rhdf5

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Contents

1 Introduction **1**

2 Installation of the HDF5 package **1**

3 High level R -HDF5 functions **1**
3.1 Creating an HDF5 file and group hierarchy 1
3.2 Writing and reading objects 2
3.3 Writing and reading with subsetting, chunking and compression 2
3.4 Saving multiple objects to an HDF5 file (h5save) 6
3.5 List the content of an HDF5 file 6
3.6 Dump the content of an HDF5 file 7
3.7 Reading HDF5 files with external software 8

4 Low level HDF5 functions **8**
4.1 Creating an HDF5 file and a group hierarchy 8
4.2 Writing data to an HDF5 file 8

5 Session Info **9**

1 Introduction

The package is an R interface for HDF5. On the one hand it implements R interfaces to many of the low level functions from the C interface. On the other hand it provides high level convenience functions on R level to make a usage of HDF5 files more easy.

2 Installation of the HDF5 package

To install the package rhdf5, you need a current version (>2.15.0) of R (www.r-project.org). After installing R you can run the following commands from the R command shell to install the bioconductor package rhdf5.

```
> source("http://bioconductor.org/biocLite.R")
> biocLite("rhdf5")
```

3 High level R -HDF5 functions

3.1 Creating an HDF5 file and group hierarchy

An empty HDF5 file is created by

```
> library(rhdf5)
> h5createFile("myhdf5file.h5")
```

```
[1] TRUE
```

The HDF5 file can contain a group hierarchy. We create a number of groups and list the file content afterwards.

```
> h5createGroup("myhdf5file.h5","foo")

[1] TRUE

> h5createGroup("myhdf5file.h5","baa")

[1] TRUE

> h5createGroup("myhdf5file.h5","foo/foobaa")

[1] TRUE

> h5ls("myhdf5file.h5")

  group   name     otype dclass dim
0     /    baa H5I_GROUP
1     /    foo H5I_GROUP
2  /foo foobaa H5I_GROUP
```

3.2 Writing and reading objects

Objects can be written to the HDF5 file. Attributes attached to an object are written as well, if `write.attributes=TRUE` is given as argument to `h5write`. Note that not all R-attributes can be written as HDF5 attributes.

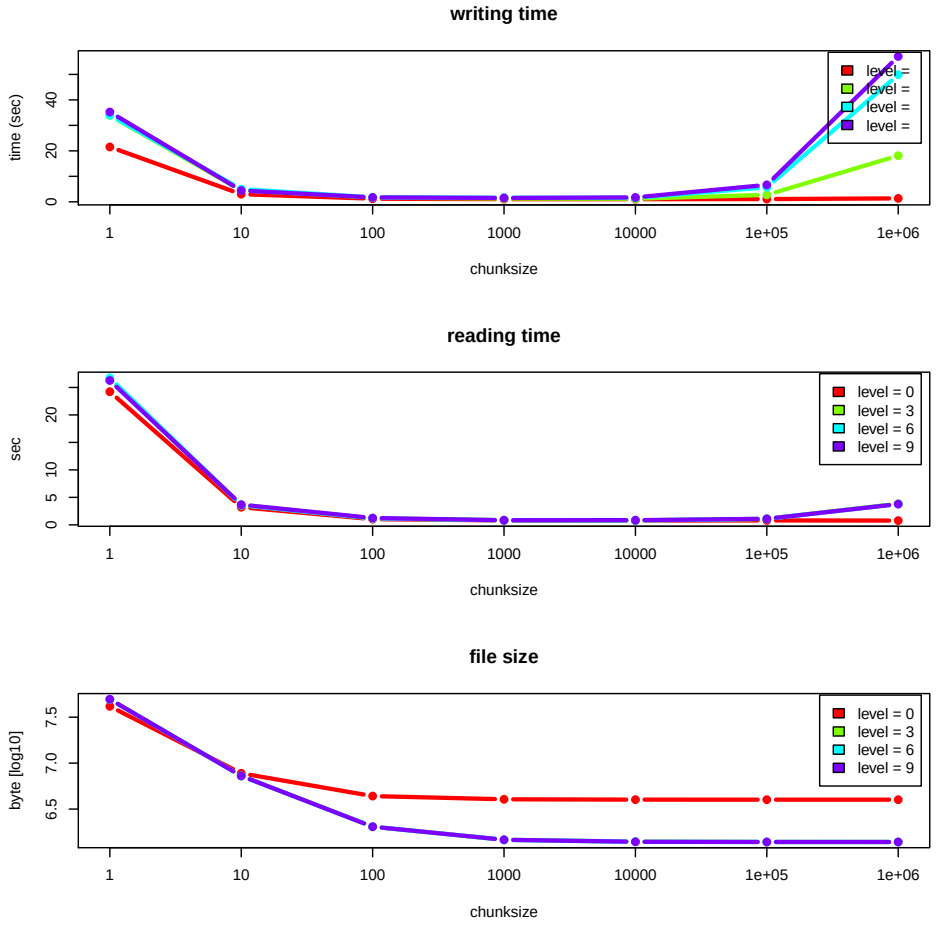
```
> A = matrix(1:10,nr=5,nc=2)
> h5write(A, "myhdf5file.h5","foo/A")
> B = array(seq(0.1,2.0,by=0.1),dim=c(5,2,2))
> attr(B, "scale") <- "liter"
> h5write(B, "myhdf5file.h5","foo/B")
> C = matrix(paste(LETTERS[1:10],LETTERS[11:20], collapse=""),
+   nr=2,nc=5)
> h5write(C, "myhdf5file.h5","foo/foobaa/C")
> df = data.frame(1L:5L,seq(0,1,length.out=5),
+   c("ab","cde","fghi","a","s"), stringsAsFactors=FALSE)
> h5write(df, "myhdf5file.h5","df")
> h5ls("myhdf5file.h5")

        group   name       otype   dclass       dim
0           /    baa   H5I_GROUP
1           /     df H5I_DATASET COMPOUND         5
2           /    foo   H5I_GROUP
3        /foo      A H5I_DATASET  INTEGER     5 x 2
4        /foo      B H5I_DATASET    FLOAT 5 x 2 x 2
5        /foo foobaa   H5I_GROUP
6 /foo/foobaa      C H5I_DATASET   STRING     2 x 5

> D = h5read("myhdf5file.h5","foo/A")
> E = h5read("myhdf5file.h5","foo/B")
> F = h5read("myhdf5file.h5","foo/foobaa/C")
> G = h5read("myhdf5file.h5","df")
```

If a dataset with the given `name` does not yet exist, a dataset is created in the HDF5 file and the object `obj` is written to the HDF5 file. If a dataset with the given `name` already exists and the datatype and the dimensions are the same as for the object `obj`, the data in the file is overwritten. If the dataset already exists and either the datatype or the dimensions are different, `h5write` fails.

3.3 Writing and reading with subsetting, chunking and compression

The rhdf5 package provides two ways of subsetting. One can specify the submatrix with the R-style index lists or with the HDF5 style hyperslabs. Note, that the two next examples below show two alternative ways for reading and writing the exact same submatrices. Before writing subsetting or hyperslabbing, the dataset with full dimensions has to be created in the HDF5 file. This can be achieved by writing once an array with full dimensions as in section 3.2 or by creating a dataset. Afterwards the dataset can be written sequentially.

Influence of chunk size and compression level The chosen chunk size and compression level have a strong impact on the reading and writing time as well as on the resulting file size. In an example an integer vector of size 10e7is written to an hdf5 file. The file is written in subvectors of size 10'000. The definition of the chunk size influences the reading as well as the writing time. In the chunk size is much smaller or much larger than actually used, the runtime performance decreases dramatically. Furthermore the file size is larger for smaller chunk sizes, because of an overhead. The compression can be much more efficient when the chunk size is very large. The following figure illustrates the runtime and file size behaviour as a function of the chunk size for a small toy dataset.



After the creation of the dataset, the data can be written sequentially to the hdf5 file. Subsetting in R-style needs the specification of the argument index to h5read and h5write.

```
> h5createDataset("myhdf5file.h5", "foo/S", c(5,8),
+                 storage.mode = "integer", chunk=c(5,1), level=7)

[1] TRUE

> h5write(matrix(1:5,nr=5,nc=1), file="myhdf5file.h5",
+         name="foo/S", index=list(NULL,1))
> h5read("myhdf5file.h5", "foo/S")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    0    0    0    0    0    0    0
[2,]    2    0    0    0    0    0    0    0
[3,]    3    0    0    0    0    0    0    0
[4,]    4    0    0    0    0    0    0    0
[5,]    5    0    0    0    0    0    0    0
```

```
> h5write(6:10, file="myhdf5file.h5",
+         name="foo/S", index=list(1,2:6))
> h5read("myhdf5file.h5", "foo/S")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6    7    8    9   10    0    0
[2,]    2    0    0    0    0    0    0    0
[3,]    3    0    0    0    0    0    0    0
[4,]    4    0    0    0    0    0    0    0
[5,]    5    0    0    0    0    0    0    0

> h5write(matrix(11:40,nr=5,nc=6), file="myhdf5file.h5",
+         name="foo/S", index=list(1:5,3:8))
> h5read("myhdf5file.h5", "foo/S")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0   12   17   22   27   32   37
[3,]    3    0   13   18   23   28   33   38
[4,]    4    0   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40

> h5write(matrix(141:144,nr=2,nc=2), file="myhdf5file.h5",
+         name="foo/S", index=list(3:4,1:2))
> h5read("myhdf5file.h5", "foo/S")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0   12   17   22   27   32   37
[3,]  141  143   13   18   23   28   33   38
[4,]  142  144   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40

> h5write(matrix(151:154,nr=2,nc=2), file="myhdf5file.h5",
+         name="foo/S", index=list(2:3,c(3,6)))
> h5read("myhdf5file.h5", "foo/S")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0  151   17   22  153   32   37
[3,]  141  143  152   18   23  154   33   38
[4,]  142  144   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40

> h5read("myhdf5file.h5", "foo/S", index=list(2:3,2:3))

     [,1] [,2]
[1,]    0  151
[2,]  143  152

> h5read("myhdf5file.h5", "foo/S", index=list(2:3,c(2,4)))

     [,1] [,2]
[1,]    0   17
[2,]  143   18

> h5read("myhdf5file.h5", "foo/S", index=list(2:3,c(1,2,4,5)))

     [,1] [,2] [,3] [,4]
[1,]    2    0   17   22
[2,]  141  143   18   23
```

The HDF5 hyperslabs are defined by some of the arguments `start`, `stride`, `count`, and `block`. These arguments are not effective, if the argument `index` is specified.

```
> h5createDataset("myhdf5file.h5", "foo/H", c(5,8), storage.mode = "integer",
+                 chunk=c(5,1), level=7)

[1] TRUE

> h5write(matrix(1:5,nr=5,nc=1), file="myhdf5file.h5", name="foo/H",
+         start=c(1,1))
> h5read("myhdf5file.h5", "foo/H")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    0    0    0    0    0    0    0
[2,]    2    0    0    0    0    0    0    0
[3,]    3    0    0    0    0    0    0    0
[4,]    4    0    0    0    0    0    0    0
[5,]    5    0    0    0    0    0    0    0

> h5write(6:10, file="myhdf5file.h5", name="foo/H",
+         start=c(1,2), count=c(1,5))
> h5read("myhdf5file.h5", "foo/H")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6    7    8    9   10    0    0
[2,]    2    0    0    0    0    0    0    0
[3,]    3    0    0    0    0    0    0    0
[4,]    4    0    0    0    0    0    0    0
[5,]    5    0    0    0    0    0    0    0

> h5write(matrix(11:40,nr=5,nc=6), file="myhdf5file.h5", name="foo/H",
+         start=c(1,3))
> h5read("myhdf5file.h5", "foo/H")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0   12   17   22   27   32   37
[3,]    3    0   13   18   23   28   33   38
[4,]    4    0   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40

> h5write(matrix(141:144,nr=2,nc=2), file="myhdf5file.h5", name="foo/H",
+         start=c(3,1))
> h5read("myhdf5file.h5", "foo/H")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0   12   17   22   27   32   37
[3,]  141  143   13   18   23   28   33   38
[4,]  142  144   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40

> h5write(matrix(151:154,nr=2,nc=2), file="myhdf5file.h5", name="foo/H",
+         start=c(2,3), stride=c(1,3))
> h5read("myhdf5file.h5", "foo/H")

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    6   11   16   21   26   31   36
[2,]    2    0  151   17   22  153   32   37
[3,]  141  143  152   18   23  154   33   38
[4,]  142  144   14   19   24   29   34   39
[5,]    5    0   15   20   25   30   35   40
```

```
> h5read("myhdf5file.h5", "foo/H",
+        start=c(2,2), count=c(2,2))

     [,1] [,2]
[1,]    0  151
[2,]  143  152

> h5read("myhdf5file.h5", "foo/H",
+        start=c(2,2), stride=c(1,2),count=c(2,2))

     [,1] [,2]
[1,]    0   17
[2,]  143   18

> h5read("myhdf5file.h5", "foo/H",
+        start=c(2,1), stride=c(1,3),count=c(2,2), block=c(1,2))

     [,1] [,2] [,3] [,4]
[1,]    2    0   17   22
[2,]  141  143   18   23
```

3.4 Saving multiple objects to an HDF5 file (h5save)

A number of objects can be written to the top level group of an HDF5 file with the function `h5save` (as analogonanalogous to the R function `save`).

```
> A = 1:7;  B = 1:18; D = seq(0,1,by=0.1)
> h5save(A, B, D, file="newfile2.h5")
> h5dump("newfile2.h5")

$A
[1] 1 2 3 4 5 6 7

$B
 [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18

$D
 [1] 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
```

3.5 List the content of an HDF5 file

The function `h5ls` provides some ways of viewing the content of an HDF5 file.

```
> h5ls("myhdf5file.h5")

        group   name       otype   dclass       dim
0           /    baa   H5I_GROUP
1           /     df H5I_DATASET COMPOUND         5
2           /    foo   H5I_GROUP
3        /foo      A H5I_DATASET  INTEGER     5 x 2
4        /foo      B H5I_DATASET    FLOAT 5 x 2 x 2
5        /foo      H H5I_DATASET  INTEGER     5 x 8
6        /foo      S H5I_DATASET  INTEGER     5 x 8
7        /foo foobaa   H5I_GROUP
8 /foo/foobaa      C H5I_DATASET   STRING     2 x 5

> h5ls("myhdf5file.h5", all=TRUE)

        group   name         ltype corder_valid corder cset       otype
0           /    baa H5L_TYPE_HARD        FALSE      0    0   H5I_GROUP
1           /     df H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
```

```
2           /    foo H5L_TYPE_HARD        FALSE      0    0   H5I_GROUP
3        /foo      A H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
4        /foo      B H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
5        /foo      H H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
6        /foo      S H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
7        /foo foobaa H5L_TYPE_HARD        FALSE      0    0   H5I_GROUP
8 /foo/foobaa      C H5L_TYPE_HARD        FALSE      0    0 H5I_DATASET
  num_attrs   dclass          dtype  stype rank       dim    maxdim
0         0                                0
1         0 COMPOUND   HST_COMPOUND SIMPLE    1         5         5
2         0                                0
3         0  INTEGER  H5T_STD_I32LE SIMPLE    2     5 x 2     5 x 2
4         0    FLOAT H5T_IEEE_F64LE SIMPLE    3 5 x 2 x 2 5 x 2 x 2
5         0  INTEGER  H5T_STD_I32LE SIMPLE    2     5 x 8     5 x 8
6         0  INTEGER  H5T_STD_I32LE SIMPLE    2     5 x 8     5 x 8
7         0                                0
8         0   STRING     HST_STRING SIMPLE    2     2 x 5     2 x 5
```

```
> h5ls("myhdf5file.h5", recursive=2)
```

```
  group   name       otype   dclass       dim
0     /    baa   H5I_GROUP
1     /     df H5I_DATASET COMPOUND         5
2     /    foo   H5I_GROUP
3  /foo      A H5I_DATASET  INTEGER     5 x 2
4  /foo      B H5I_DATASET    FLOAT 5 x 2 x 2
5  /foo      H H5I_DATASET  INTEGER     5 x 8
6  /foo      S H5I_DATASET  INTEGER     5 x 8
7  /foo foobaa   H5I_GROUP
```

3.6 Dump the content of an HDF5 file

The function `h5dump` is similar to the function `h5ls`. If used with the argument `load=FALSE`, it produces the same result as `h5ls`, but with the group structure resolved as a hierarchy of lists. If the default argument `load=TRUE` is used all datasets from the HDF5 file are read.

```
> h5dump("myhdf5file.h5",load=FALSE)
```

```
$baa
NULL

$df
  group name       otype   dclass dim
1     /   df H5I_DATASET COMPOUND   5

$foo
$foo$A
  group name       otype  dclass   dim
1     /    A H5I_DATASET INTEGER 5 x 2

$foo$B
  group name       otype dclass       dim
1     /    B H5I_DATASET  FLOAT 5 x 2 x 2

$foo$H
  group name       otype  dclass   dim
1     /    H H5I_DATASET INTEGER 5 x 8

$foo$S
```

```
  group name       otype  dclass   dim
1     /    S H5I_DATASET INTEGER 5 x 8

$foo$foobaa
$foo$foobaa$C
  group name       otype dclass   dim
1     /    C H5I_DATASET STRING 2 x 5
```

```
> D <- h5dump("myhdf5file.h5")
```

3.7 Reading HDF5 files with external software

The content of the HDF5 file can be checked with the command line tool `h5dump` (available on linux-like systems with the HDF5 tools package installed) or with the graphical user interface `HDFView` (http://www.hdfgroup.org/hdf-java-html/hdfview/) available for all major platforms.

```
> system("h5dump myhdf5file.h5")
```

Please note, that arrays appear as transposed matrices when opening it with a C-program (h5dump or HDFView). This is due to the fact the fastest changing dimension on C is the last one, but on R it is the first one (as in Fortran).

4 Low level HDF5 functions

4.1 Creating an HDF5 file and a group hierarchy

Create a file.

```
> library(rhdf5)
> h5file = H5Fcreate("newfile.h5")
> h5file
```

```
HDF5 FILE

        name /
    filename
```

and a group hierarchy

```
> h5group1 <- H5Gcreate(h5file, "foo")
> h5group2 <- H5Gcreate(h5file, "baa")
> h5group3 <- H5Gcreate(h5group1, "foobaa")
> h5group3
```

```
HDF5 GROUP

        name /foo/foobaa
    filename
```

4.2 Writing data to an HDF5 file

Create 4 different simple and scalar data spaces. The data space sets the dimensions for the datasets.

```
> d = c(5,7)
> h5space1 = H5Screate_simple(d,d)
> h5space2 = H5Screate_simple(d,NULL)
> h5space3 = H5Scopy(h5space1)
> h5space4 = H5Screate("H5S_SCALAR")
> h5space1
```

```
HDF5 DATASPACE

        rank 2
        size 7 x 5
     maxsize 7 x 5
```

```
> H5Sis_simple(h5space1)
```

```
[1] TRUE
```

Create two datasets, one with integer and one with floating point numbers.

```
> h5dataset1 = H5Dcreate( h5file, "dataset1", "H5T_IEEE_F32LE", h5space1 )
> h5dataset2 = H5Dcreate( h5group2, "dataset2", "H5T_STD_I32LE", h5space1 )
> h5dataset1
```

```
HDF5 DATASET

        name /dataset1
    filename
        type H5T_IEEE_F32LE
        rank 2
        size 7 x 5
     maxsize 7 x 5
```

Now lets write data to the datasets.

```
> A = seq(0.1,3.5,length.out=5*7)
> H5Dwrite(h5dataset1, A)
> B = 1:35
> H5Dwrite(h5dataset2, B)
```

To release resources and to ensure that the data is written on disk, we have to close datasets, dataspaces, and the file. There are different functions to close datasets, dataspaces, groups, and files.

```
> H5Dclose(h5dataset1)
> H5Dclose(h5dataset2)
> H5Sclose(h5space1)
> H5Sclose(h5space2)
> H5Sclose(h5space3)
> H5Sclose(h5space4)
> H5Gclose(h5group1)
> H5Gclose(h5group2)
> H5Gclose(h5group3)
> H5Fclose(h5file)
```

5 Session Info

```
> sessionInfo()
```

```
R version 2.15.0 (2012-03-30)
Platform: x86_64-unknown-linux-gnu (64-bit)

locale:
 [1] LC_CTYPE=en_US.UTF-8       LC_NUMERIC=C
 [3] LC_TIME=en_US.UTF-8        LC_COLLATE=C
 [5] LC_MONETARY=en_US.UTF-8    LC_MESSAGES=en_US.UTF-8
 [7] LC_PAPER=C                 LC_NAME=C
 [9] LC_ADDRESS=C               LC_TELEPHONE=C
[11] LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C
```

```
attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] rhdf5_2.0.2

loaded via a namespace (and not attached):
[1] tools_2.15.0   zlibbioc_1.2.0
```