >,
    amgcl::solver::cg<Backend>
    >,
    amgcl::solver::cg<Backend>
    > NestedSolver;
```

const Precond &**precond** () **const**

Returns reference to the constructed preconditioner.

const IterativeSolver &**solver** () **const**

Returns reference to the constructed iterative solver.

Precond::matrix **const** &**system_matrix** () **const**

Returns the system matrix in the backend format.

void **get_params** (boost::property_tree::ptree &p) **const**

Stores the parameters used during construction into the property tree p.

size_t **size** () **const**

Returns the size of the system matrix.

struct **params**

Combined parameters of the bundled preconditioner and the iterative solver.

Public Members

template<>

Precond::params **precond**

Preconditioner parameters.

template<>

IterativeSolver::params **solver**

Iterative solver parameters.

1.2 Components

1.2.1 Matrix adapters

Matrix adapters in AMGCL allow 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 access to the nonzero matrix values. An example of creating an adapter is provided in [Adapting custom matrix class](#).

Boost tuple adapter

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

The Boost tuple adapter allows to use a `boost::tuple` of a matrix size and its three [CRS](#) format components (row pointer array, column indices array, and values array) as input matrix to AMGCL solvers. The arrays are allowed to be in any format recognized by the [Boost.Range](#) library as a random access range. Common examples are STL vectors and Boost [iterator ranges](#).

Example:

```
// boost::tie creates a tuple of references, which avoids copying.
Solver solve( boost::tie(n, ptr, col, val) );

// A (cheap) copy is required when iterator ranges are created on the fly:
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())
) );
```

Boost.uBLAS adapter

```
#include <amgcl/adapters/ublas.hpp>
```

The `Boost.uBLAS` adapter allows to use uBLAS sparse matrices as input to AMGCL solvers. It also allows to use uBLAS dense vectors with `amgcl::backend::builtin`.

Example:

```
namespace ublas = boost::numeric::ublas;

ublas::compressed_matrix<double> A;
...
Solver solve(A);

ublas::vector<double> rhs, x;
...
solve(rhs, x);
```

Zero copy adapter

```
#include <amgcl/adapters/zero_copy.hpp>
```

In general, AMGCL copies the adapted input matrix into its internal structures, so that the matrix may be safely destroyed or reused as soon as the solver setup is complete. However, the memory overhead of the copying may be too large, especially for large problems that eat up almost all of available RAM. The zero copy adapter allows to use raw pointers to CRS arrays as input matrix for MAGCL solvers. The data from the arrays is never copied during setup, and the user has to make sure the arrays stay alive long enough. However, unless the backend used is `amgcl::backend::builtin`, the input matrix will be copied into the backend structures when the setup is finished. This would still allow to save some memory in case of GPGPU backends.

The one requirement is that the integer types stored in row pointers and column indices arrays have to be binary compatible with `ptrdiff_t`, and the value type has to be the value type of the backend.

Example:

```
Solver solve( amgcl::adapter::zero_copy(n, &ptr[0], &col[0], &val[0]) );
```

1.2.2 Backends

A backend in AMGCL is a class that defines matrix and vector types together with several operations on them, such as creation, matrix-vector products, elementwise vector operations, inner products etc. The `<amgcl/backend/interface.hpp>` file defines an interface that each backend should extend. The AMG hierarchy is

moved to the specified backend upon construction. The solution phase then uses types and operations defined in the backend. This enables transparent acceleration of the solution phase with OpenMP, OpenCL, CUDA, or any other technologies.

In order to use a backend, user must include its definition from the corresponding file inside `amgcl/backend` folder. On the user side of things, only the types of the right-hand side and the solution vectors should be affected by the choice of AMGCL backend. Here is an example of using the `builtin` backend. First, we need to include the appropriate header:

```
#include <amgcl/backend/builtin.hpp>
```

Then, we need to construct the solver and apply it to the vector types supported by the backend:

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

typedef amgcl::make_solver<
    amgcl::amg<Backend, amgcl::coarsening::aggregation, amgcl::relaxation::spai0>,
    amgcl::solver::gmres<Backend>
> Solver;

Solver solve(A);

std::vector<double> rhs, x; // Initialized elsewhere

solve(rhs, x);
```

Now, if we want to switch to a different backend, for example, in order to accelerate the solution phase with a powerful GPU, we just need to include another backend header, and change the definitions of `Backend`, `rhs`, and `x`. Here is an example of what needs to be done to use the `VexCL` backend.

Include the correct header:

```
#include <amgcl/backend/builtin.hpp>
```

Change the definition of `Backend`:

```
typedef amgcl::backend::vexcl<double> Backend;
```

Change the definition of the vectors:

```
vex::vector<double> rhs, x;
```

That's it! Well, almost. In case the backend requires some parameters, we also need to provide those. In particular, the `VexCL` backend should know what `VexCL` context to use:

```
// Initialize VexCL context on a single GPU:
vex::Context ctx(vex::Filter::GPU && vex::Filter::Count(1));

// Create backend parameters:
Backend::params backend_prm;
backend_prm.q = ctx;

// Pass the parameters to the solver constructor:
Solver solve(A, Solver::params(), backend_prm);
```

Builtin

```
#include <amgcl/backend/builtin.hpp>
```

```
template <typename ValueType>
```

```
struct amgcl::backend::builtin
```

The builtin backend does not have any dependencies except for the Boost libraries, and uses OpenMP for parallelization. Matrices are stored in the CRS format, and vectors are instances of `std::vector<value_type>`. There is no usual overhead of moving the constructed hierarchy to the builtin backend, since the backend is used internally during setup.

Public Types

```
typedef amgcl::detail::empty_params params
```

The backend has no parameters.

```
struct provides_row_iterator
```

Inherits from `true_type`

VexCL

```
#include <amgcl/backend/vexcl.hpp>
```

```
template <typename real, class DirectSolver = solver::vexcl_skyline_lu<real>>
```

```
struct amgcl::backend::vexcl
```

The backend uses the VexCL library for accelerating solution on the modern GPUs and multicore processors with the help of OpenCL or CUDA technologies. The VexCL backend stores the system matrix as `vex::SpMat<real>` and expects the right hand side and the solution vectors to be instances of the `vex::vector<real>` type.

```
struct params
```

The VexCL backend parameters.

Public Members

```
template<>
```

```
std::vector<vex::backend::command_queue> q
```

Command queues that identify compute devices to use with VexCL.

```
template<>
```

```
bool fast_matrix_setup
```

Do CSR to ELL conversion on the GPU side.

This will result in faster setup, but will require more GPU memory.

```
struct provides_row_iterator
```

Inherits from `false_type`

1.2.3 Preconditioners

1.2.4 Iterative solvers

AMGCL provides several iterative solvers, but it should be easy to use AMGCL preconditioners with a user-provided solver as well. Each solver in AMGCL is a class template. Its single template parameter specifies the backend to use.

This allows to preallocate necessary resources at class construction. Obviously, the solver backend has to coincide with the preconditioner backend.

Each of the solvers in AMGCL provides two overloads for the `operator()`:

```
boost::tuple<size_t, scalar_type> operator () (const Matrix &A, const Precond &P, const Vec1 &rhs,
                                             Vec2 &&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 `boost::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].

```
boost::tuple<size_t, scalar_type> operator () (const Precond &P, const Vec1 &rhs, Vec2 &&x) const
```

Computes the solution for the given right-hand side `rhs`. The system matrix is the same that was used for the setup of the preconditioner `P`. Returns the number of iterations made and the achieved residual as a `boost::tuple`. The solution vector `x` provides initial approximation on input and holds the computed solution on output.

Conjugate Gradient

```
#include <amgcl/solver/cg.hpp>
```

```
template <class Backend, class InnerProduct = detail::default_inner_product>
```

```
class amgcl::solver::cg
```

Conjugate Gradients method. An effective method for symmetric positive definite systems [Barr94].

Public Functions

```
cg (size_t n, const params &prm = params (), const backend_params &backend_prm = back-
    end_params(), const InnerProduct &inner_product = InnerProduct())
    Preallocates necessary data structures for the system of size n.
```

```
struct params
```

Solver parameters.

Public Members

```
template<>
```

```
size_t maxiter
```

Maximum number of iterations.

```
template<>
```

```
scalar_type tol
```

Target relative residual error.

```
template<>
```

```
scalar_type abstol
```

Target absolute residual error.

BiConjugate Gradient Stabilized (BiCGSTAB)

```
#include <amgcl/solver/bicgstab.hpp>
```

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

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

Public Functions

```
bicgstab (size_t n, const params &prm = params (), const backend_params &backend_prm = back-
end_params(), const InnerProduct &inner_product = InnerProduct())
    Preallocates necessary data structures for the system of size n.
```

```
struct params
    Solver parameters.
```

Public Members

```
template<>
preconditioner::side::type pside
    Preconditioning kind (left/right).
```

```
template<>
size_t maxiter
    Maximum number of iterations.
```

```
template<>
scalar_type tol
    Target relative residual error.
```

```
template<>
scalar_type abstol
    Target absolute residual error.
```

BiCGSTAB(L)

```
#include <amgcl/solver/bicgstabl.hpp>
template <class Backend, class InnerProduct = detail::default_inner_product>
class amgcl::solver::bicgstabl
```

BiCGStab(L) method. Generalization of BiCGStab method [Sidi93].

Public Functions

```
bicgstabl (size_t n, const params &prm = params (), const backend_params &backend_prm =
backend_params(), const InnerProduct &inner_product = InnerProduct())
    Preallocates necessary data structures for the system of size n.
```

```
struct params
    Solver parameters.
```

GMRES

```
#include <amgcl/solver/gmres.hpp>
```

```
template <class Backend, class InnerProduct = detail::default_inner_product>
```

```
class amgcl::solver::gmres
```

Generalized Minimal Residual (GMRES) method. The Generalized Minimal Residual method is an extension of MINRES (which is only applicable to symmetric systems) to unsymmetric systems [Barr94].

Public Functions

```
gmres (size_t n, const params &prm = params (), const backend_params &backend_prm = back-  
end_params(), const InnerProduct &inner_product = InnerProduct())  
Preallocates necessary data structures for the system of size n.
```

```
struct params
```

Solver parameters.

Public Members

```
template<>
```

```
unsigned M
```

Number of iterations before restart.

```
template<>
```

```
preconditioner::side::type pside
```

Preconditioning kind (left/right).

```
template<>
```

```
unsigned maxiter
```

Maximum number of iterations.

```
template<>
```

```
scalar_type tol
```

Target relative residual error.

```
template<>
```

```
scalar_type abstol
```

Target absolute residual error.

LGMRES

```
#include <amgcl/solver/lgmres.hpp>
```

```
template <class Backend, class InnerProduct = detail::default_inner_product>
```

```
class amgcl::solver::lgmres
```

“Loose” GMRES. The LGMRES algorithm [BaJM05] is designed to avoid some problems in the convergence in restarted GMRES, and often converges in fewer iterations.

Public Functions

```
lgmres (size_t n, const params &prm = params (), const backend_params &bprm = back-  
end_params(), const InnerProduct &inner_product = InnerProduct())  
Preallocates necessary data structures for the system of size n.
```


struct params

Solver parameters.

Public Members

template<>

unsigned **M**

Number of inner GMRES iterations per each outer iteration.

template<>

unsigned **K**

Number of vectors to carry between inner GMRES iterations.

According to [BaJM05], good values are in the range of 1..3. However, note that if you want to use the additional vectors to accelerate solving multiple similar problems, larger values may be beneficial.

template<>

bool **always_reset**

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.

template<>

bool **store_Av**

Whether LGMRES should store also $A*v$ in addition to vectors v .

template<>

preconditioner::side::type **pside**

Preconditioning kind (left/right).

template<>

size_t **maxiter**

Maximum number of iterations.

template<>

scalar_type **tol**

Target relative residual error.

template<>

scalar_type **abstol**

Target absolute residual error.

FGMRES

```
#include <amgcl/solver/fgmres.hpp>
```

```
template <class Backend, class InnerProduct = detail::default_inner_product>
```

```
class amgcl::solver::fgmres
```

Flexible GMRES method. Flexible version of the GMRES method [Saad03].

Public Functions

```
fgmres (size_t n, const params &prm = params (), const backend_params &bprm = back-
end_params(), const InnerProduct &inner_product = InnerProduct())
Preallocates necessary data structures for the system of size n.
```

struct params

Solver parameters.

Public Members

template<>

unsigned **M**

Number of inner GMRES iterations per each outer iteration.

template<>

unsigned **maxiter**

Maximum number of iterations.

template<>

scalar_type **tol**

Target relative residual error.

template<>

scalar_type **abstol**

Target absolute residual error.

1.3 Runtime interface

The compile-time configuration of the solvers used in AMGCL is not always convenient, especially if the solvers are used inside a software package or another library. That is why AMGCL provides runtime interface, which allows to postpone the configuration until, well, runtime. The classes inside `amgcl::runtime` namespace correspond to their compile-time alternatives, but the only template parameter they have is the backend to use.

Since there is no way of knowing 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. The runtime interface provides some enumerations for this purpose. For example, to select smoothed aggregation for coarsening, we could do this:

```
boost::property_tree::ptree prm;  
prm.put("precond.coarsening.type", amgcl::runtime::coarsening::smoothed_aggregation);
```

The enumerations provide functions for converting to/from strings, so the following would work as well:

```
prm.put("precond.coarsening.type", "smoothed_aggregation");
```

Here is an example of using a runtime-configurable solver:

```
#include <amgcl/backend/builtin.hpp>  
#include <amgcl/runtime.hpp>  
  
...  
  
boost::property_tree::ptree prm;  
prm.put("precond.coarsening.type", amgcl::runtime::coarsening::smoothed_aggregation);  
prm.put("precond.relaxation.type", amgcl::runtime::relaxation::spai0);  
prm.put("solver.type", amgcl::runtime::solver::gmres);  
  
amgcl::make_solver<  
    amgcl::runtime::amg<Backend>,&br/>
```

```
amgcl::runtime::iterative_solver<Backend>
> solve(A, prm);
```

1.3.1 Classes

AMG preconditioner

```
template <class Backend>
class amgcl::runtime::amg
    Runtime-configurable AMG preconditioner.

    Inherits from noncopyable
```

Public Functions

```
template <class Matrix>
amg (const Matrix &A, params prm = params(), const backend_params &backend_prm = back-
    end_params())
    Constructs the AMG hierarchy for the system matrix A. prm is an in-
    stance of boost::property_tree::ptree class. The property tree
    may contain parameters "coarsening.type" and "relax.type". Default val-
    ues are amgcl::runtime::coarsening::smoothed_aggregation and
    runtime::relaxation::spai0. The rest of the property tree should copy the structure of
    the corresponding amgcl::amg::params struct. For example, when smoothed aggregation is selected
    for coarsening, one could:
```

```
prm.put("coarsening.aggr.eps_strong", 1e-2);
```

Note: Any parameters that are not relevant to the selected AMG components are silently ignored.

```
template <class Vec1, class Vec2>
void cycle (const Vec1 &rhs, Vec2 &x) const
    Performs single V-cycle for the given right-hand side rhs and solution x.
```

```
template <class Vec1, class Vec2>
void apply (const Vec1 &rhs, Vec2 &x) const
    Performs single V-cycle for the given right-hand side rhs after clearing x. This is intended for use as a
    preconditioning procedure.
```

```
const matrix &system_matrix () const
    Returns the system matrix in the backend format
```

```
size_t size () const
    Returns the problem size at the finest level.
```

Friends

```
std::ostream &operator<< (std::ostream &os, const amg &a)
    Prints some info about the AMG hierarchy to the output stream.
```

```
enum amgcl::runtime::coarsening::type
    Values:
```

ruge_stuben

Ruge-Stueben coarsening.

aggregation

Aggregation.

smoothed_aggregation

Smoothed aggregation.

smoothed_aggr_emin

Smoothed aggregation with energy minimization.

enum `amgcl::runtime::relaxation::type`

Relaxation schemes.

Values:

gauss_seidel

Gauss-Seidel smoothing.

ilu0

Incomplete LU with zero fill-in.

iluk

Level-based incomplete LU.

ilut

Incomplete LU with thresholding.

damped_jacobi

Damped Jacobi.

spai0

Sparse approximate inverse of 0th order.

spai1

Sparse approximate inverse of 1st order.

chebyshev

Chebyshev relaxation.

Iterative solver

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

class `amgcl::runtime::iterative_solver`

This is runtime wrapper around AMGCL iterative solver types. Allows to select the actual solver at runtime.

Public Functions

iterative_solver (`size_t n`, `params prm = params()`, **const** `backend_params &bprm = backend_params()`, **const** `InnerProduct &inner_product = InnerProduct()`)

Constructs the iterative solver for the problem size `n`. The property tree `solver_prm` may contain “type” entry that would determine the actual type of the iterative solver. Default value: `amgcl::runtime::solver::bicgstab`.

Note: Any parameters that are not relevant to the selected solver are silently ignored.

template <**class** Matrix, **class** Precond, **class** Vec1, **class** Vec2>

`boost::tuple<size_t, scalar_type> operator ()` (Matrix `const &A`, Precond `const &P`, Vec1 `const &rhs`, Vec2 `&&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 `boost::tuple`. The solution vector `x` provides initial approximation in 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 Precond, class Vec1, class Vec2>`

`boost::tuple<size_t, scalar_type> operator ()` (Precond `const &P`, Vec1 `const &rhs`, Vec2 `&&x`) `const`

Computes the solution for the given right-hand side `rhs`. The system matrix is the same that was used for the setup of the preconditioner `P`. Returns the number of iterations made and the achieved residual as a `boost::tuple`. The solution vector `x` provides initial approximation in input and holds the computed solution on output.

`enum amgcl::runtime::solver::type`

Values:

`cg`

Conjugate gradients method.

`bicgstab`

BiConjugate Gradient Stabilized.

`bicgstabl`

BiCGStab(ell)

`gmres`

GMRES.

`lgmres`

LGMRES.

`fgmres`

FGMRES.

`idrs`

IDR(s)

1.4 Examples

1.4.1 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 $\Omega = [0, 1] \times [0, 1]$:

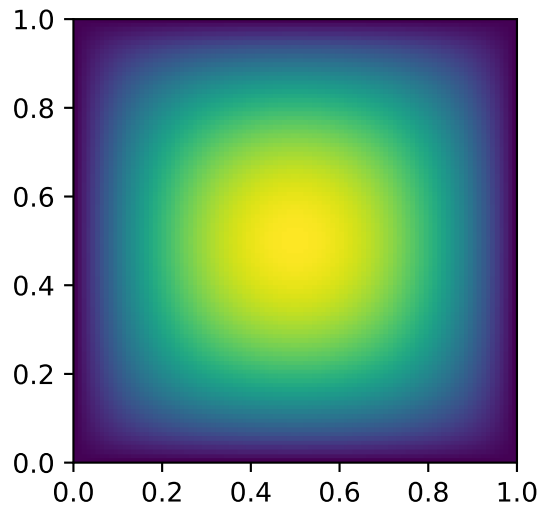
$$-\Delta u = 1, u \in \Omega \quad u = 0, u \in \partial\Omega$$

The solution to the problem looks like this:

Here is how the problem may be discretized on a uniform $n \times n$ grid:

```
#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;
}

```

1.4.2 Adapting custom matrix class

This example shows how to adapt a custom matrix class for use with AMGCL solvers. Let's say the user application declares the following class to store its sparse matrices:

```

class sparse_matrix {
public:
    typedef std::map<int, double> sparse_row;

    sparse_matrix(int n, int m) : _n(n), _m(m), _rows(n) { }

    int nrows() const { return _n; }
    int ncols() const { return _m; }
    int nonzeros() const {
        int nnz = 0;
        for(auto &row : _rows) nnz += row.size();
        return nns;
    }

    // Get a value at row i and column j
    double operator()(int i, int j) const {
        sparse_row::const_iterator elem = _rows[i].find(j);
        return elem == _rows[i].end() ? 0.0 : elem->second;
    }

    // Get reference to a value at row i and column j
    double& operator()(int i, int j) { return _rows[i][j]; }

    // Access the whole row
    const sparse_row& operator[](int i) const { return _rows[i]; }
private:
    int _n, _m;
    std::vector<sparse_row> _rows;
};

```

Using `std::map` to store sparse rows is probably not the best idea performance-wise, but it may be convenient during

assembly phase. Also, AMGCL will copy the matrix to internal structures during construction, so setup performance should not be affected by the choice of the input matrix type too much.

In order to make the above class work as input matrix for AMGCL, we have to specialize a few templates inside `amgcl::backend` namespace (the templates are declared inside `<amgcl/backend/interface.hpp>`). First we need to let AMGCL know the value type of the matrix:

```
namespace amgcl {
namespace backend {

template <> struct value_type<sparse_matrix> {
    typedef double type;
};
```

We also need to tell how to get the dimensions of the matrix and the number of its nonzero elements:

```
// Number of rows in the matrix
template<> struct rows_impl<sparse_matrix> {
    static int get(const sparse_matrix &A) { return A.nrows(); }
};

// Number of cols in the matrix
template<> struct cols_impl<sparse_matrix> {
    static int get(const sparse_matrix &A) { return A.ncols(); }
};

// Number of nonzeros in the matrix. This may be just a rough estimate.
template<> struct nonzeros_impl<sparse_matrix> {
    static int get(const sparse_matrix &A) { return A.nonzeros(); }
};
```

The last and the most involved part is providing a row iterator for the custom matrix type. In order to do this we need to define a `row_iterator<sparse_matrix>::type` class and specialize `row_begin_impl<sparse_matrix>` template that would return the iterator over the given row of the matrix. Here goes:

```
// Here we define row_iterator<sparse_matrix>::type
template<> struct row_iterator<sparse_matrix> {
    struct iterator {
        sparse_matrix::sparse_row::const_iterator _it, _end;

        // Take the matrix and the row number:
        iterator(const sparse_matrix &A, int row)
            : _it(A[row].begin()), _end(A[row].end()) { }

        // Check if the iterator is valid:
        operator bool() const {
            return _it != _end;
        }

        // Advance to the next nonzero element.
        iterator& operator++() {
            ++_it;
            return *this;
        }

        // Column number of the current nonzero element.
        int col() const { return _it->first; }
    };
};
```



```

        // Value of the current nonzero element.
        double value() const { return _it->second; }
    };

    typedef iterator type;
};

// Provide a way to obtain the row iterator for the given matrix row:
template<> struct row_begin_impl<sparse_matrix> {
    typedef typename row_iterator<sparse_matrix>::type iterator;
    static iterator get(const sparse_matrix &A, int row) {
        return iterator(A, row);
    }
};

} // namespace backend
} // namespace amgcl

```

After this, we can directly use our matrix type to create an AMGCL solver:

```

// Discretize a 1D Poisson problem
const int n = 10000;

sparse_matrix A(n, n);
for(int i = 0; i < n; ++i) {
    if (i == 0 || i == n - 1) {
        // Dirichlet boundary condition
        A(i,i) = 1.0;
    } else {
        // Internal point.
        A(i, i-1) = -1.0;
        A(i, i) = 2.0;
        A(i, i+1) = -1.0;
    }
}

// Create an AMGCL solver for the problem.
typedef amgcl::backend::builtin<double> Backend;

amgcl::make_solver<
    amgcl::amg<
        Backend,
        amgcl::coarsening::aggregation,
        amgcl::relaxation::spai0
    >,
    amgcl::solver::cg<Backend>
> solve( A );

```

Note: The complete source code of the example may be found at [examples/custom_adapter.cpp](#).

1.5 Benchmarks

The performance of the library on shared and distributed memory systems was tested on two example problems in a three dimensional space: simple scalar Poisson problem and a non-scalar Navier-Stokes problem. The source code for the benchmarks is available at https://github.com/ddemidov/amgcl_benchmarks.

The first example we consider 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:

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p &= \mathbf{b}, \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned}$$

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.

1.5.1 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.

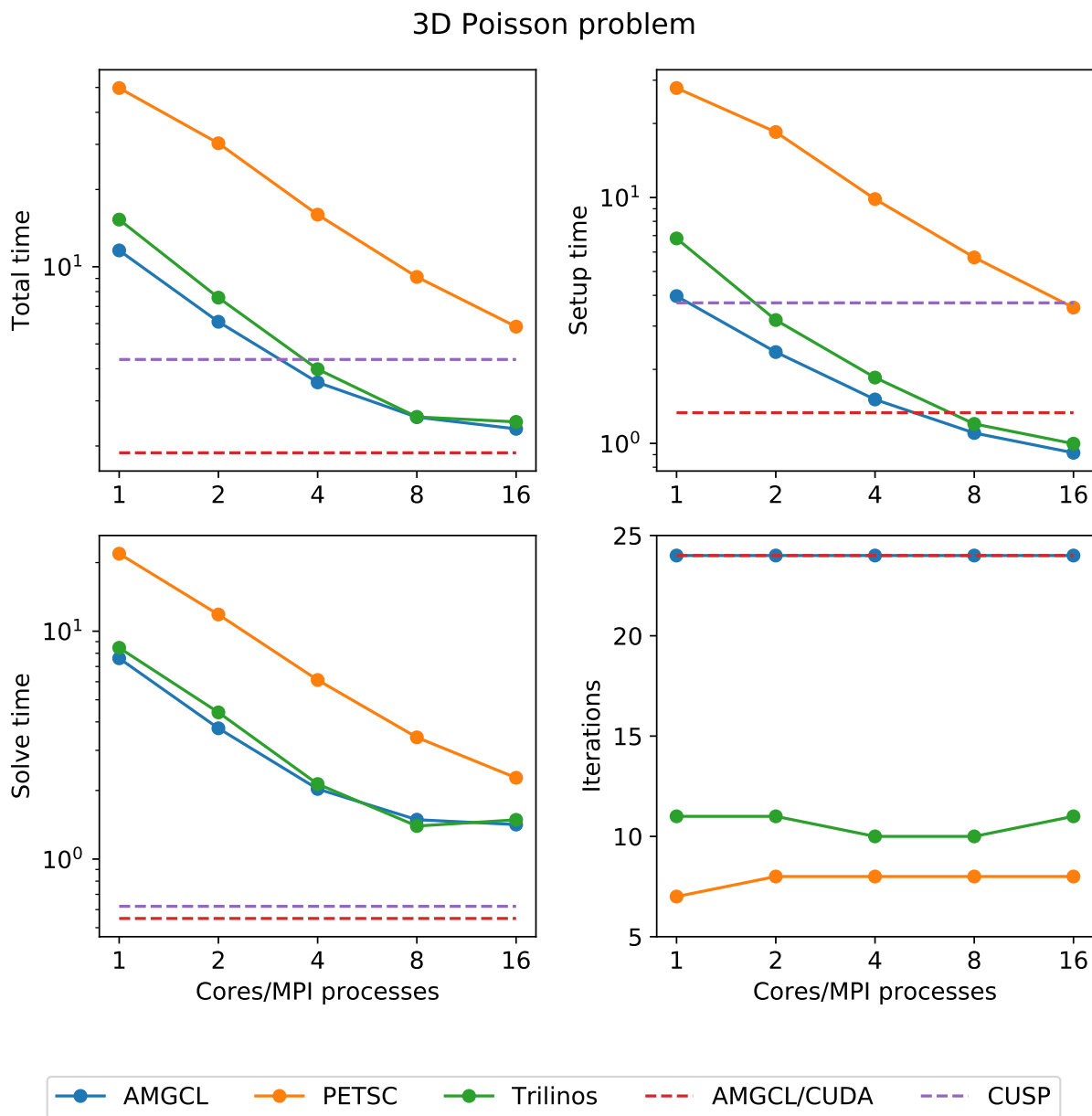
3D Poisson problem

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



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.

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.

1.5.2 Distributed memory benchmarks

Support for distributed memory systems in AMGCL is implemented using the subdomain deflation method. Here we demonstrate performance and scalability of the approach 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-known Trilinos ML package. The benchmarks were run on MareNostrum 4 and PizDaint 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.

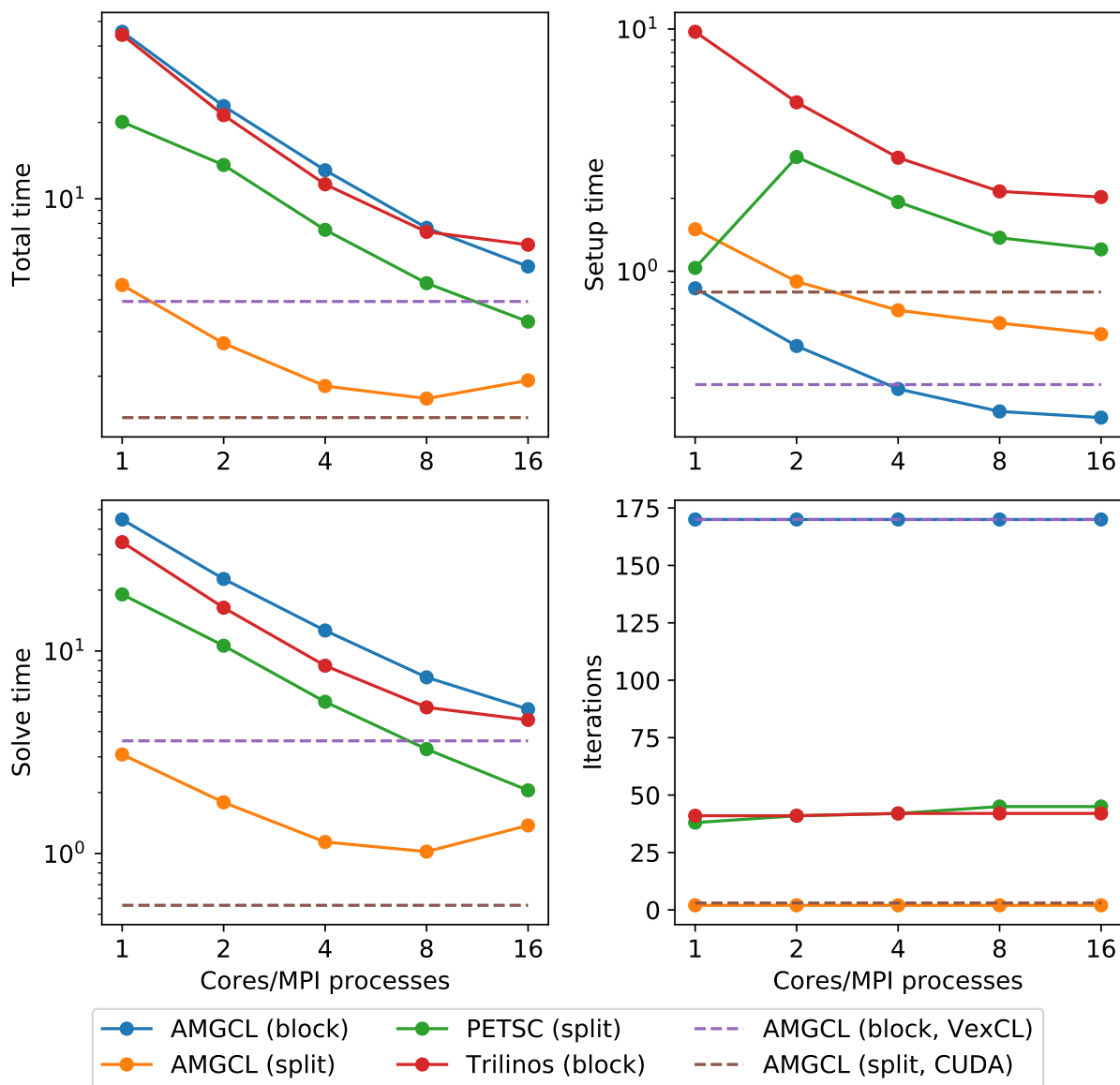
3D Poisson problem

The AMGCL implementation uses a BiCGStab(2) iterative solver preconditioned with subdomain deflation. Smoothed aggregation AMG is used as the local preconditioner. The Trilinos implementation uses CG solver preconditioned with smoothed aggregation AMG with default settings.

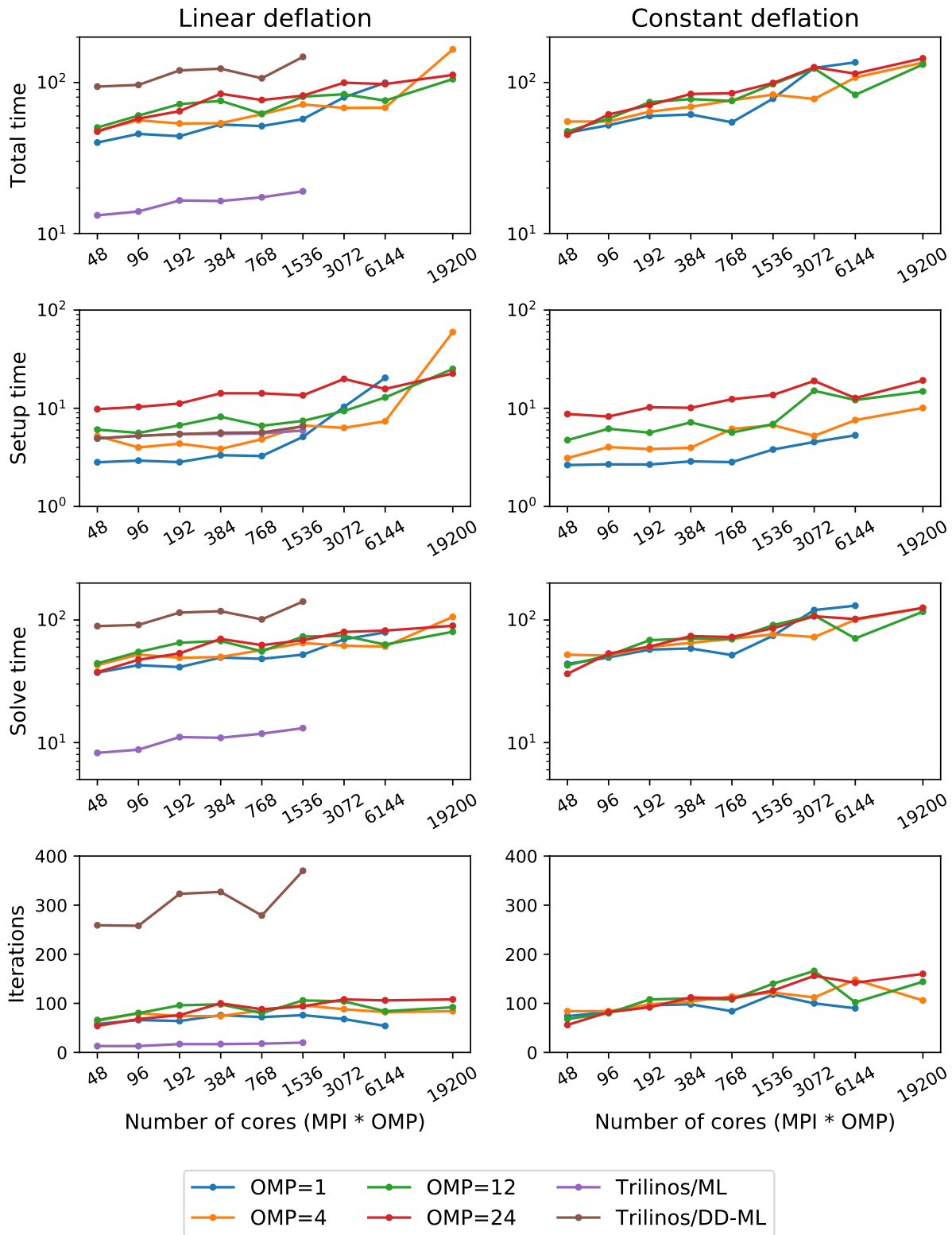
The figure below shows weak scaling of the solution on the MareNostrum 4 cluster. Here the problem size is chosen to be proportional to the number of CPU cores with about 100^3 unknowns per core. The rows in the figure from top to bottom show total computation time, time spent on constructing the preconditioner, 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 768 MPI processes, because the library runs out of memory for larger configurations. The AMGCL data points for 19200 cores with ‘OMP=1’ are missing for the same reason. AMGCL plots in the left and the right columns correspond to the linear deflation and the constant deflation correspondingly

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 AMGCL loses about 6-8% efficiency whenever number of cores doubles. This, however, is much better than we managed to obtain for the Trilinos library, which loses about 36% on each step.

3D Navier-Stokes problem



Weak scaling of the Poisson problem on the MareNostrum 4 cluster



If we look at the AMGCL results for the linear deflation alone, we can see that the ‘OMP=1’ line stops scaling properly at 1536 cores, and ‘OMP=4’ loses scalability at 6144 cores. We refer to the following table for the explanation.

Cores	Setup		Solve			Iterations
	Total	Factorize E	Total	RHS for E	Solve E	
<i>Linear deflation, OMP=1</i>						
384	3.33	0.04	49.35	0.82	0.08	76
1536	5.12	1.09	52.13	1.83	0.80	76
6144	20.39	15.42	79.23	31.81	4.30	54
<i>Constant deflation, OMP=1</i>						
384	2.88	0.00	58.52	0.73	0.01	98
1536	3.80	0.02	74.42	2.51	0.10	118
6144	5.31	0.24	130.76	63.52	0.52	90
<i>Linear deflation, OMP=4</i>						
384	3.86	0.00	49.90	0.15	0.01	74
1536	6.68	0.05	64.91	0.66	0.13	96
6144	7.36	0.76	60.74	2.87	0.79	82
19200	59.72	51.11	105.96	30.86	9.54	84
<i>Constant deflation, OMP=4</i>						
384	3.97	0.00	65.11	0.30	0.00	104
1536	6.73	0.00	76.44	1.01	0.01	122
6144	7.57	0.02	100.39	4.30	0.10	148
19200	10.08	0.74	125.41	48.67	0.83	106

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’ and the ‘Solve’ columns are further split into subcolumns detailing time required for factorization and solution of the coarse system. It is apparent from the table that weak scalability is affected by two factors. First, 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. Second factor is the solution of the coarse problem, which in our experiments is dominated by communication; namely, most of the coarse solve time is spent on gathering the deflated problem right-hand side for solution on the master MPI process.

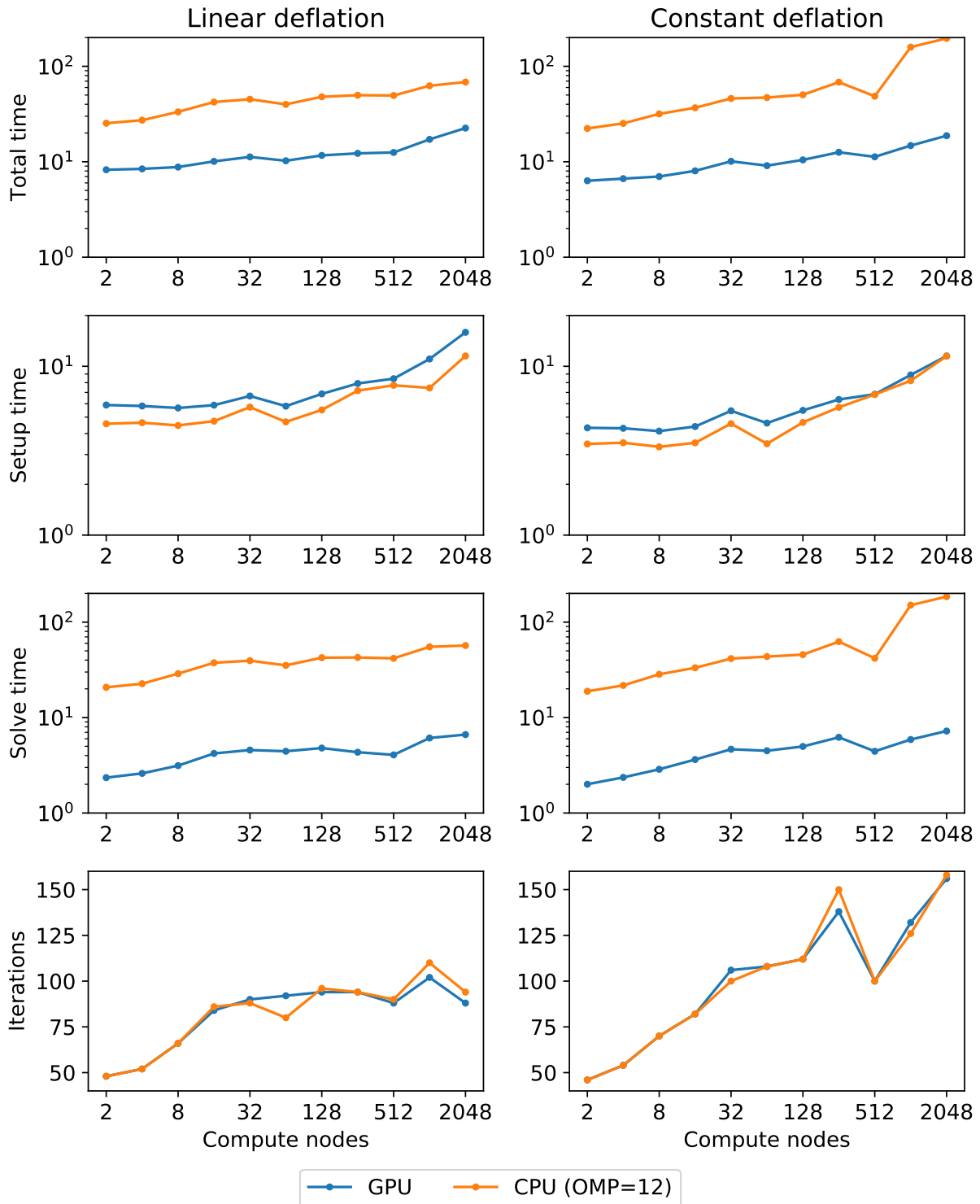
The constant deflation scales better since the deflation matrix is four times smaller than for a corresponding linear deflation case. Hence, the setup time is not affected that much by factorization of the coarse problem. The communication bottleneck is still present though, as is apparent from the table above.

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.

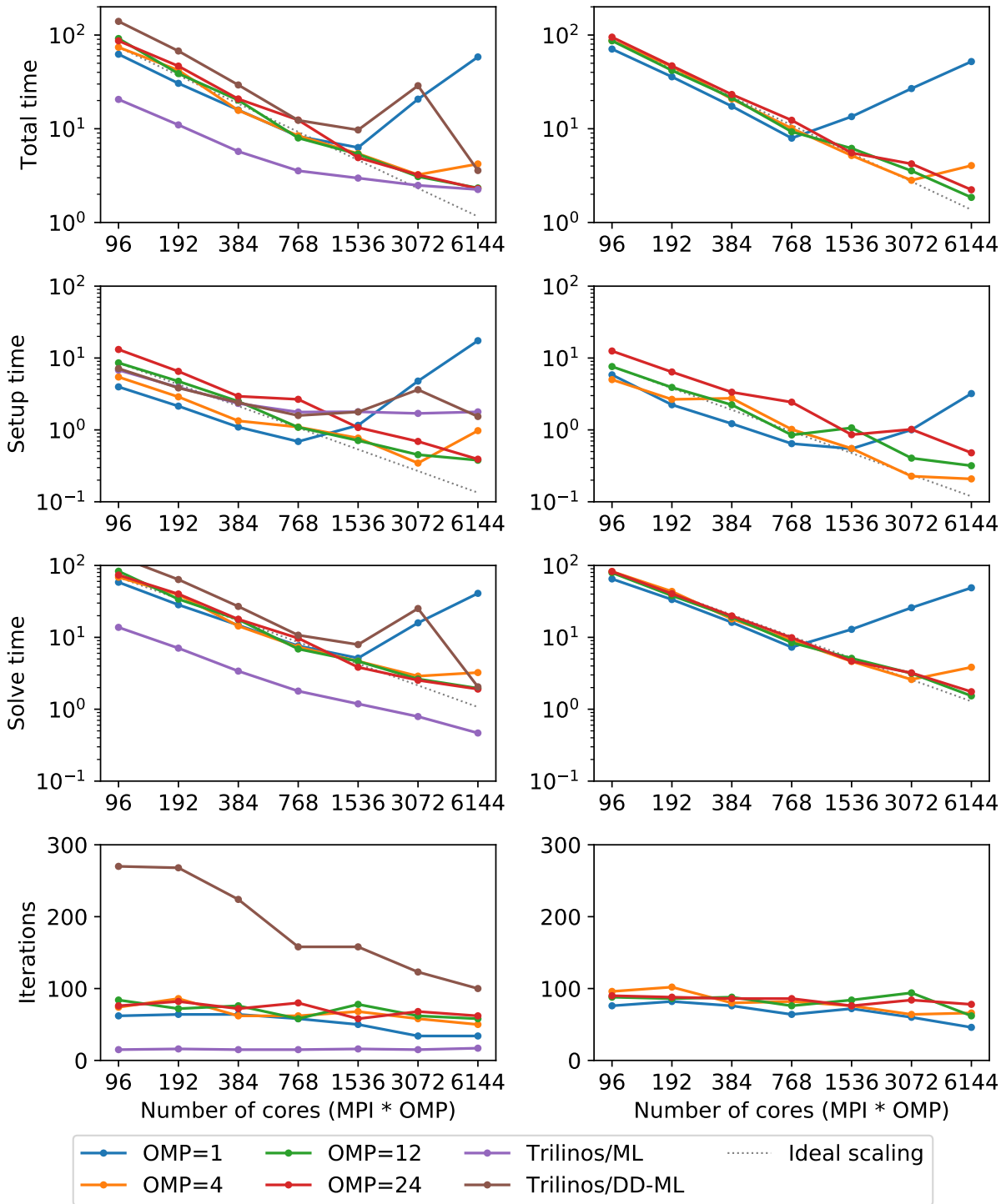
Next figure shows weak scaling of the Poisson problem on the PizDaint cluster. The problem size here is chosen so that each node owns about 200^3 unknowns. We only show the results of the AMGCL library on this cluster to compare performance of the OpenMP and CUDA backends. Intel Xeon E5-2690 v3 CPU is 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.

The figure below 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.

Weak scaling of the Poisson problem on PizDaint cluster



Strong scaling of the Poisson problem on the MareNostrum 4 cluster
 Linear deflation Constant deflation



Here AMGCL scales much better than Trilinos, and is close to ideal for both kinds of deflation. As in the weak scaling case, we see a drop in scalability at about 1536 cores for ‘OMP=1’, but unlike before, the drop is also observable for the constant deflation case. This 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 following table, and it is apparent that the same factorization and coarse solve communication bottlenecks as in the weak scaling scenario come into play. Unfortunately, we were not able to obtain detailed profiling info for the constant deflation, but it should be obvious that in this case communication is the main limiting factor, as the coarse problem factorization costs much less due to reduced size of the deflated space.

Cores	Setup		Solve			Iterations
	Total	Factorize E	Total	RHS for E	Solve E	
<i>Linear deflation, OMP=1</i>						
384	1.01	0.03	14.77	1.04	0.07	64
1536	1.16	0.76	5.15	0.71	0.48	50
6144	17.43	15.58	40.93	34.23	2.72	34
<i>Constant deflation, OMP=1</i>						
384	1.22		16.16			76
1536	0.55		12.92			72
6144	3.20		48.91			46
<i>Linear deflation, OMP=4</i>						
384	1.34	0.00	14.38	0.13	0.01	62
1536	0.77	0.03	4.66	0.40	0.08	68
6144	0.98	0.76	3.24	0.78	0.48	50
<i>Constant deflation, OMP=4</i>						
384	2.75		18.05			80
1536	0.55		4.63			76
6144	0.21		3.83			66

Next figure shows strong scaling AMGCL results for OpenMP and CUDA backends on the PizDaint cluster. The problem size here is 256^3 unknowns. The scalability curves show similar trends as on the MareNostrum 4 cluster, but the GPU scaling is a bit further from ideal due to higher overheads required for managing the GPU and transferring the communication data between the GPU and CPU memories. As in the weak scaling case, the GPU backend is about 9 times faster than the CPU backend during solution phase, and about 3 times faster overall.

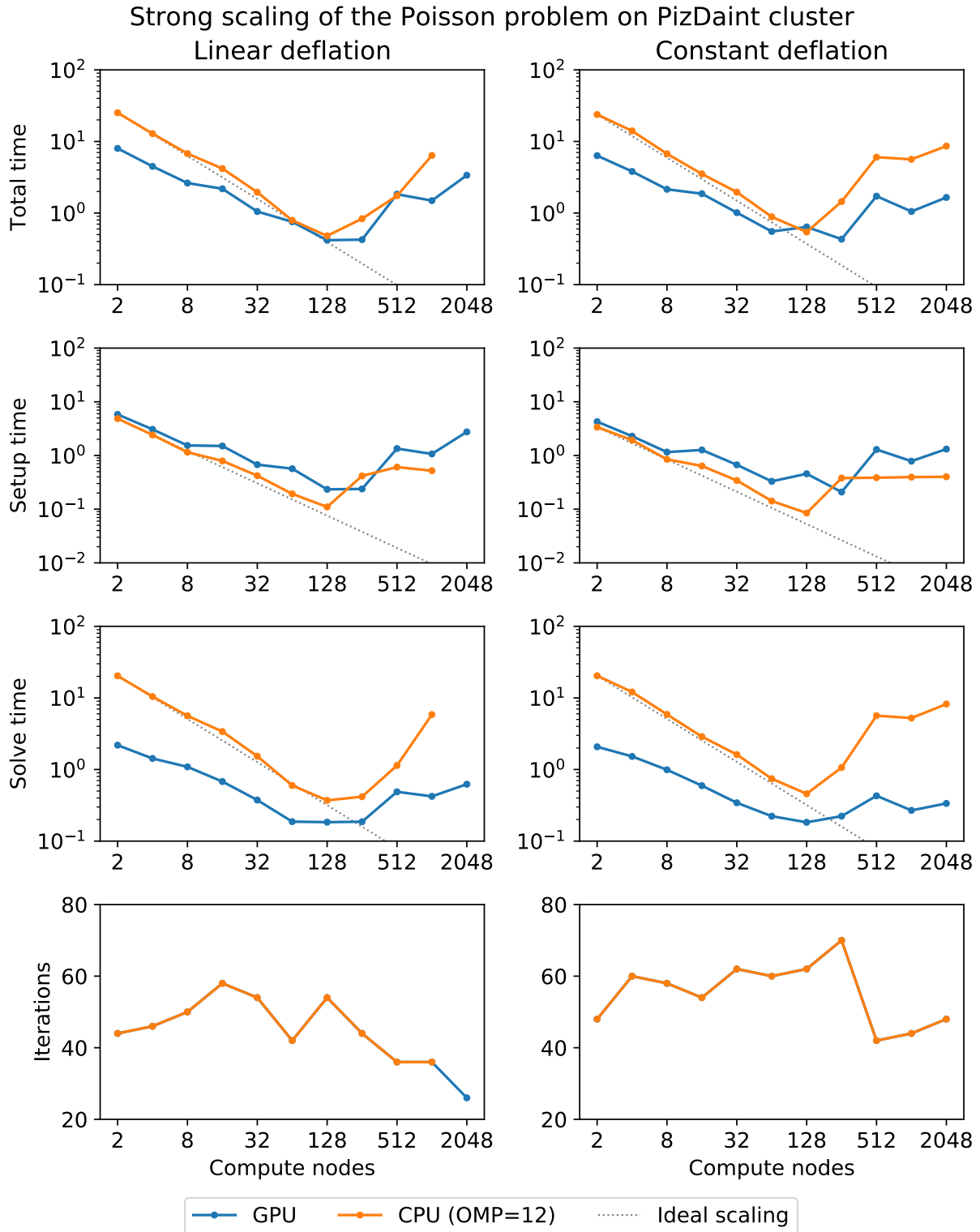
An interesting observation is that convergence of the method improves with growing number of MPI processes. In other words, the number of iterations required to reach the desired tolerance decreases with as the number of subdomains grows, since the deflated system is able to describe the main problem 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’.

3D Navier-Stokes problem

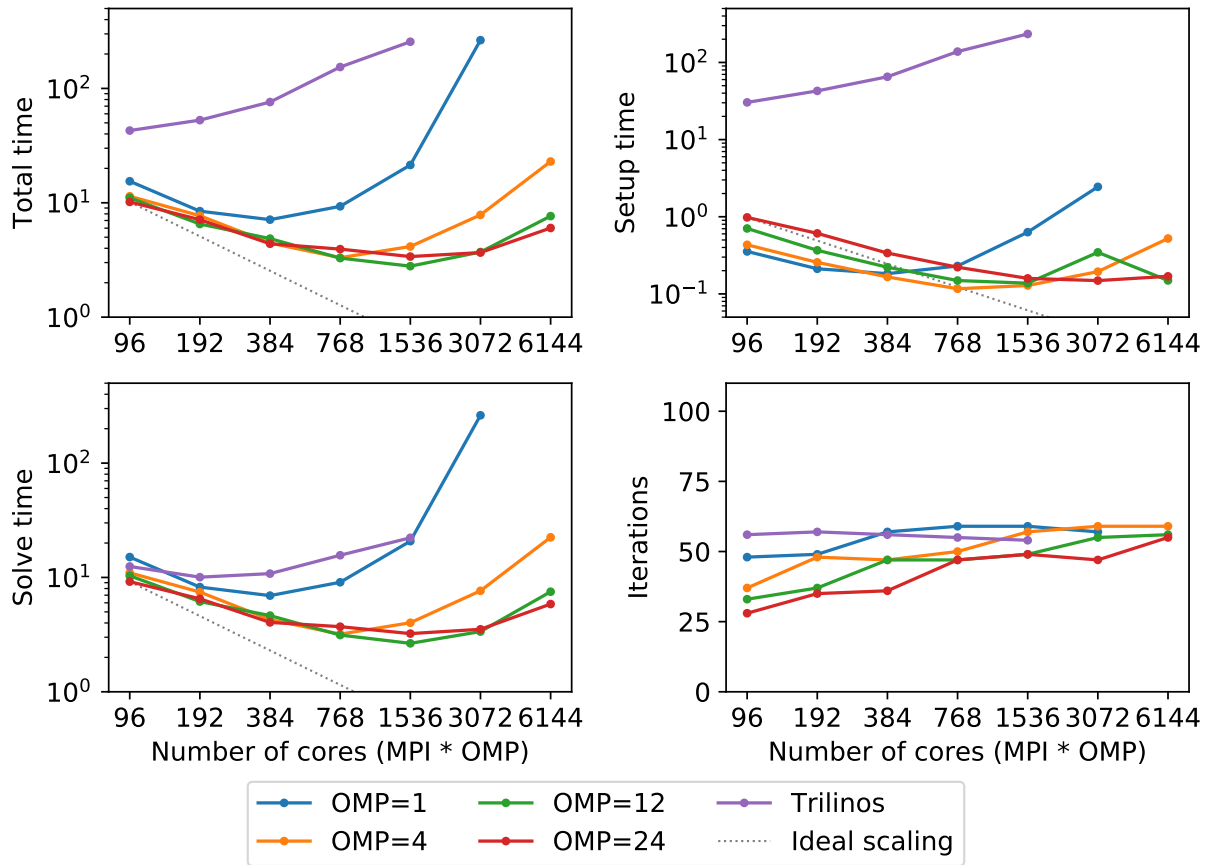
The system matrix in these tests contains 4773588 unknowns and 281089456 nonzeros. AMGCL library uses field-split approach with the `mpi::schur_pressure_correction` preconditioner. Trilinos ML does not provide field-split type preconditioners, and uses the nonsymmetric smoothed aggregation variant (NSSA) applied to the monolithic problem. Default NSSA parameters were employed in the tests.

The 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



Strong scaling of the Navier-Stokes problem on MareNostrum 4 cluster



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 context the use of OpenMP within each domain pays off and allows delivering a greater level of scalability.

1.6 Bibliography

1.7 Indices and tables

- [genindex](#)
- [search](#)

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A

- amgcl::backend::builtin (C++ class), 9
- amgcl::backend::builtin::params (C++ type), 9
- amgcl::backend::builtin::provides_row_iterator (C++ class), 9
- amgcl::backend::vexcl (C++ class), 9
- amgcl::backend::vexcl::params (C++ class), 9
- amgcl::backend::vexcl::provides_row_iterator (C++ class), 9
- amgcl::backend::vexcl<real, DirectSolver>::params::fast_matrix_setup (C++ member), 9
- amgcl::backend::vexcl<real, DirectSolver>::params::q (C++ member), 9
- amgcl::make_solver (C++ class), 5
- amgcl::make_solver::apply (C++ function), 5
- amgcl::make_solver::get_params (C++ function), 6
- amgcl::make_solver::make_solver (C++ function), 5
- amgcl::make_solver::operator() (C++ function), 5
- amgcl::make_solver::params (C++ class), 6
- amgcl::make_solver::precond (C++ function), 6
- amgcl::make_solver::size (C++ function), 6
- amgcl::make_solver::solver (C++ function), 6
- amgcl::make_solver::system_matrix (C++ function), 6
- amgcl::make_solver<Precond, IterativeSolver>::params::precond (C++ member), 6
- amgcl::make_solver<Precond, IterativeSolver>::params::solver (C++ member), 6
- amgcl::runtime::amg (C++ class), 15
- amgcl::runtime::amg::amg (C++ function), 15
- amgcl::runtime::amg::apply (C++ function), 15
- amgcl::runtime::amg::cycle (C++ function), 15
- amgcl::runtime::amg::size (C++ function), 15
- amgcl::runtime::amg::system_matrix (C++ function), 15
- amgcl::runtime::coarsening::aggregation (C++ enumerator), 16
- amgcl::runtime::coarsening::ruge_stuben (C++ enumerator), 15
- amgcl::runtime::coarsening::smoothed_aggr_emin (C++ enumerator), 16
- amgcl::runtime::coarsening::smoothed_aggregation (C++ enumerator), 16
- amgcl::runtime::coarsening::type (C++ type), 15
- amgcl::runtime::iterative_solver (C++ class), 16
- amgcl::runtime::iterative_solver::iterative_solver (C++ function), 16
- amgcl::runtime::iterative_solver::operator() (C++ function), 16, 17
- amgcl::runtime::relaxation::chebyshev (C++ enumerator), 16
- amgcl::runtime::relaxation::damped_jacobi (C++ enumerator), 16
- amgcl::runtime::relaxation::gauss_seidel (C++ enumerator), 16
- amgcl::runtime::relaxation::ilu0 (C++ enumerator), 16
- amgcl::runtime::relaxation::iluk (C++ enumerator), 16
- amgcl::runtime::relaxation::ilut (C++ enumerator), 16
- amgcl::runtime::relaxation::spai0 (C++ enumerator), 16
- amgcl::runtime::relaxation::spai1 (C++ enumerator), 16
- amgcl::runtime::relaxation::type (C++ type), 16
- amgcl::runtime::solver::bicgstab (C++ enumerator), 17
- amgcl::runtime::solver::bicgstabl (C++ enumerator), 17
- amgcl::runtime::solver::cg (C++ enumerator), 17
- amgcl::runtime::solver::fgmres (C++ enumerator), 17
- amgcl::runtime::solver::gmres (C++ enumerator), 17
- amgcl::runtime::solver::idrs (C++ enumerator), 17
- amgcl::runtime::solver::lgmres (C++ enumerator), 17
- amgcl::runtime::solver::type (C++ type), 17
- amgcl::solver::bicgstab (C++ class), 10
- amgcl::solver::bicgstab::bicgstab (C++ function), 11
- amgcl::solver::bicgstab::params (C++ class), 11
- amgcl::solver::bicgstab<Backend, InnerProduct>::params::abstol (C++ member), 11
- amgcl::solver::bicgstab<Backend, InnerProduct>::params::maxiter (C++ member), 11
- amgcl::solver::bicgstab<Backend, InnerProduct>::params::pside (C++ member), 11

amgcl::solver::bicgstab<Backend, InnerProduct>::params::tol (C++ member), 11
 amgcl::solver::bicgstabl (C++ class), 11
 amgcl::solver::bicgstabl::bicgstabl (C++ function), 11
 amgcl::solver::bicgstabl::params (C++ class), 11
 amgcl::solver::cg (C++ class), 10
 amgcl::solver::cg::cg (C++ function), 10
 amgcl::solver::cg::params (C++ class), 10
 amgcl::solver::cg<Backend, InnerProduct>::params::abstol (C++ member), 10
 amgcl::solver::cg<Backend, InnerProduct>::params::maxiter (C++ member), 10
 amgcl::solver::cg<Backend, InnerProduct>::params::tol (C++ member), 10
 amgcl::solver::fgmres (C++ class), 13
 amgcl::solver::fgmres::fgmres (C++ function), 13
 amgcl::solver::fgmres::params (C++ class), 14
 amgcl::solver::fgmres<Backend, InnerProduct>::params::abstol (C++ member), 14
 amgcl::solver::fgmres<Backend, InnerProduct>::params::M (C++ member), 14
 amgcl::solver::fgmres<Backend, InnerProduct>::params::maxiter (C++ member), 14
 amgcl::solver::fgmres<Backend, InnerProduct>::params::tol (C++ member), 14
 amgcl::solver::gmres (C++ class), 12
 amgcl::solver::gmres::gmres (C++ function), 12
 amgcl::solver::gmres::params (C++ class), 12
 amgcl::solver::gmres<Backend, InnerProduct>::params::abstol (C++ member), 12
 amgcl::solver::gmres<Backend, InnerProduct>::params::M (C++ member), 12
 amgcl::solver::gmres<Backend, InnerProduct>::params::maxiter (C++ member), 12
 amgcl::solver::gmres<Backend, InnerProduct>::params::pside (C++ member), 12
 amgcl::solver::gmres<Backend, InnerProduct>::params::tol (C++ member), 12
 amgcl::solver::lgmres (C++ class), 12
 amgcl::solver::lgmres::lgmres (C++ function), 12
 amgcl::solver::lgmres::params (C++ class), 12
 amgcl::solver::lgmres<Backend, InnerProduct>::params::abstol (C++ member), 13
 amgcl::solver::lgmres<Backend, InnerProduct>::params::always_reset (C++ member), 13
 amgcl::solver::lgmres<Backend, InnerProduct>::params::K (C++ member), 13
 amgcl::solver::lgmres<Backend, InnerProduct>::params::M (C++ member), 13
 amgcl::solver::lgmres<Backend, InnerProduct>::params::maxiter (C++ member), 13
 amgcl::solver::lgmres<Backend, InnerProduct>::params::pside (C++ member), 13

O

operator() (C++ function), 10
 operator<< (C++ function), 15