Large Scale Parallel Computations in R through Elemental

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Abstract

Even though in recent years the scale of statistical analysis problems has increased tremendously, many statistical software tools are still limited to single-node computations. However, statistical analyses are largely based on dense linear algebra operations, which have been deeply studied, optimized and parallelized in the high-performance-computing community. To make high-performance distributed computations available for statistical analysis, and thus enable large scale statistical computations, we introduce RElem, an open source package that integrates the distributed dense linear algebra library Elemental into R. While on the one hand, RElem provides direct wrappers of Elemental’s routines, on the other hand, it overloads various operators and functions to provide an entirely native R experience for distributed computations. We showcase how simple it is to port existing R programs to RElem and demonstrate that RElem indeed allows to scale beyond the single-node limitation of R with the full performance of Elemental without any overhead.

Keywords: Linear Algebra, Elemental, Distributed, Parallel, R.

1. Introduction

In many scientific fields ranging from Chemistry and Biology to Meteorology, data-sets of increasing size are analyzed with statistical methods on a daily basis. Such analyses are often performed with the help of R, an open-source software and programming language focused on and designed for statistical computations. R is supported by both a large community and CRAN, a well-developed contribution system with over 9000 open-source packages. R’s user-base has steadily grown since its first release in 1993 and in many disciplines it has become the
RElem
de-facto standard for statistical computations. However, statistical analyses are constantly evolving, most notably, in the size of their databases. In fields like computational biology, it is quite common that analyses are performed on workstations, and take days to complete. Other problems are simply too large to fit in even modern main memories.

In the field of scientific computing, which is often only loosely connected with the statistical computing community, large scale problems are routinely solved through distributed parallel computing: In clusters, the combined resources and processing power of multiple interconnected computers make processing large data-sets feasible and fast. For dense linear algebra operations, which are at the core of statistical computing, there exist highly optimized libraries for both shared-memory and distributed systems.

While R already makes use of such optimized libraries, namely BLAS\textsuperscript{1} and LAPACK\textsuperscript{2}, for single-node computations, it cannot profit from modern distributed memory libraries for larger data-sets. In this paper, we overcome this limitation by integrating R with the state-of-the-art distributed linear algebra library Elemental: We propose the R-package RElem. RElem provides the functionality and performance of Elemental in R and thereby enables large scale computations in native R. RElem not only provides wrappers to Elemental, but replicates R’s operators and methods, allowing the use of native R scripts in distributed computing nodes.

The remainder of this paper is structured as follows: In Sec. 2 we summarize currently available distributed computing packages for R and provide an overview of the distributed Elemental library. 2. In Sec. 3 we then present how RElem connects R and Elemental in and describe its usage in Sec. 4. Finally, in Sec. 5 we demonstrate the performance and large-scale capabilities of RElem and, in Sec. 6 draw conclusions and potential future directions.

2. Distributed parallelism in R

With the advent of multi-core processors, R began to embrace shared memory parallelism. Several built-in routines use multi-threading capabilities or rely on parallel high-performance kernels, such as the BLAS. On the contrary, distributed parallelism is not natively available in R.

There are several packages that address this issue and enable multi-node execution in R. Most of these packages are built on top of the Message Passing Interface (MPI), which enables the communication between different processes. MPI enables the Single Program Multiple Data (SPMD) parallel programming paradigm, where all computing nodes execute the same program using a portion of the global data. Processes synchronize with each other using messages, which can be point-to-point or collective among processes.

A low-level interface to this parallelism model in R is provided by RMPI, a package that exposes MPI routines in R but leaves the parallelization task to the user.

Other packages such as Snow and Snowfall apply one function to or perform reductions on a whole distributed data set in parallel. These packages achieve good performance and their use is straightforward for simple parallelization tasks such as numerical integration (Schmidberger, Morgan, Eddelbuettel, Yu, Tierney, and Mansmann 2009).

\textsuperscript{1}Basic Linear Algebra Subprograms
\textsuperscript{2}Linear Algebra PACKage
The package collection *Programming Big Data in R* (pbdR) (Ostrouchov, Chen, Schmidt, and Patel 2012) provides mechanisms and routines to handle big amounts of data in distributed environments. In particular, the module pdbDMAT offers distributed dense linear algebra functionality based on the ScaLAPACK library (a distributed memory parallelization of LAPACK) (Choi, Dongarra, Pozo, and Walker 1992). It also implements native R interfaces to and operators on distributed matrices, making it accessible without extensive knowledge of distributed computing in general or ScaLAPACK in particular.

However, in the field of parallel dense linear algebra, ScaLAPACK (1992) is nowadays seen as a legacy library that is still widely used, but no longer represents the state of the art. For instance, it does not contain more recent developments on distributed linear algebra for key routines, such as eigenvalue decomposition (Gutheil, Münchhalfen, and Grotendorst 2014). To provide R users access to the state of the art in dense linear algebra, we therefore see the necessity to provide a more newer alternative. For this purpose, we use Elemental (Poulson, Marker, van de Geijn, Hammond, and Romero 2013), a modern distributed linear algebra library that incorporates the latest algorithms and modern programming standards. Elemental is a recent (2013) and actively developed library. Since its open source license (BSD) allows it to be included in proprietary software, it is an ideal basis for distributed computations both in academia and industry.

In contrast to legacy libraries such as BLAS, LAPACK, and ScaLAPACK, Elemental embraces modern programming paradigms to provide a simpler object-oriented programming interface. At the center of this interface are distributed matrices, which encapsulate not only their data but also their size and distributed storage format. All of Elemental's computational and input/output routines implicitly operate on these formats, performing optimized matrix communications, replications, and redistributions as necessary, while keeping the memory overhead minimal. Hence, while the distributed storage formats are fully transparent and accessible by the user, knowledge of such is not required to use the library.

To extend the availability of Elemental beyond its native C++ environment, recent releases include C and Python interfaces that cover the majority of the library's functionality. To also make the powerful functionality and features of Elemental available to the statistical programming community, we embrace the task of integrating the library with R.

### 3. RElem

This section introduces RElem, our novel interface package that provides Elemental features and functionality in native R. We begin with an overview of RElem's design and structure and in the following subsections focus on its implementation.

The R programming language is in part so widely used in statistical computing and data analysis not so much because of its inherent feature set but because of its large and well maintained package system and simple extensibility. It can natively interface with Fortran and C routines, and separate packages provide interaction with other languages such as Java and C++ (Eddelbuettel and François 2011).

Our first attempt to connect R with Elemental was to use the interface code generator SWIG (Beazley 1996) to directly interface with Elemental's core C++ interface. However, we soon ran into complications due to the extensive use of templating and C++11 features within Elemental. As an alternative, we turned to Elemental's C interface, which also serves as the
basis for the library’s Python interface.

With C as a starting point, there are two interfacing mechanisms provided by R: On the one hand, the routine \texttt{.C} operates as a simple C wrapper that reinterprets R data as basic C data types; on the other hand, the routine \texttt{.Call} provides a low-level interface to compiled C object files. As arguments, \texttt{.Call} passes and operates on internal R objects, the so-called SEXP C structures.

Since \texttt{Elemental} operates on matrices and other complex objects that are neither basic C data types nor known to R, the \texttt{.C} interface is not applicable and we have to employ R’s \texttt{.Call} interface. This means that a separate layer between R’s internal SEXP objects and \texttt{Elemental}’s C interface is required. However, this also allows to directly benefit from much of R’s features, such as object methods, garbage collection, and type checking.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure1.png}
\caption{\texttt{RElem}’s integration scheme.}
\end{figure}

In the following, we present the layered structure of \texttt{RElem} from bottom to top as depicted in Fig. 1: We begin with a short description of \texttt{Elemental}’s C interface and describe its mapping to R’s internal SEXP format. We then provide an overview of the R wrappers using the
.Call interface: The definition of Elemental matrix types and routines in R, as well as the representation of Elemental’s object-oriented methods of matrix classes. We conclude with the extension Elemental’s functionality by overloading R operators and functions to provide an interface very similar to native R.

3.1. Elemental’s C interface

To provide a simple interface to languages other than C++, Elemental offers a C compatibility API and headers. In this API, Elemental’s templated class system is translated into fully typed C structures and functions:

- The templated classes are instantiated with El as a prefix (corresponding to the C++ namespace El), and suffixes indicating the data-types, e.g., ElMatrix_d for a local double-precision matrix. The instantiations are implemented as anonymous structures that are essentially pointers to the C++ objects.

- Templated routines are similarly instantiated, e.g., the C++ function MaxNorm(A) in C becomes ElMaxNormDist_c(A, &val) for distributed single-precision complex matrix. C++ return values are implemented as the last argument by reference, and each routine returns an error code representing errors thrown in the corresponding C++ routine.

- Instance methods are implemented as routines that take a reference to the instance as a first argument; e.g., A.Width() becomes ElMatrixWidth_i(A) for local integer matrices.

3.2. RElem’s C-layer

Since RElem relies on R’s .Call routine to interact with Elemental, the construction of a C-layer that connects R’s SEXP structures and Elemental’s C interface is necessary. This layer contains a wrapper for each of Elemental’s C-routines. In these wrappers, we already simplify some abstractions from the C interface by implementing return values as such, instead of final arguments by reference.

```c
SEXP maxNormDist_d(SEXP RptrA){
    SEXP ans = PROTECT(allocVector(REALSXP, 1));
    ElMaxNormDist_d(toDistMatrix_d(RptrA), REAL(ans));
    UNPROTECT(1);
    return ans;
}
```

Listing 1: maxNormDist_d in RElem’s C-layer.

As an example, listing 1 shows the definition for maxNormDist_d that serves as a wrapper for Elemental’s ElMaxNormDist_d. The routine begins by allocating a double-precision return value using R’s internal allocator and types\(^3\). It then invokes Elemental’s C interface, passing arguments extracted from the SEXP objects: toDistMatrix_d is an RElem routine that casts the external pointer stored in a SEXP object to a ElDistMatrix_d, and REAL is an R macro

\(^3\)The PROTECT and UNPROTECT are necessary to indicate to R’s garbage collection that the allocated object is in use.
that provides a pointer to the double precision slot in a SEXP. Finally, the SEXP representing the result is returned.

3.3. R Matrix and Function Wrappers

The C-layer described above allows to load and access Elemental’s C interface in R through the .Call syntax. In order to offer not a mere copy of Elemental’s C interface but mirror its original object-oriented C++ functionality in R, RElem contains wrappers for all Elemental data types (e.g., matrices) and routines (e.g., MaxNorm).

Just as Elemental, RElem represents both local and distributed matrices (as well as few other objects) as classes. Each of these classes contains 1) an external pointer to an Elemental object, and 2) a datatype indicator needed to select the corresponding typed C-layer routines.

```r
ElDistMatrix <- setClass(
  "ElDistMatrix",
  representation(
    ptr = "externalptr",
    datatype = "character"
  )
)
```

Listing 2: R class ElDistMatrix.

As an example, listing 2 presents the definition of the class ElDistMatrix. In addition to the class name, the class declaration routine SetClass is passed the class “representation” containing its attributes: The external pointer ptr references the Elemental matrix as a C pointer and the character datatype indicates the type of data in this matrix, i.e., double-precision real (d) or complex (z), or integer-precision (i). Note that, in contrast to Elemental’s C interface, which has separate structures and routines for each data-type, thanks to this mechanism RElem has only one distributed matrix class that encapsulates the data-type as an attribute.

```r
MaxNorm <- function(MatrixA) {
  .Call(
    paste0("maxNorm", .getSuffix(MatrixA)),
    MatrixA@ptr
  )
}
```

Listing 3: R wrapper for MaxNorm.

As shown in the example of MaxNorm in listing 3, To translate Elemental functions on matrices to R, we need to use the .Call interface. The name of the function called in RElem’s C-layer is constructed from two parts: the name MaxNorm and a type-dependent suffix that is constructed from the information encapsulated in the matrix object by .getSuffix. E.g., for a complex distributed matrix, the result would be MaxNormDist_z, while for a real local matrix, it would be MaxNorm_d. The selected C-function is then invoked with the external pointer to the Elemental matrix (MatrixA@ptr) as an argument. The return value of the C-function and thus .Call is implicitly returned by the R wrapper.

---

4We use R’s recommended S4 object system.
Class constructors are implemented by overloading R’s \texttt{initialize} function as shown for \texttt{DistMatrix} in listing 4. Of the constructor’s four arguments, the first (\texttt{tag}) indicates the data type and determines the correct C-layer constructor, while the remaining three relate to \texttt{Elemental}’s data distribution and are passed directly to this constructor and further to \texttt{Elemental}’s C interface. However, all arguments are optional: By default, matrices use double-precision (\texttt{d}) as a data-type and the remaining arguments map to the default C++ argument and template values. The \texttt{Elemental} object is initialized through the C-layer constructor and the corresponding C-layer destructor is associated to the instance to integrate with R’s garbage collection. Finally the newly created instance is returned.

3.4. Matrix Methods

Methods on matrix instances, such as \texttt{A.Height()}, which yields the matrix height, require a slightly different treatment from functions that operate on such matrices as arguments. What makes the issue surprisingly complicated (from a programming language point of view) is that R does not have a direct equivalent to instance methods and, in particular, the dot \texttt{.} is not a reserved symbol in R, i.e., it can appear as part of a variable name. To overcome this shortcoming, we use the same approach as many other R libraries and resort to the dollar character \texttt{\$} as a substitute for the dot \texttt{.} in C++. Technically, \texttt{\$} is a binary operator in R that takes the left and right hand side as arguments (such as +), i.e., \texttt{A\$arg} is equivalent to \texttt{A(arg)}.

```r
setMethod(
  "initialize",
  signature(.Object="ElDistMatrix"),
  function(.Object, tag="d", colDist="MC", rowDist="MR",
          grid=new("ElGrid")) {
    .Object@datatype <- tag
    .Object@ptr <- .Call(
      paste0("newDistMatrixSpecific_", tag),
      colDist, rowDist, grid@ptr
    )
    reg.finalizer(.Object@ptr,
      .ElDestroy(tag, "destroyDistMatrix")
    )
    return(.Object)
  }
)
```

Listing 4: \texttt{DistMatrix} constructor.
Listing 5: Method accessor $ for ElDistMatrix.

```
DistMatrixFunctions <- list(
  "Get" = MatrixGet,
  "Set" = MatrixSet,
  "Height" = MatrixHeight,
  "Width" = MatrixWidth,
  "LDim" = MatrixLDim,
  "Empty" = MatrixEmpty,
...
)
```

Listing 6: Mapping of instance methods to functions for ElDistMatrix (excerpt).

Listing 5 shows how `setMethod` overloads the operator $ for the class `ElDistMatrix`: The associated function receives as arguments both the matrix instance and the name of the method. It first looks up the method name in `DistMatrixFunctions` (listing 6) returning an R function (upon failure an error is thrown); the matched function is implemented as part of the R-layer, as described in the previous section. The operator function for $ returns an anonymous function that wraps the matched function, passing the matrix instance as a first argument and any additional arguments (masked as ...).

3.5. Operator and Function Overloading

While the classes, functions, and methods described above are already sufficient to cover Elemental’s full functionality, RElem further overloads several R functions and operators to simplify many operations and provide a native experience to R users.

```
setMethod("+",
  signature(e1="ElDistMatrix", e2="ElDistMatrix"),
  function(e1, e2) {
    if (e1@datatype != e2@datatype)
      stop("Matrices must have the same datatype")
    if (e1$Height() != e2$Height() && e1$Width() != e2$Width())
      stop("Matrices must have the same size")
    matA <- DistMatrix(e1@datatype)
    Copy(e1, matA)
    Axpy(1.0, e2, matA)
    matA
  }
)
```

Listing 7: Operator + for ElDistMatrix.

---

5 `setMethod` takes three arguments: a method name, a signature specifying the arguments and their types, and a function.
The overloading arithmetic operators, such as +, `%*%` and `*`\(^6\) through `setMethod` is very similar to the already overloaded operator `$`, yet requires a few additional argument checks and a memory allocation for the return value. The overloading of `+` for `ElDistMatrix` is shown in listing 7: The operator receives two distributed matrices; first, it is ensured that both the matrix data-types and their sizes match; then a new matrix is created and initialized with a copy of the first operand; finally, the actual computation is performed by `Axpy`, an `Elemental` function named after the `BLAS` counterpart that scales (in this case by 1.0) and adds one matrix to another; the new matrix is returned.

```r
setMethod(
  "[",
  signature(x="ElDistMatrix"),
  function(x, i, j, ...) {
    if (length(i) == 1 && length(j) == 1)
      return(MatrixGet(x, i - 1, j - 1))
    g <- Grid()
    DistMatrixGrid(x, g)
    V <- DistMatrix(grid=g, tag=x@datatype);
    ViewNormal(V, x, i[1] - 1, tail(i, 1), j[1] - 1, tail(j, 1))
    V
  }
)
```

Listing 8: Indexing overloading in R for `ElDistMatrix`.

In R, arrays and tables can be indexed not only to access single elements but to address portions of such objects; e.g., indexing allows to extract certain rows or columns from matrices. Since this is also a very common operation in dense linear algebra, `Elemental` provides so-called “matrix views”. We use this feature to overload R’s indexing operator `[` as show for `ElDistMatrix` in listing 8: If the provided indices `i` and `j` identify a single matrix element, this is returned as a scalar; otherwise, a submatrix is extracted.

```r
setMethod(
  "print",
  signature(x="ElDistMatrix"),
  function(x) {
    Print(x)
  }
)
```

Listing 9: Overloading of R’s `print` for `ElDistMatrix`.

Native R methods are overloaded very similarly, as shown for `print` and `ElDistMatrix` instances in listing 9: The overload simply maps R’s `print` to `RElem`’s `Print` wrapper function.

```r
setMethod(
  "prcomp",
  signature(x="ElDistMatrix"),
  function(x, retx=TRUE, center=TRUE, scale.=FALSE, 
          tol=NULL, ...) {
    x_centered <- scale(x, center, scale.)
    ...
  }
)
```

\(^6\) matrix-matrix and element-wise multiplication.
\[ x_{\text{center}} \leftarrow \text{attr}(x_{\text{centered}}, \text{"scaled:center"}) \]

\[ s \leftarrow \text{svd}(x_{\text{centered}}, nu=0) \]

\[ s$d \leftarrow (1 / \text{sqrt}(x$\text{Height}() - 1)) * s$d \]

\[ \text{list(sdev=s$d, rotation=s$v, center=x\_center)} \]

Listing 10: Overloading of R’s SVD-based PCA routine \texttt{prcomp} for \texttt{ElDistMatrix}.

Other core R operations, such as the principal component analysis (PCA), do not have a direct counterpart in \texttt{Elemental}, but can be assembled from \texttt{Elemental} routines. For instance, the PCA routine \texttt{prcomp}, which is based on the singular value decomposition (SVD) of the \( n \times m \) dataset \( X \) with \( n \) observations of \( m \) variables, is overloaded in \texttt{RElem} as outlined in listing 10: First, \texttt{scale}, which is also overloaded in \texttt{RElem}, centers (and optionally scales) the input \( X \) to ensure that the average of each observed variable is 0: \( \tilde{X} = X - \bar{X} \); the center \( \bar{X} \) is extracted since it is one of \texttt{prcomp}’s list of return values. Now \texttt{svd} performs the core singular value decomposition \( U \Sigma V^T = \tilde{X} \) through \texttt{Elemental}’s SVD. While the principle components are directly given by the right singular vectors \( V \) stored in \texttt{s$d}, the variance \( \sigma \) for each vector is computed from the singular values (diagonal elements of \( \Sigma \)), and then stored in \texttt{s$v} as \( \sigma = \frac{\Sigma}{\sqrt{n-1}} \). The returned data structure consists of the principle components, their variance, and the matrix center.

4. Usage

This section offers a brief introduction to \texttt{RElem} from the user’s perspective: We start by describing \texttt{RElem}’s installation process, then introduce its parallel execution across multiple processes, and conclude by comparing distributed \texttt{RElem} scripts with native R, and with \texttt{Elemental}.

4.1. Installation

\texttt{RElem} is provided as a standard R package and installed through the command

\[ \texttt{R CMD INSTALL RElem.zip} \]

Since \texttt{Elemental} is not distributed and compiled along with \texttt{RElem}, the installation script searches the file system for a valid \texttt{Elemental} installation and compiles \texttt{RElem} accordingly using \texttt{Elemental} headers. \texttt{RElem} has been successfully installed and tested on both Linux and OS X.\footnote{Windows is currently not supported by \texttt{Elemental} but is also uncommon on distributed memory cluster systems.}

4.2. Parallel Launch

Since \texttt{Elemental} is based on MPI and is typically launched in parallel with \texttt{mpirun}, so is \texttt{RElem}: \texttt{mpirun} is used to run one instance of R per process, each of which receives the same input file. \texttt{Elemental} is loaded locally on each process and performs all interaction with MPI — the R instances are at no point confronted with communication and are actually unaware
that they are running in parallel. A user might for instance run an RElem script `myScript.R` on 64 processes using

```
mpirun -n 64 R -f myScript.R
```

### 4.3. Syntax and Interface

The component to successfully run RElem is the R script that uses it. To give an impression not only of how RElem is used but also of how it compares to pure R and Elemental, let us start with a simple example in pure R that loads a Hermitian matrix from a file `data.txt`, and computes its eigendecomposition, storing the result (eigenvalues and eigenvectors) in the structure `ans`:

```r
A <- read.table("data.txt")
ans <- eigen(A)
```

Listing 11: Pure R eigen decomposition.

To convert the above code to use RElem’s distributed matrices, only few changes are necessary:

```r
library(Relem)
A <- read.table.dist("data.txt")
ans <- eigen(A)
```

Listing 12: RElem eigen decomposition.

Besides loading RElem, the script only needs the addition of `.dist` to the `read.table` routine, which then loads the passed file as `ElDistMatrix`.

If we compare the above RElem script with a C++ code performing the same operation, we notice that the RElem version is considerably shorter:

```c++
#include "El.hpp"
using namespace El;
int main(int argc, char *argv[]) {
  Initialize(argc, argv);
  DistMatrix<double> A, w, X;
  Read(A, "data.txt");
  HermitianEig(LOWER, A, w, X);
  return 0;
}
```

Listing 13: Elemental C++ eigen decomposition.

### 5. Performance and Scalability

In this chapter we present the performance and scalability of RElem; we compare it with both pure R and Elemental and show computations only made possible in R through RElem. We demonstrate that RElem translates both Elemental’s performance and scalability directly to R with minimal overhead.

Our test environment is a computing cluster of nodes equipped with two 12-core Intel Xeon
E5-2680 processors (Haswell microarchitecture) and 64GB of main memory. We use R version 3.1.0, Elemental version 0.85, and link to Intel’s Math Kernel Library (MKL) version 11.3.

5.1. Performance: R vs. RElem

We begin with a performance comparison on a single node (24 cores) between R linked to multi-threaded MKL, and RElem using Elemental’s MPI-based parallelization; as test-cases we use two basic linear algebra operations: the multiplication of two $6,000 \times 6,000$ matrices (gemm, the central and most optimized operation in dense linear algebra) and the solution of a linear system with 12,000 unknowns and 1,000 right-hand sides.

![Figure 2: Execution time in R and RElem.](image-url)

Figure 2: Execution time in R and RElem.

Figure 2 presents the execution time of these two operations for both R and RElem, with increasing number of cores (threads in R, processes in RElem): Up to small differences, the libraries are on-par with one another, as neither is clearly faster than the other.

Note that an alternative would be to run one instance of RElem per node and rely on multi-threaded mkl for shared memory parallel performance.

5.2. Scalability: R vs. RElem

The main goal of RElem is to extend R’s processing capabilities beyond the memory and compute limitations of a single node. Hence, in the following, we consider a Principle Component Analysis (prcomp) with 5,000 variables and between 125,000 and 875,000 observations, i.e., an input matrix that is between 4.66GB and 41.90GB.

Figure 3 presents the execution time of the PCA of both R and RElem for increasing problem sizes. First off, already on a single node, RElem is between 18% and 43% faster than native R since Elemental offers a faster singular value decomposition algorithm than MKL. Furthermore, since during the PCA computation multiple copies of the input matrix are created, both
R and RElem can only solve problems of up to 12GB in size (roughly 320,000 observations) on a single node. While this limitation cannot possibly be overcome in native R, it is easily addressed in RElem by adding more processes. In addition to speeding up single-node analyses, each added compute node allows to linearly increase the size of the processed problem by 12GB.

5.3. Overhead over Elemental

The previous experiments have shown the performance and scalability advantages of RElem compared to R; in the following, we consider RElem as an interface to Elemental and study its overhead in execution time and memory consumption.

We begin by analyzing the execution time overhead of RElem over Elemental: For this purpose, we consider the multiplication of two matrices of size $12,000 \times 12,000$ and the solution of a linear system with 20000 unknowns and 1000 right-hand sides (both problems take up around 3GB).

Figure 4 shows the execution time of these two operations for both RElem and Elemental: The two different setups are virtually identical, showing that RElem causes no relevant overhead over Elemental for large computations. This behavior was expected since RElem only introduces very light-weight wrapping layers around Elemental’s core functions. Measurements of simple query routines such as \texttt{A.Width()} (In RElem: \texttt{A$\%\%$Width()}) confirm this observation and suggest a marginal overhead of, on average, 0.6ms per function call.

Next, we study the memory overhead of RElem over Elemental: for this purpose, we consider a principal component analysis with 5000 variables and between 125,000 and 725,000 observations (between 3.66GB and 27.00GB) on three compute nodes (72 cores).

Figure 5 presents the peak memory requirements of this computation per process for both RElem and Elemental: Independent of the problem size, the memory overhead of RElem is constant at about 30MB per process. This corresponds to the memory footprint of the
6. Conclusions

The presented package RElem enables large scale distributed computations in R through the state-of-the-art linear algebra library Elemental. RElem allows R users to tackle enormous problems on compute clusters that pure R cannot possibly process being limited to a single shared memory processor.
By not only translating Elemental’s interface to R but giving it a native R feeling by overloading various operators and functions, we created a package that both offers full access to Elemental for experienced users, and allows for a seamless transition to distributed memory computations for R users.

Nonetheless, RElem is a light-weight interface from R to Elemental that in both execution time and memory requirements introduces virtually no overhead at all. We demonstrated both RElem’s performance and its scalability beyond the memory-limitations of a single compute nodes.

RElem is available both on GitHub under the open-source MIT licence (https://github.com/HPAC/RElem).

Future plans for RElem include the support for sparse linear algebra routines available in Elemental.

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