

Chapter 1

Linear solvers

The purpose of this tutorial is to show how to specify different linear solvers for `oomph-lib`'s Newton solver.

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1.1 Overview

As discussed in the [bottom-up discussion of `oomph-lib`'s data structure](#), by default `oomph-lib`'s Newton solver, `Problem::newton_solve(...)` solves the linear systems arising during the Newton iteration with its default linear solver, `SuperLUSolver`, a wrapper to Demmel, Eistenstat, Gilbert, Li & Liu's sparse direct solver `SuperLU`.

`oomph-lib` provides a large number of alternative linear solvers that may be used instead. All linear solvers within the library are derived from the base class `LinearSolver` which contains a single pure virtual function

```
virtual void solve(Problem* const& problem_pt, DoubleVector& result) = 0;
```

whose task it is to compute the solution $\delta\mathbf{x}$ (returned in the vector `result`) of the linear system

$$\mathcal{J}\delta\mathbf{x} = -\mathbf{r}$$

where `r` and \mathcal{J} are the global Jacobian and the residual vector, computed by the `Problem` pointed to by `problem_pt`. The `LinearSolver` class also defines linear-algebra-type interfaces that allow the solution of linear systems with matrices other than the `Problem`'s Jacobian matrix. However, these methods may not be implemented for all linear solvers.

1.2 List of available linear solvers

`oomph-lib`'s linear solvers can be sub-divided into serial and parallel, and direct and iterative linear solvers. Here is a quick overview of the available linear solvers. If you are viewing this document online, the links take you directly to the solvers' class references which explain any solver-specific member functions.

- **Serial solvers:**

– Direct solvers:

- * `SuperLUSolver`: oomph-lib's default linear solver, a wrapper to Demmel, Eistenstat, Gilbert, Li & Liu's sparse direct solver `SuperLU`.
- * `HSL_MA42`: A wrapper to the frontal solver MA42 from the `HSL library`. This solver is available free-of-charge for UK academics. The source code can be dropped into the oomph-lib distribution; see the instructions in the dummy code

`external_src/oomph_hsl/dummy_frontal.f`

- * `DenseLU`: A direct solver, based on the LU decomposition of the Jacobian matrix which is stored as a dense matrix. Given that the Jacobian matrices arising from most problems are sparse, this is likely to be a very inefficient solver. It is mainly used by the derived (and even more inefficient!) solver `FD_LU`.
- * `FD_LU`: Almost certainly the world's most inefficient solver. It computes the Jacobian matrix by finite differencing the global residual vector, without taking any sparsity into account. Mainly used by developers as a last-resort sanity check.

– Iterative solvers:

- * oomph-lib provides its own implementations of various standard iterative linear solvers. They are derived from the base class `IterativeLinearSolver` and are typically templated by the matrix type used to store the Jacobian matrix. In most cases you will want to set the template argument MATRIX to `CRDoubleMatrix`:
 - `GMRES`: A Krylov subspace solver for symmetric and non-symmetric linear systems. The memory usage increases with each iteration but the iteration can be restarted.
 - `BiCGStab`: A Krylov subspace method for symmetric and non-symmetric linear systems. The memory requirement remains constant throughout the iteration.
 - `CG`: The classical conjugate gradient method for symmetric positive definite matrices. The memory requirement remains constant throughout the iteration.
 - `GS`: Gauss-Seidel – a stationary iterative solver.
- * oomph-lib also provides wrappers to third-party iterative linear solvers. These tend to provide their own implementations of GMRES, BiCGStab, CG, etc. but are not necessarily derived from oomph-lib's own `IterativeLinearSolver` base class.
 - `HypreSolver`: A wrapper to the high-performance linear solvers/preconditioners from the `Scalable Linear Solvers Project`.

- `TrilinosAztecOOsolver`: A wrapper to the linear solvers from the [Trilinos Project](#).

- **Parallel solvers:**
 - **Direct solvers:**
 - * When `oomph-lib` is compiled with MPI support, its default linear solver `SuperLUSolver` becomes a wrapper to Demmel, Eistenstat, Gilbert, Li & Liu's parallel sparse direct solver `SuperLU_DIST`. This behaviour can be over-ruled with the member function `SuperLUSolver::set_solver_type(...)` whose argument must specify one of the three options listed in the enumeration `SuperLUSolver::Type`. This allows the serial solver `SuperLU` to be used even if `oomph-lib` is compiled with MPI support.

 - * `MumpsSolver` : is a wrapper to the `MUMPS` multifrontal solver that is available when `oomph-lib` is compiled with MPI support and support for MUMPS.
 - **Iterative solvers:**
 - * `HypreSolver`: A wrapper to the high-performance linear solvers/preconditioners from the [Scalable Linear Solvers Project](#).

 - * `TrilinosAztecOOsolver`: A wrapper to the linear solvers from the [Trilinos Project](#).

1.3 How to change the LinearSolver

1.3.1 Direct solvers

Changing `oomph-lib`'s linear solver is straightforward. For instance, to change the linear solver to `oomph-lib`'s `DenseLU` solver, simply create an instance of this solver and pass a pointer to it to the `Problem`. This most easily done in the `Problem` constructor:

```
// Change solver to DenseLU
linear_solver_pt()=new DenseLU;
```

In any subsequent calls to `oomph-lib`'s Newton solver, `DenseLU` will now be used to solve the linear systems arising during the Newton iteration.

1.3.2 Iterative linear solvers and preconditioners

The specification of an iterative linear solver is just as easy: For instance, to specify `oomph-lib`'s conjugate gradient solver `CG` (storing the Jacobian matrix in compressed row format) as the linear solver, add

```
// Change solver to CG
IterativeLinearSolver* solver_pt=new CG<CRDoubleMatrix>;
linear_solver_pt()=solver_pt;
```

to the problem constructor. We note that, by default, `oomph-lib`'s `IterativeLinearSolvers` perform the preconditioning using the trivial "identity preconditioner". Most Krylov subspace solvers perform very poorly without some sort of preconditioning.

Specific preconditioners may be implemented by deriving from the Preconditioner base class, by implementing its two pure virtual functions

```
/// Apply the preconditioner. Pure virtual generic interface
/// function. This method should apply the preconditioner operator to the
/// vector r and return the vector z.
virtual void preconditioner_solve(const DoubleVector& r,
                                  DoubleVector& z) = 0;
```

and

```
/// Setup the preconditioner. Pure virtual generic interface
/// function.
virtual void setup() = 0;
```

Note that, by default, oomph-lib's IterativeLinearSolvers employ left preconditioning.

oomph-lib provides fully-functional implementations of several general-purpose preconditioners. For instance, the zero-fill-in incomplete LU factorisation preconditioner ILU(0) may be employed by adding the lines

```
// Specify preconditioner
solver_pt->preconditioner_pt() = new ILUZeroPreconditioner<CRDoubleMatrix>;
```

to the Problem constructor.

Of particular interest is the availability of an "exact preconditioner"

[SuperLUPreconditioner](#) whose use guarantees the convergence of any iterative solver within a single iteration – useful for code development.

1.3.3 Third-party iterative linear solvers and preconditioners

oomph-lib provides wrappers to various third-party iterative linear solvers and preconditioners. We stress that these solvers are not necessarily implemented as oomph-lib IterativeLinearSolvers since their interfaces for the specification of preconditioners, etc may differ from those employed by oomph-lib.

1.3.3.1 Trilinos

oomph-lib provides wrappers to the iterative linear solvers/preconditioners from the [Trilinos Project](#). The demo code [TrilinosSolver_test.cc](#) demonstrates how use various combinations of solvers/preconditioners. Here is a brief overview:

Trilinos solvers

The wrappers to Trilinos' Krylov subspace solvers are implemented as oomph-lib IterativeLinearSolvers, allowing them to be used via the standard interfaces described above. For instance, to use oomph-lib's wrapper to Trilinos' Aztec solver, using Trilinos' ML multilevel preconditioner, set the solvers and preconditioners as usual:

```
// Create a Trilinos Solver
TrilinosAztecOOSolver* linear_solver_pt = new TrilinosAztecOOSolver;

// Create the Trilinos ML preconditioner
TrilinosMLPreconditioner* preconditioner_pt = new TrilinosMLPreconditioner;

// Set the preconditioner pointer
linear_solver_pt->preconditioner_pt() = preconditioner_pt;

// Set linear solver
problem.linear_solver_pt() = linear_solver_pt;
```

The actual Krylov subspace solver used by the Trilinos solver is specified by passing an enumerated flag (defined as static member data in the TrilinosAztecOOSolver class) to the solver. For instance, Trilinos' CG, GMRES and BiCGStab solvers are selected with

```
linear_solver_pt->solver_type() = TrilinosAztecOOSolver::CG;
or
linear_solver_pt->solver_type() = TrilinosAztecOOSolver::GMRES;
or
linear_solver_pt->solver_type() = TrilinosAztecOOSolver::BiCGStab;
```

respectively.

Trilinos preconditioners

oomph-lib provides wrappers to Trilinos' ML and IFPACK preconditioners that allows them to be used as oomph-lib Preconditioners that may be used with oomph-lib's own IterativeLinearSolvers. Here is an example that shows how to build an instance of oomph-lib's GMRES, preconditioned with its wrapper to Trilinos' IFPACK preconditioner:

```
// Create oomph-lib linear solver
IterativeLinearSolver* linear_solver_pt=new GMRES<CRDoubleMatrix>;

// Create Trilinos IFPACK preconditioner as oomph-lib Preconditioner
Preconditioner* preconditioner_pt=new TrilinosIFPACKPreconditioner;

// Pass pointer to preconditioner to oomph-lib IterativeLinearSolver
linear_solver_pt->preconditioner_pt()=preconditioner_pt;
```

1.3.3.2 Hypre

oomph-lib provides wrappers to the high-performance linear solvers/preconditioners from the [Scalable Linear Solvers Project](#). The demo code `HypreSolver_test.cc` demonstrates how to use various combinations of solvers/preconditioners. Here is a brief overview:

Hypre solvers

The wrappers to Hypre's Krylov subspace and AMG solvers are implemented as oomph-lib `LinearSolvers` (not `IterativeLinearSolvers!`) so the interfaces for the specification of preconditioners etc. differ from those for oomph-lib's own `IterativeLinearSolvers`.

The `HypreSolver` is set like any other `LinearSolver`:

```
// Create a new Hypre linear solver
HypreSolver* hypre_linear_solver_pt = new HypreSolver;

// Set the linear solver for problem
problem.linear_solver_pt() = hypre_linear_solver_pt;
```

The actual solver used by the `HypreSolver` is specified by passing an enumerated flag (defined as static member data in the `HypreSolver` class) to the solver. For instance, Hypre's AMG, CG, GMRES and BiCGStab solvers are selected with

```
hypre_linear_solver_pt->hypre_method() = HypreSolver::BoomerAMG;
or
hypre_linear_solver_pt->hypre_method() = HypreSolver::CG;
or
hypre_linear_solver_pt->hypre_method() = HypreSolver::GMRES;
or
hypre_linear_solver_pt->hypre_method() = HypreSolver::BiCGStab;
```

respectively.

These Krylov subspace methods may then be preconditioned by Hypre's own (internal) preconditioners, again by specifying the method via an enumerated flag. So, to use no preconditioning, or to precondition with BoomerAMG (and AMG-based preconditioner), Euclid (an ILU preconditioner) or ParaSails (a sparse approximate inverse preconditioner), set:

```
hypre_linear_solver_pt->internal_preconditioner()=HypreSolver::None;
or
hypre_linear_solver_pt->internal_preconditioner()=HypreSolver::BoomerAMG;
or
hypre_linear_solver_pt->internal_preconditioner()=HypreSolver::Euclid;
or
hypre_linear_solver_pt->internal_preconditioner()=HypreSolver::ParaSails;
```

respectively.

Hypre preconditioners

oomph-lib provides wrappers to Hypre's preconditioners that allows them to be used as oomph-lib Preconditioners that may be used with oomph-lib's own `IterativeLinearSolvers`. Here is an example that shows how to build an instance of oomph-lib's BiCGStab and to use the `HyprePreconditioner` as the preconditioner:

```
// Build and instance of BiCGStab and pass it to the problem
oomph_linear_solver_pt = new BiCGStab<CRDoubleMatrix>;

problem.linear_solver_pt() = oomph_linear_solver_pt;
```

Now we build an instance of a `HyprePreconditioner`

```
// Create a new Hypre preconditioner
HyprePreconditioner* hypre_preconditioner_pt = new HyprePreconditioner;
```

and set it as the Preconditioner for oomph-lib's BiCGStab solver:

```
oomph_linear_solver_pt->preconditioner_pt()=hypre_preconditioner_pt;
```

The actual preconditioning methodology to be used by the `HyprePreconditioner` is again selected via enumerated flags, i.e.

```
hypre_preconditioner_pt->hypre_method() = HyprePreconditioner::BoomerAMG;
or
hypre_preconditioner_pt->hypre_method() = HyprePreconditioner::Euclid;
or
hypre_preconditioner_pt->hypre_method() = HyprePreconditioner::ParaSails;
```

1.4 Problem-specific preconditioners

In addition to "general-purpose" preconditioners like ILU, oomph-lib provides a number of problem-specific preconditioners which are typically based on the library's block preconditioning framework. Separate documentation is available for these:

- We provide a (very!) detailed discussion of oomph-lib's [block preconditioning framework](#).
 - Another tutorial discusses oomph-lib's "[general purpose](#)" [block preconditioners](#).
 - The NavierStokesSchurComplementPreconditioner for Navier-Stokes problems is described in its [own tutorial](#).
 - The FSIPreconditioner for monolithically-discretised fluid-structure interaction problems is described in its [own tutorial](#).
 - We provide a [preconditioner for large-displacement solid mechanics problems in which boundary displacements are prescribed](#).
 - The previous preconditioner is mainly used as a subsidiary block preconditioner for the [solution of fluid-structure interaction problems with \(pseudo-\)solid fluid mesh updates](#).
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1.5 PDF file

A [pdf version](#) of this document is available. \