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Mazen Ali
Christopher Davis

Dr. Andreas Borchert
Prof. Dr. Stefan Funken
Prof. Dr. Karsten Urban

Institute for Numerical Mathematics

A Reimplementation of the Finite Element Method Software Package using FLENS

Mazen Ali, Christopher Davis

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0 Introduction

The primary objective of the High Performance Computing lecture course is the parallelisation of various numerical methods, with a particular focus on the Finite Element Method. For this project we have been supplied with a (subsection of a) software package (which we shall henceforth refer to as *the FEM package*) that computes the solution to the Poisson partial differential equation using the Finite Element Method. This package is self-contained - it includes its own custom matrix/vector classes, and its own implementations of linear algebra operations on these types. Our goal is to make improvements to the package with the help of FLENS.

FLENS (*Flexible Library for Efficient Numerical Solutions*) is a C++ library, written by Dr. Michael Lehn, which offers a comprehensive collection of matrix and vector classes. Included is a C++ -based BLAS (*Basic Linear Algebra Subfunctions*) implementation, which provides linear algebra operations, such as matrix-vector multiplication, on these types.

The advantages of using FLENS in the FEM package are numerous. Firstly, use of an external library for matrix/vector types adds standardisation to the package. A user who is unfamiliar with the FEM package, but has experience of FLENS from other projects, for example, would benefit from such standardisation. Secondly, the library can be linked, with almost trivial effort, to any optimised BLAS or LAPACK libraries that are available, such as *ATLAS* or *Goto BLAS*, for instant performance increases of BLAS operations. Thirdly, FLENS offers overloaded operators for linear algebra operations. We recognise that users from different backgrounds may have a preference regarding the notation used for such operations, be it the tradition BLAS notation:

```
1 ||    blas::mv(NoTrans, One, A, p, Zero, Ap);
```

or notation more akin to that of MATLAB:

```
1 ||    Ap = A*p;
```

(for the matrix-vector product of some matrix A, vector p). With FLENS, we have the choice.

We therefore summarise the aims of this project as follows:

1. Replace all data storage objects in the FEM package with FLENS-based objects.
2. Where possible replace linear algebra operations with BLAS equivalents via the FLENS framework, to allow for speed-up from optimised BLAS libraries.
3. Offer two versions of solvers, one using BLAS notation, one using overloaded operators.

1 Part I (Christopher Davis)

1.1 Matrix and Vector Types

A major task when converting the FEM package to the FLENS framework is the transition from the package's custom storage types to FLENS-based types. Of course, some types, such as the package's `Vector` class, have exact FLENS equivalents. Others, however, contain bespoke objects and methods for MPI communications. Clearly we must create our own custom storage types in the latter cases.

1.1.1 Equivalent Types and Index Base

We adopt the following direct type conversions from the FEM package to FLENS framework:

$$\begin{aligned} \texttt{Vector} &\rightarrow \texttt{DenseVector}\langle\texttt{Array}\langle\texttt{double}\rangle\ \rangle \\ \texttt{IndexVector} &\rightarrow \texttt{DenseVector}\langle\texttt{Array}\langle\texttt{int}\rangle\ \rangle \end{aligned}$$

However we must note that the default index base in FLENS is 1, as opposed to that of the package, which has index base 0. We accept this default value, despite the awkwardness it adds to the transition, because 1 is the natural choice of index base with respect to the mesh geometry. The numbering of the mesh nodes starts at 1, and assembly of the system of linear equations frequently accesses vector elements corresponding to node identities. For example in the FEM package:

```
1 || someVec_FEMpackage(nodeID - 1) = someValue;
```

as opposed to using FLENS:

```
1 || someVec_FLENS(nodeID) = someValue;
```

Whilst this is a purely cosmetic change, it may help to avoid future problems caused by forgetting to subtract 1 from node identities. For consistency, we implemented all FLENS matrices/vectors with this default index base of 1.

FLENS includes a CRS (*Column-Row-Storage*) storage scheme for sparse matrices, offering a direct conversion from the FEM package's `CRSMatrix` class. However, these FLENS CRS matrices must be initialised via conversion from a FLENS sparse matrix with a coordinate storage scheme. Thus the conversion effects a change in the initialisation of the matrix object, but not requiring the creation of a custom matrix class.

1.1.2 TypeI and TypeII

The FEM package adopts the nomenclature defined in the lecture course, of *TypeI* and *TypeII* to distinguish between vectors that contain values corresponding to the problem posed on a compute node's local mesh, or on the global mesh:

- **TypeI**: global values.
- **TypeII**: local values.

We adopt this definition in this paper and in our code, and refer to these types as *MPI vector types*.

1.1.3 FLENSDataVector

The FEM package's `DataVector` class is the package's primary custom vector type. Members are comprised of:

- A `Vector` object: stores the values/elements of the `DataVector`.
- A `Coupling` object: contains mesh geometry information required for MPI communications.
- A `vectorType` enumerated type: determines the MPI vector type of the vector (see Section 1.1.2).

We propose a FLENS-based replacement for this class called `FLENSDataVector`, which incorporates a few small, yet profound, modifications to the general structure.

Firstly, we make the obvious choice of using a FLENS `DenseVector⟨Array⟨double⟩ ⟩` to store our vector values/elements. We choose to *derive* our class from this FLENS type, rather than specifying a `DenseVector` as a member object. I.e. we use an 'is-a' `DenseVector` approach, rather than a 'has-a' `DenseVector` approach. The advantage is that our class inherits all methods and overloaded operators from the `DenseVector` class, and can therefore be passed directly to the FLENS BLAS functions. This lends itself to a more parsimonious implementation - under the 'has-a' approach we would need to overload every BLAS function, for example:

```
1  double
2  dot(FLENSDataVector x, FLENSDataVector y) {
3       blas::dot(x.vec, y.vec);
4  }
```

and clutter our `FLENSDataVector` class with trivial operators, such as:

```
1  double &
2  operator()(int index) {
3       return vec(index);
4  }
```

neither of which are desirable.

The `Coupling` object is stored as a constant reference - the same way as in the FEM package.

Next we consider the enumerated type that specifies the MPI vector type in the FEM package's `DataVector`. Here we wish to change the structure somewhat - whilst setting the MPI vector type in this fashion is easy and flexible, allowing the type to be changed as and when required, we find this to be *too* flexible, and not ideal from a software design perspective. To help explain the situation, we consider a blind man and his socks.

> *The man in question loves to wear socks, and therefore does so at all times. He commands an extensive collection, comprising a wide range of different colours. Each morning he changes his socks, taking care to pair the dirty socks together so that they remain paired after washing. His system appears to work well - he always wears matching socks, and as a result leads a successful life. But what if one morning, whilst in the midst of changing his socks, he is distracted by the telephone ringing, and as such neglects to change one of his socks - now his socks don't match! Whilst we would like to think that some kind person may notify him of his mistake, the world can be a cruel place. Odd socks are rarely tolerated by modern societies, and so his life's achievements would probably crumble around him.*

Returning to the world of the FEM package, we hope that the difficulties that could arise from the enumerated type are clearer - there is no way of determining whether the values contained in a TypeI `DataVector` are actually global values. There is always the chance that some rogue function changed the type without modifying the values, or vice-versa. Such a problem would not make for an enjoyable debugging task.

Thus our `FLENSDataVector` is implemented as a template class, requiring the MPI vector type to be defined (permanently) at instantiation. The following classes are permitted as specialisation types:

- `class FLvNonMPI`
- `class FLvTypeI`
- `class FLvTypeII`

Clever implementation of the `FLENSDataVector` constructors limits specialisation of the vector class *only* to these types, as well as ensuring that a Coupling object is specified for MPI types (and not for the non-MPI). We achieve this by adding specialisations of the constructor template function for these types, for example:

```
1 template <>
2 FLENSDataVector<FLvNonMPI>::FLENSDataVector(int n)
3         :       DenseVector<Array<double> >(n),
4                 coupling(Coupling())
5 {
6         //Permits instatiation of FlNonMPI specialisation.
7 }
```

and we add a line to the unspecialised constructor that will cause an error at *compile time* if scope ever reaches there (which would be due to a wrong type specialisation):

```
template <typename VTYPE>
FLENSDataVector<VTYPE>::FLENSDataVector(int n)
        :       coupling(Coupling())
{
        VTYPE::CHK;                     //<-- If scope ever reaches here,
                                        //compilation will fail.
                        //e.g. if FLENSDataVector<double> instantiated.
}
```

Thus the following instantiation would cause a compiler error:

```
FLENSDataVector<double>  oops(5);
```

As such, we have limited the potential for undefined behaviour.

All communication-related methods of the FEM package's `DataVector` were added to the `FLENSDataVector` with no significant changes. For MPI type conversion methods, we force the object to be converted to be of the destination type. For example:

```
FLENSDataVector<FLvTypeI> myVec(5, Coupling());

////////////////////////////////////////////
// *** fill with local (type II) values *** //
////////////////////////////////////////////

myVec.typeII_2_I();             //<-- perfect
myVec.typeI_2_II();             //<-- would cause compiler error
```

1.1.4 BLAS Overloading

Most BLAS functions can be used in place of the FEM package's linear algebra routines without modification. The `copy` and `dot` functions, however, require attention.

Copying between two `FLENSDataVectors` of the same MPI vector type can use the BLAS copy function without further assistance. The types match, and we can't do anything about the constant reference to the Coupling object (this must be left to the user to ensure), so we just need to transfer the element values.

When copying vectors of differing MPI vector types, we overload the BLAS copy function. From within this overloaded function, we call the BLAS copy function to copy the vector element values by *upcasting* the `FLENSDataVectors` to their parent class `DenseVector⟨Array⟨double⟩ ⟩`, then perform the appropriate MPI type conversion, for example:

```
void
copy(FLENSDataVector<FLvTypeII> &orig, FLENSDataVector<FLvTypeI> &dest)
{

        //Copy data as usual (masquerading as a DenseVector :) ):
        blas::copy(*static_cast<DenseVector<Array<double> > *>(&orig),
                   *static_cast<DenseVector<Array<double> > *>(&dest));

        //Perform vector type conversion:
        dest.typeII_2_I();
}
```

We use a similar technique for the dot product - the dot product of the two supplied vectors is calculated using BLAS via upcasting, and then the appropriate MPI communication is performed.

By ensuring that our overloaded functions still use the FLENS BLAS implementation, we maintain the possibility for objective (2) in the Introduction.

We point out that our use of 'proper' object types to define the MPI vector types means that the many type asserts present in the FEM package's linear algebra subroutines, such as:

```
double dot(DataVector &u, DataVector &v)
{
        if(u.type==nonMPI && v.type==nonMPI)
          return u.values.dot(v.values);

        // we only multiply typeI and typeII vectors
        assert(u.type != v.type);               //<--assert
```

are no longer required. All type checking is moved to compile time, an advantage in terms of both runtime efficiency and ease of debugging.

1.2 The CG Solver

1.2.1 Implementation

In this section we look at the implementation of the conjugate gradient method for solving a system of linear equations. The solver was initially integrated into the FEM package via a wrapper, the details of which are described below in Section 2.1.

The CG solver uses many linear algebra operations, and is therefore a prime candidate for using BLAS functions. For example, we replaced FEM package function calls such as:

```
CRSmatVec(p,A,x);
add(r2,p,-1.);
```

with the more widely recognised BLAS equivalent:

```
1 blas::mv(NoTrans, One, A, x, Zero, p);
2 blas::axpy(-One, p, r2);
```

As claimed in objective (3) in the Introduction, we also offer a version of the CG solver where such BLAS functions are overloaded, providing a MATLAB-style notation:

```
1 p = A*x;
2 r2 = r2 - p;
```

The CG solver containing this notation is contained in Flens_supl/overloaded.

1.2.2 Testing

We undertook some benchmarking on the Pacioli compute cluster. We examined the performance of the new FEM implementation, with respect to:

1. Serial vs. parallel performance.
2. Performance boost from GotoBLAS (provided by the OpenBLAS library).

Testing was conducted using a 2-d mesh with four domains (hence requiring 4 computation processes). For full homogeneity, the program was executed such that each process was run on separate (identical) nodes, rather than making use of multiple processors/cores on fewer nodes. Thus all communications were performed over the Infiniband network using the MPI.

Figure 1 shows the compute times required to assemble the FEM system. This part of computation requires no communication between processes, and makes use of no BLAS subroutines. The results follow our logical predictions, and can be summarised as follows:

- The parallel implementation is, on average, 4.2x faster than the serial implementation for a given number of mesh elements.
- GotoBLAS is of no benefit here.

Figure 2 shows the compute times required to solve the system of linear equations. This part of computation does require communication between processes, and does make extensive use of BLAS subroutines. The results again follow our predictions, and can be summarised as follows:

- The parallel implementation is, on average, only 1.8x faster than the serial implementation for a given number of mesh elements. Thus we see that the communication here acts as a bottleneck, with a detrimental effect on compute times.

- The near-trivial linking of the OpenBLAS library effects a 1.34x performance increase in the serial implementation and a 1.43x performance increase in the parallel implementation, on average. This 'free' improvement was only possible due to the use of FLENS.

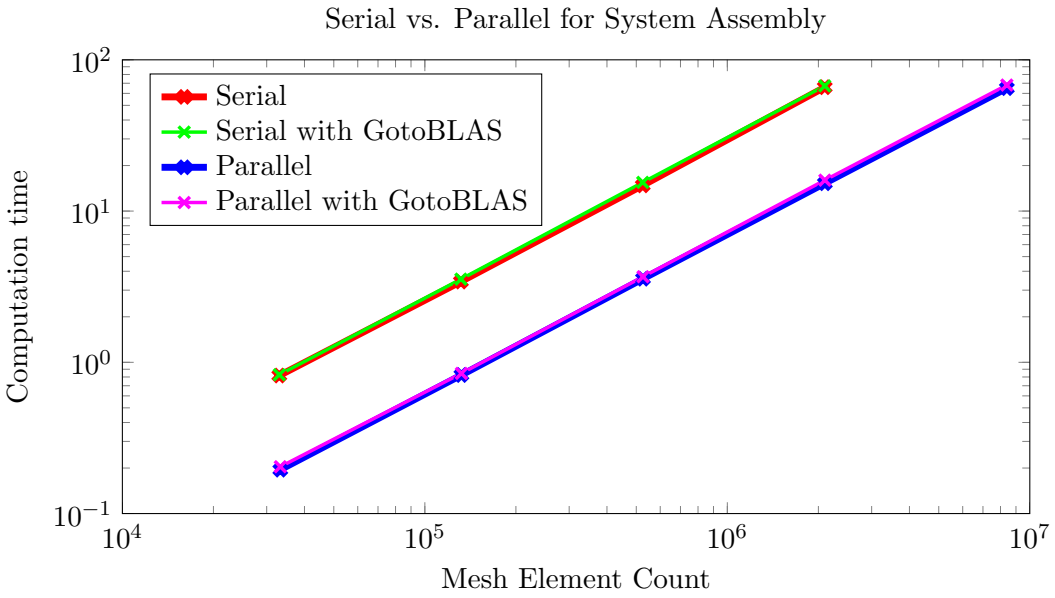


Figure 1: Compute times to perform system assembly.

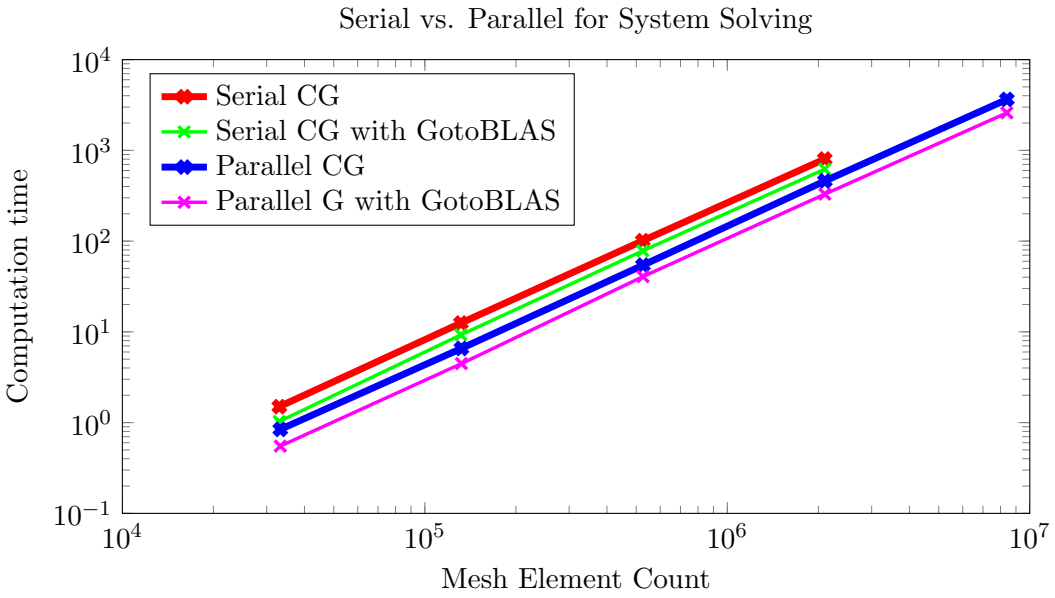


Figure 2: Compute times to perform system assembly.

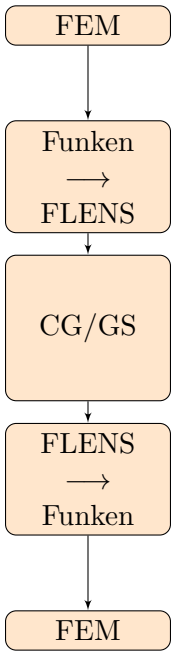
2 Part II (Mazen Ali)

This section continues describing the performed changes to the FEM package in order to replace the provided LinearAlgebra library with FLENS. Note that the Makefiles have to be slightly adjusted as well, please refer to the provided package. Further adjustments, not described here, were performed for the main functions (main-serial and main-parallel).

2.1 GS Solver

One of the main components of the FEM package is the solver that provides the end-result. Implemented in the FEM package were the CG (*Conjugate Gradient*) and the GS (*Gauss-Seidel*) solvers, parallel and serial versions. The adapting of the CG-Solver to FLENS was described in the previous section.

Analogue to the CG solver, the GS solver was initially integrated into FEM via a wrapper. Schematically the wrapper does the following:



Function wrapper

The wrappers transform the data from the original format to FLENS and from FLENS back to the original format upon completion of the solving procedure. This functionality is provided in Flens_supl by the headers funk2flens.h and flens2funk.h. For the solvers the transformation is required for a

matrix and a vector type. Although for the Poisson problem and the chosen basis functions it suffices to consider transformations for sparse matrices, Flens_supl includes both transformations for sparse and dense matrices, as well as a GS-solver for dense matrix classes (possible future utilization as pre-conditioner for e.g. multigrid in problems with resulting non-sparse systems).
The implemented transformation in Flens_supl copies the data manually from the original storing format into FLENS and back. However, FLENS also provides other alternatives for transforming data to FLENS using *Matrix/Vector-Views*. The concept is illustrated below, where data from the original storing format is transformed to FLENS:

```
int
main()
{
        // Typedefs
        typedef flens::DenseVector<flens::Array<double> >
                                                        Fl_Vec;
        typedef flens::DenseVector<flens::Array<double>::View>
                                                        VecView;
        typedef flens::Array<double>::View
                                                        View;

        // Initialize with 0s
        Vector  v_funk(5); // Funken
        VecView v_flens_view = View(5, v_funk.data()); // Flens View
        Fl_Vec  v_flens = v_flens_view; // Flens

        // Change values
        v_funk(0) = 1;
        v_flens_view(5) = 1;

        // Print
        cout << "funk=" << endl;
        print(v_funk, 0, 4);
        cout << endl;
        cout << "flens_view=" << endl;
        print(v_flens_view, 1, 5);
        cout << endl;
        cout << "flens=" << endl;
        print(v_flens, 1, 5);
        return 0;
};
```

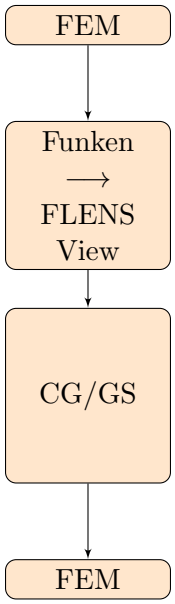
which would produce the output:

```
 $ funk=
1 0 0 0 1
flens_view=
1 0 0 0 1
flens=
0 0 0 0 0
```

FLENS views can be thus used in two ways: reference data from any other linear algebra package,

as long as it provides access to the underlying C-Array, maintaining all the functionality of FLENS; or initialize FLENS non-view data structures via the internal FLENS copy constructor, thus avoiding copying the values manually.

Note that this offers another form of "wrapping" for the solvers which does not involve data copying. The original data can be referenced via FLENS Matrix/Vector-Views using non-const view for the solutions vector and const views for the rest. The idea is schematically illustrated below:



Function wrapper w. Views

After completing the modification process for all data structures in the FEM package the wrappers for the solvers are turned off, since not required any more.

The implementation of the solvers themselves remained mostly unchanged. The required changes included:

- Index base: by default the index base in FLENS is 1 (FORTRAN style), as opposed to the original data structures where the index base is 0 (C style). FLENS provides the possibility to set the index base (and range), as well as operators to access first and last indexes of its data structures. Thus, it is possible to utilize these operators in order to provide maximum flexibility w.r.t. choice of index base. However, we decided not to follow this approach, since this would make the code longer and less readable and the mentioned flexibility does not provide any foreseeable advantages. Thus, the index base was assumed to be 1 in all FEM data structures, as by default in FLENS, and the code was modified accordingly.

- CRS matrices access: FLENS CRS matrices can be accessed much in the same way as the original CRS matrices:

```
const auto &_rows = A.engine().rows();
const auto &_cols = A.engine().cols();
const auto &_vals = A.engine().values();
```

The keyword *auto* is recognized by the C++11 standard, i.e. this necessitates the use of a C++11 conform compiler, such as g++ version 4.7 or higher[1]. Compile via:

```
$ g++ hello.cpp -std=c++11 <options>
```

The keyword *auto* allows the compiler to deduce the type of the declared variable, applying rules similar to template argument deduction during function calls. Hence, this saves the programmer a lot of typing and makes the code more readable for the user.
engine() is the storage mechanism for FLENS and for CRS matrices it contains the getter methods rows(), cols() and values(), that return the corresponding vectors of type *DenseVector*. In order to preserve the functionality of FLENS data structures, it is recommended to use references instead of pointers to the data (which would also be possible). Usage of the attained vectors is analogue to the standard usage of CRS data structures, e.g. as implemented in the original FEM package.

Note, however, that FLENS sparse matrices do not allow to access elements directly (which can otherwise result in unintentional densifying), i.e.:

```
A(2,2)          += 3;      // works fine for CoordStorage
double _tmp     = A(2,2); // compile error
```

The second access would produce a compile error for all sparse FLENS classes. Thus, for retrieving values of the matrix a search loop is required.

- Underscore operator _ : FLENS provides the utility of an underscore operator that can be used to set or copy portions of matrices and vectors, similar as in e.g. MATLAB:

```
const Underscore<IndexType> _
// Set MyVector to 3rd column of MyMatrix (must be same length)
MyVector = MyMatrix(_,3);
// Set Myvector's elements 1 to 3 to first elements of first row
MyVector(_(1,3)) = MyMatrix(1,_(1,3));
```

The underscore operator substituted the original set() and memcpy() calls of the LinearAlgebra data structures.

- Type I,II vectors: the original *DataVector*s were replaced by templated *FLENSDataVector*s that were described in Part I. As already mentioned, this preserves type safety. Usage is in many ways identical to the original DataVectors, main difference being that type conversions are performed during copy operations or during explicit method calls, such as typeII_2_I or vice-versa.

[1] Note that this is required for the entire FLENS library.

- Templates: Both solvers were templated, as well as most of Flens_supl headers. The only exceptions are some of the headers that were used as temporary "adapters" to introduce FLENS into the original FEM package. Apart from some minor flexibility, this would allow to utilize Flens_supl via headers only. Note that the FLENS library is headers only as well.

The dense GS solver required the same modifications, CRS matrix access excluded. The GS solver was tested and debugged.

2.2 Data Structures

In this section the adjustments for the Mesh and Coupling data structures are briefly described.

2.2.1 Mesh

Apart from the self explanatory data type changes, the required adjustments included:

- Index Base: as described in previous section.
- Read and write methods: Flens_supl includes the templated read and write methods, implemented similar to the original read and write methods of the FEM package.
- Const-Correctness: note that another advantage of the FLENS library is that it ensures const-correctness. Therefore the constructor calls had to be modified accordingly. E.g. in the original Mesh constructor the input vector *_dirichlet* is declared as *const* although write access is required, which would cause a compile error in FLENS.
- Underscore operator _: as described in the previous section.
- CRS_sort: for the method provideGeometricData() the original FEM package utilized the constructor for the CRSMatrix class to sort the values of a vector. The constructor accepted 3 vectors of same size, the first contained the row index, the second the column index and the third the corresponding value in the matrix. This functionality is provided by the templated header function CRS_sort.h, implemented analogue to the constructor call of the original FEM package. Alternatively, this can be done entirely without intermediary headers, utilizing the FLENS CoordStorage format and converting to GeCRSMatrix:

```
// Initialize (_numRows, _numCols assumed to be already computed in a preceding
    for-loop)
flens::GeCRSMatrix<flens::CRS<ElementType> >
                                vals_crs;
flens::GeCoordMatrix<flens::CoordStorage<ElementType> >
                                vals_coord(_numRows, _numCols);
// Fill
for (IndexType i=1; i<=rowi.length(); ++i)
{
        if (vals(i)!=0)
        {
                vals_coord(rowi(i), coli(i)) += vals(i);
        }
}
// Convert
vals_crs = vals_coord;
// Access
const auto &_vals = vals_crs.engine().values();
```

The latter way requires less writing but internally does more than actually necessary. However, even for large vectors this does not have a substantial influence on run-time, so that the end-choice is a matter of taste.

After adjusting the Mesh class, the dependencies in Fem.cpp have to be adjusted accordingly. The modified data structures were tested and debugged.

2.2.2 Coupling

Other than the self explanatory data type changes, no further modifications for the Coupling class were required. The dependencies have to be adjusted accordingly in Mesh, Fem, FLENSDataVector and the GS solver. The modifications were tested and debugged.

2.3 Debugging notes

The modifications described above required extensive debugging for both parts, as well as the merging process. Since this amounted to the biggest portion of the entire work time, this section will illustrate on a simple example of a common segmentation fault how to debug using core dumps. This will hopefully save future users a lot of time when modifying the FEM package.

The FLENS library utilizes *assert()* to ensure the index is not out of bounds. However, since these assertions are "hidden" deep in the templates and there is no exception handling implemented, the resulting error message will not provide any useful information about the origin of the faulty access. The system will attempt to produce a core dump, which is however turned off by default on most modern OSs. For example, the following code will produce a segmentation fault:

```
1 int
2 main()
3 {
4         flens::DenseVector <flens::Array<double> > V(5);
5         V(6) = 3;
6         return 0;
7 };
```

Compile and run:

```
$ g++ seg_fault.cpp -o seg_fault -g
$ ./seg_fault
seg_fault:  /usr/local/FLENS/flens/storage/array/array.tcc:108:
flens::Array<T, I, A>::ElementType& flens::Array<T, I, A>::operator()
(flens::Array<T, I, A>::IndexType) [with T = double; I = flens::IndexOptions<>;
A = std::allocator<double>; flens::Array<T, I, A>::ElementType = double;
flens::Array<T, I, A>::IndexType = int]:  Assertion 'index<=lastIndex()' failed.
Aborted (core dumped)
```

As can be seen at the end of the error message, it claims that a core was dumped, which does not have to be true. To indeed enable core dumping type in the command line:

```
$ ulimit -c unlimited
```

Instead of *unlimited* you can specify any other data size (in number of 512-byte blocks). After running the executable again, the crash now generates a core dump, by default in the same directory. Note that for debugging it is advisable to compile with the -g option, since the resulting machine code then contains more information. To analyze the produced core one can e.g. use the standard gdb debugger and proceed by typing:

```
$ gdb -c core seg_fault
```

where the executable has to be specified as well, otherwise the machine code messages will not be "linked" with the source code. The last statements will usually be some calls to the kernel, e.g. a request to terminate the program. Working up the core file, one then can get to the observed error message:

```
Program terminated with signal 6, Aborted.
#0 0x00007f3fa01f1425 in raise () from /lib/x86_64-linux-gnu/libc.so.6
(gdb) up
#1 0x00007f3fa01f4b8b in abort () from /lib/x86_64-linux-gnu/libc.so.6
(gdb)
#2 0x00007f3fa01ea0ee in ??  () from /lib/x86_64-linux-gnu/libc.so.6
(gdb)
#3 0x00007f3fa01ea192 in __assert_fail () from /lib/x86_64-linux-gnu/libc.so.6
(gdb)
#4 0x0000000000400835 in operator() (index=6, this=0x7fff85fc2108)
at /usr/local/FLENS/flens/storage/array/array.tcc:108
108 ASSERT(index<=lastIndex());
```

Working up further will lead to preceding calls and then finally to the origin of the faulty access:

```
4 0x0000000000400835 in operator() (index=6, this=0x7fff85fc2108)
at /usr/local/FLENS/flens/storage/array/array.tcc:108
108 ASSERT(index<=lastIndex());
(gdb)
#5 operator() (index=6, this=0x7fff85fc2100)
at /usr/local/FLENS/flens/vectortypes/impl/densevector.tcc:201
201 return _array(index);
(gdb)
#6 main () at seg_fault.cpp:22
22 V(6) = 3;
```

Obviously the benefits of analyzing core dumps extend to any sort of program crashes and it is generally a good way to make debugging much more efficient.

Unfortunately, the approach does not apply in general to MPI. Though a core dump can still be generated, the content of the core is usually useless for debugging purposes. This, together with the fact that standard debuggers are not suited for parallel programs, often forces the programmer to debug "by hand", i.e. via cout and Barrier().

3 Flens_supl (Mazen+Chris)

This section summarizes the headers in Flens_supl.

- CRS_sort.h: sorting function required in Mesh; accepts a vector of values with the corresponding row and column coordinates, returns a sorted vector values; sorted according to the order in a CRS matrix; templated;
- FLENSDataVector.h: Type I and II (2 separate data types) data vectors derived from FLENS DenseVector; required for parallel computations; methods implemented as in the original FEM package; templated;
- FLENS_read_write.h: read method for FLENS and write methods for FLENS dense vectors and matrices; implemented as in the original FEM package; templated;
- cg_mpi_blas.h: CG sparse solver for MPI; implemented as in the original FEM package; templated;
- cg_nompi_blas.h: CG sparse solver; standard implementation; templated;
- gs_mpi_blas.h: GS sparse and dense solvers for MPI; implemented as in the original FEM package; templated;
- gs_nompi_blas.h: GS sparse and dense solvers; standard implementation; templated;
- flens2c.h: converts FLENS DenseVector to C array; initially required for wrapping the original package with FLENS data structures; not required in the final version; non-templated;
- flens2funk.h: converts data from FLENS data structures to the original FEM package; initially required for wrapping; not required in the final version; templated;
- funk2flens.h: converts data from the original FEM package to FLENS; initially required for wrapping; not required in the final version; templated;
- wrappers.h: wraps the CG and GS solvers for use with the data structures from the original FEM package; not required in the final version; non-templated;

A Appendix

In this appendix we offer instructions on how to set up and run our software package on both a desktop computer and on the Pacioli compute cluster. We assume the target device is of the UNIX family, and already has the following installed:

- gcc of at least version 4.7
- git
- MPI

A.1 Desktop

1. Make a new directory where you would like the magic to happen.
   ```
   $ mkdir FEMtastic
   ```
2. Add our package (the directory called HPC_FLENS) to this new directory.
3. Get and build FLENS:
   ```
   $ git clone https://github.com/michael-lehn/FLENS.git
   $ cd ./FLENS
   $ make
   $ cd ..
   ```
4. Our makefiles assume FLENS is located under /usr/local/FLENS, so copy it there. If this isn't possible, the makefiles will require some minor modifications (change the FLENS link flags to wherever you wish to store FLENS).
   ```
   $ cp -rvf ./FLENS /usr/local/FLENS
   ```
5. Build our package:
   ```
   $ cd ./HPC_FLENS
   $ make
   ```
6. Run our package.
   Replace n with the number of mesh refinements you desire (less than 8 is sensible), and cg can be replaced by gs to use the Gaus-Seidel solver (a great choice for when you have a lot of time on your hands):
   (a) Serial implementation:
   ```
   $ ./main-serial ./input/Square_one_domain n cg 1
   ```
   (b) Parallel implementation:
   ```
   $ mpirun -np 4 main-parallel ./input/Square_four_domains n cg 1
   ```
7. Sit back and watch it work its magic.

A.2 Pacioli

1. Log in to Pacioli and make a new directory where you would like the magic to happen.
   ```
   $ mkdir FEMtastic
   ```
2. Use scp to add our package (the directory called HPC_FLENS) to this new directory.
3. Get and build FLENS:
   ```
   $ git clone https://github.com/michael-lehn/FLENS.git
   $ cd ./FLENS
   $ make
   $ cd ..
   ```
   (no copying of FLENS to /usr/local is required here, our makefiles know we're now on Pacioli ☺).
4. Load the required modules:
   ```
   $ module load gcc/4.7.2
   $ module load sge/6.2u5
   $ module load openmpi/gcc/64/1.4.2
   ```
5. Build our package:
   ```
   $ cd ./HPC_FLENS
   $ make
   ```
6. Submit the appropriate jobscript to the queue (modify the commands in it first, if you so wish):
   (a) Serial:
   ```
   $ qsub batchscript_hpc_flens_serial.qs
   ```
   (b) Parallel:
   ```
   $ qsub batchscript_hpc_flens_parallel.qs
   ```
7. Wait for the job to be processed. Since the parallel version demands exclusive use of 4 nodes, this may take some time if the queue is busy. Once complete, there will be an output file created in the HPC_FLENS directory. This will have the name of the job submitted, appended by `.o`, followed by the job ID number. It contains the standard output from the program.

A.3 GotoBLAS

Notes:

- GotoBLAS offers highly machine-specific optimisations. We performed testing on the single processor (AMD Opteron 252) nodes of Pacioli (nodes 1-16, according to the UZWR website[2]). The frontend is (apparently[2]) identical to these nodes, and therefore can be used to build GotoBLAS. Creativity would be required to build the library for use on the nodes with different hardware.

[2] http://www.uni-ulm.de/en/einrichtungen/uzwr/hardware-and-software/hardware.html

- We found some issues with certain nodes (prime suspect: Node 16), whereby computation times were increased significantly (∼10x) when using GotoBLAS. We suspect that this is due to a node that isn't actually identical to the others, despite what [2] claims, and as such the 'optimised' code is in fact the opposite. Therefore care should be taken to use the GotoBLAS library *only* on processors for which it was configured/built.

To link FLENS with GotoBLAS (on Parcioli), perform steps 1-4 of A.2, then:

1. Get GotoBLAS in the form of OpenBLAS:
   ```
   $ git clone git://github.com/xianyi/OpenBLAS
   ```
2. Make OpenBLAS:
   ```
   $ cd ./OpenBLAS
   $ make FC=gfortran
   $ cd ..
   ```
3. Install OpenBLAS:
   ```
   $ mkdir gotoins
   $ cd ./OpenBLAS
   $ make PREFIX=../gotoins FC=gfortran install
   $ cd ..
   ```
4. Add OpenBLAS to the linker directory path:
   ```
   $ export LD_LIBRARY_PATH=/home/__your username__/gotoins/lib:$LD_LIBRARY_PATH
   ```
5. Build our package with GotoBLAS options:
   ```
   $ cd ./HPC_FLENS
   $ make goto
   ```
6. Submit the appropriate jobscript with 'goto' in its name, in the same way as in A.2.