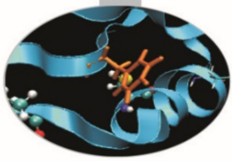
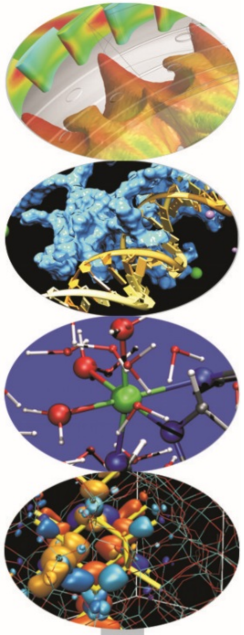


Introducion to R and parallel libraries



Giorgio Pedrazzi, CINECA
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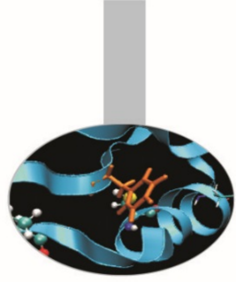
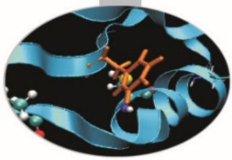
School of Data Analytics and Visualisation
Milan, 09/06/2015



Outline

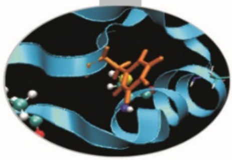
- Overview
  - What is R
  - R Console Input and Evaluation
- Data types
  - R Objects and Attributes
  - Vectors and Lists
  - Matrices
  - Factors
  - Missing Values
  - Data Frames
- Reading data
  - Reading Tabular Data
  - Reading Large Tables
- Subsetting
  - Basics
  - Lists
  - Matrices
  - Removing Missing Values
- Grouping, loops and conditional execution
  - Repetitive execution
  - Branching
  - Loops
  - Function and operators
- Parallel libraries
  - Parallel
  - foreach
- R on PICO

What is R



- R is “GNU S” — A language and environment for data manipulation, calculation and graphical display
  - similar to the award-winning S system, which was developed at Bell Laboratories by John Chambers et al.
  - a suite of operators for calculations on arrays (in particular matrices)
  - a large, coherent, integrated collection of intermediate tools for interactive data analysis
  - a collection of graphical facilities for data analysis and to display either directly at the computer or on hardcopy
  - a well-developed programming language which includes conditionals, loops, user defined recursive functions and input and output facilities
- The core of R is an ***interpreted*** computer language
  - It allows branching and looping as well as modular programming using functions
  - Most of the user-visible functions in R are written in R, calling upon a smaller set of internal primitives
  - It is possible for the user to interface to procedures written in C, C++ or FORTRAN languages for efficiency, and also to write additional primitives

R Console and evaluation



- In R, the “**<-**” symbol is the **assignment** operator (newest R versions also support “**=**“):

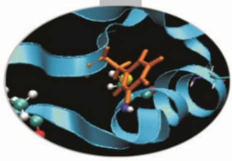
```
> x <- 5
```

The R grammar determines whether an expression is complete or not:

```
> x <-     # Incomplete expression
```

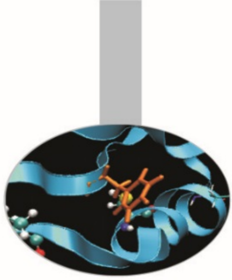
- The “**#**” character indicates a **comment**.
- When a complete expression is typed in the prompt, it is evaluated and the result of the evaluated expression is then returned. The result may be auto-printed

```
> print(x)
> x
```



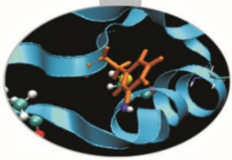
Objects

- R has six basic or “atomic” classes of objects
  - character
  - numeric (real numbers)
  - integer
  - complex
  - factor
  - logical (True/False)
- The most basic object is a vector
  - A vector can only contain objects of the same class
  - BUT: The one exception is a *list, which is represented as a vector but can contain objects of* different classes (indeed, that’s usually why we use them)
- Empty vectors can be created with the ***vector()*** function.



Attributes

- R objects can have attributes
  - names, rownames, colnames, dimnames
  - dimensions (matrices)
  - class
  - length (vectors and lists)
  - other user-defined attributes/metadata
- Attributes of an object can be accessed using the ***attributes()*** function.



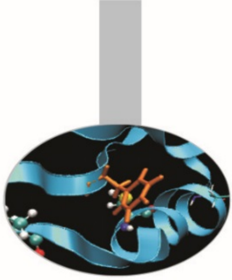
Vectors

- The ***c()*** function can be used to create vectors of objects.

```
> x <- c(0.5, 0.6) ## numeric
> x <- c(TRUE, FALSE) ## logical
> x <- c("a", "b", "c") ## character
> x <- 9:29 ## integer
```

- Using the ***vector()*** function

```
> x <- vector("numeric", length = 10)
[1] 0 1 2 3 4 5 6
```



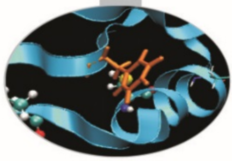
Coercion

- When different objects are mixed in a vector, ***coercion*** occurs so that every element in the vector is of the same class.
- Objects can be explicitly coerced from one class to another using the ***as.*()*** functions, if available.

```
> x <- 0:6
> class(x)
[1] "integer"
> as.numeric(x)
```

- Nonsensical coercion results in *NAs*.

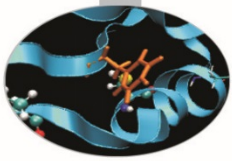
Lists



- ***Lists*** are a special type of vector that can contain elements of different classes. Lists are a very important data type in R and should be examined carefully.

```
> x <- list(1, "a", TRUE, 1 + 4i)
```

Matrices



- Matrices are vectors with a dimension attribute. The dimension attribute is itself an integer vector of length 2 (nrow, ncol)

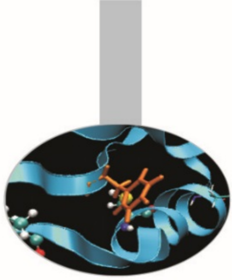
```
> m <- matrix(nrow = 2, ncol = 3)
```

- Matrices are constructed column-wise, so entries can be thought of starting in the “upper left” corner and running down the columns.

```
> m <- matrix(1:6, nrow = 2, ncol = 3)
```

- Matrices can be created by column-binding or row-binding with ***cbind()*** and ***rbind()***.

```
> x <- 1:3
> y <- 10:12
> cbind(x, y)
```

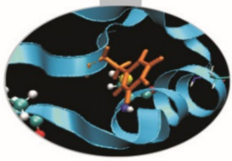


Factors

- Factors are used to represent categorical data. Factors can be unordered or ordered
- Using factors with labels is better than using integers because factors are self-describing
- The order of the levels can be set using the levels argument to ***factor()***. This can be important in linear modelling because the first level is used as the baseline level

```
> x <- factor(c("yes", "yes", "no", "yes", "no"), levels = c("yes", "no"))
```

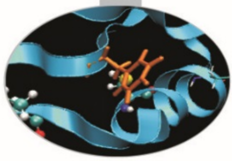
Missing values



- Missing values are denoted by ***NA*** or ***NaN*** for undefined mathematical operations
- ***is.na()*** is used to test objects if they are NA
- ***is.nan()*** is used to test for NaN
- NA values have a class also, so there are integer NA, character NA, etc.
- A NaN value is also NA but the converse is not true

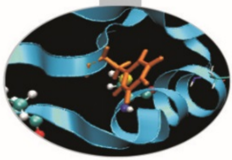
```
> x <- c(1, 2, NA, 10, 3)
> is.na(x)
[1] FALSE FALSE TRUE FALSE FALSE
```

Data Frames

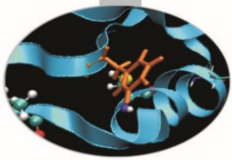


- Used to store tabular data
- Can be considered as a special type of list where every element of the list has to have the same length
- Each element of the list can be thought of as a column and the length of each element of the list is the number of rows
- Unlike matrices, they can store different classes of objects in each column
- Data frames also have special attributes called **names** and **row.names**
- Data frames are usually created by calling ***read.table()*** or ***read.csv()***
- Can be converted to a matrix by calling ***data.matrix()***

Reading and writing data

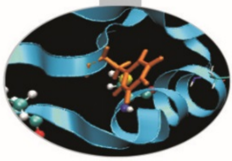


- There are a few principal functions reading data into R
  - read.table(), read.csv(): tabular data
  - readLines(): lines of a text file
  - source(): R code files (inverse of dump)
  - dget(): R code files (inverse of dput)
  - load(): saved workspaces
  - unserialize(): single R objects in binary form
- There are analogous functions for writing data to files
  - write.table()
  - writeLines()
  - dump()
  - dput()
  - save()
  - serialize()



read.table (1)

- ***read.table()*** is one of the most used functions for reading data. The most important arguments are:
  - **file**: the name of a file, or a connection
  - **header**: (logical) indicates if the file has a header line
  - **sep**: a string indicating how the columns are separated
  - **colClasses**: a character vector indicating the class of each column
  - **nrows**: the number of rows in the dataset
  - **comment.char**: a character string indicating the comment character
  - **skip**: the number of lines to skip from the beginning
  - **stringsAsFactors**: should character variables be coded as factors?
  - **quote**: the set of quoting characters



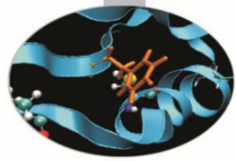
read.table (2)

- For small and moderately sized datasets, the function may be called without specifying any other argument

```
> data <- read.table(”example.txt")
```

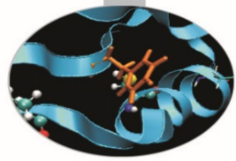
- R will automatically:
  - skip lines that begin with a # (such setting may be modified)
  - figure out how many rows the file has
  - assign a type to each column of the table
- ***read.csv()*** is identical to read.table, but the default separator is a comma.

Reading larger datasets (1)



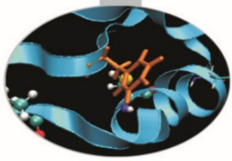
- With much larger datasets, the following precautions will make life easier and prevent R from choking.
  - Make a rough calculation of the memory required to store the dataset. If the dataset is larger than the available RAM, no further stops can be executed.
  - Set ***comment.char* = ""** if there are no commented lines in the file
  - Set ***quote* = “”**
- Hint: **always read the help pages!**
  - Example: ***?read.table***
  - Once a R package is loaded, it will be possible to read the help page of every function contained in such package

Reading larger datasets (2)



- Know your system
  - In general, when using R with larger datasets, it’s useful to know a few things about the system used.
  - How much memory is available?
  - What other applications are in use?
  - Are there other users logged into the same system?
  - What operating system?
  - Is the OS 32 or 64 bit?
- Calculating Memory Requirements
  - Having a data frame with 1,500,000 rows and 120 columns, with numeric data. Roughly, how much memory is required to store this data frame?
  - 1,500,000 × 120 × 8 bytes/numeric = 1440000000 bytes =
    = 1440000000 /2^20 bytes/MB = 1,373.29 MB = 1.34 GB

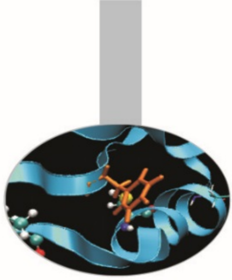
Subsetting (1)



- Some operators can be used to extract subsets of R objects:
  - **[** always returns an object of the same class as the original: it can be used to select more than one element
  - **[[** is used to extract elements of a list or a data frame; it can only be used to extract a single element and the class of the returned object will not necessarily be a list or a data frame
  - **$** is used to extract elements of a list (or data frame) by name
- Examples:

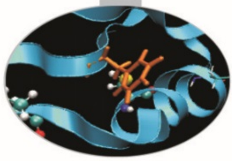
```
> x <- c("a", "b", "c", "c", "d", "a")
> x[1]
[1] "a”
> x[2]
[1] "b”
> x[1:4]
[1] "a" "b" "c" "c"
```

Subsetting (2)



- Subsetting a **list**: an example

```
> x <- list(foo = 1:4, bar = 0.6)
> x[1]
$foo
[1] 1 2 3 4
> x[[1]]
[1] 1 2 3 4
> x$bar
[1] 0.6
> x[["bar"]]
[1] 0.6
> x["bar"]
$bar
[1] 0.6
```



Subsetting (3)

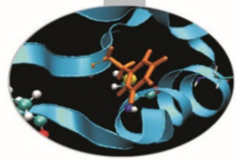
- **Matrices** can be subsetted with **[i,j]** type indices*:*

```
> x <- matrix(data=1:6, nrow=2, ncol=3)
> x[1, 2]
[1] 3
> x[2, 1]
[1] 2
```

- If the index is missing, the entire row (column) will be selected

```
> x[1, ]
[1] 1 3 5
> x[, 2]
[1] 3 4
```

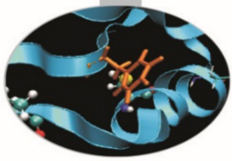
Removing missing values



- Missing values (*NAs*) can be easily removed

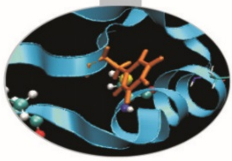
```
> x <- c(1, 2, NA, 4, NA, 5)
> bad <- is.na(x)
> x[!bad]
[1] 1 2 4 5
```

Grouped expressions



- R is an expression language in the sense that its only command type is a function or expression which returns a result.
- Commands may be grouped in braces
- {expr 1, . . . , expr m}
- The value of the group is the result of the last expression in the group evaluated

if() statement

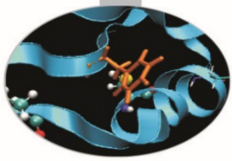


- The language includes a conditional construction:

  if (expr 1) {expr 2}

  else {expr 3}
- *(expr 1)* must evaluate to a **logical value**
- A vectorized version of such construct is the ***ifelse()*** function: this has the form *ifelse(condition, yes=a, no=b)*
- **NB: *else{}* branch is optional**

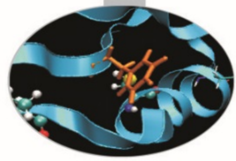
Repetitive executions (1)



- ***for()*** loop: ***for(name in (expr 1)) {expr 2}***
  where: *name* is the loop variable, *expr 1* is a vector expression (often a sequence like 1:20), and *expr 2* is often a grouped expression with its sub-expression. *expr 2* is repeatedly evaluated as name ranges through the values in the vector result of *expr 1*

- Other looping constructs are the ***repeat{}*** statement and the ***while()*** statement. The break statement can be used to terminate any loop, possibly abnormally. This is the only way to terminate *repeat{}* loops. The next statement can be used to discontinue one particular cycle and skip to the “next”.

Repetitive executions (2)



- ***for()***:

```
> for(i in 1:10) { print(i*i) }
```

- ***repeat{}***:

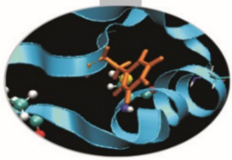
```
> i<-1
> repeat{ print(i*i);  if(i>10) break; i<-i+1 }
```

- ***while():***

```
>  i<-1
>  while(i<10) { print(i*i); i<-i+1 }
```

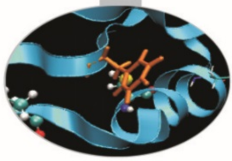
- **Hint: run these codes in your R console and look for the differences!**

The ***apply()*** family



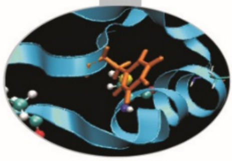
- Useful when similar tasks need to be performed multiple times for all elements of a list or for all rows (columns) of an array
- May be easier and much faster than ***for()*** loops
- Such tasks can be easily speeded up

lapply()



- ***lapply(li, function)***
- To each element of the list *li*, the function *function* is applied
- The result is a list whose elements are the individual *function* results

```
> li = list("klaus","martin","georg")
> lapply(li, toupper)
> [[1]]
> [1] "KLAUS"
> [[2]]
> [1] "MARTIN"
> [[3]]
> [1] "GEORG"
```

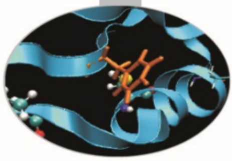


apply()

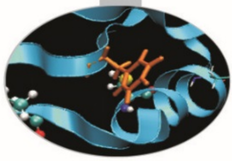
- ***apply(arr, margin, fun)***
- Apply the function *fun* along some dimensions of the array *arr*, according to *margin* (1=rows, 2=columns), and return a vector or array of the appropriate size

```
> x
     [,1] [,2] [,3]
[1,]    5    7    0
[2,]    7    9    8
[3,]    4    6    7
[4,]    6    3    5
> apply(x, 1, sum)
[1] 12 24 17 14
> apply(x, 2, sum)
[1] 22 25 20
```

Using R on PICO



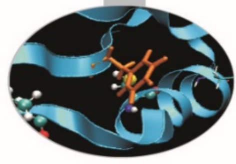
- R can be used within HPC environments
  - PBS Batch jobs: running R using **qsub batch** instructions
  - Interactive PBS Batch jobs: **interactive qsub**
  - Graphical sessions: R & Rstudio via **RCM**
- Some examples will be given using PICO
  - One of Cineca's HPC clusters
  - Made of 74 nodes of different types
    - 54 Compute nodes
    - 4 Visualization nodes
    - 2 Login nodes
    - 14 other nodes
  - 1080 cores available for computational tasks (Batch jobs only)
  - http://www.hpc.cineca.it/content/pico-user-guide



Parallel Computing with R

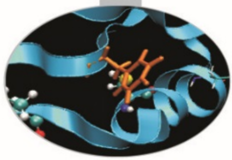
- Under some circumstances, a R job can be speeded up
- Several ways of parallelization are available
- Such methods can be divided in two broad categories:
  - **lapply-based** (*shared memory* and *distributed memory*)
  - **foreach-based** (*shared memory* and *distributed memory*)
- Parallel jobs with R & MPI-based R packages
  - parallel, doParallel, foreach, doMC
  - Rmpi,doMPI,foreach
  - Rmpi,snow,snowfall

Parallelization parameters



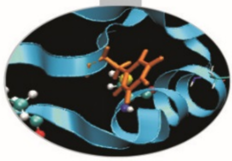
- How many cores?
  - If Rstudio is launched via RCM, only the cores of the visualization node in use can be exploited (up to 20)
- How many nodes?
  - If a **qsub** (Batch or Interactive) job is submitted, more than a single computing node can be exploited
  - The job will be queued and scheduled as any PBS Batch job
- How much memory?
- **Careful!** If too many resources are requested, the priority of the process launched will be lowered

Parallelization (**qsub** jobs)



- How to manage parallelization in qsub jobs?
  - The resources needed can be directly specified within the code:
    - Number of nodes
    - Number of processors per node
    - Memory needed
    - Maximum job time
  - The number of cores to exploit must also be specified within the R code by using the built-in functions of the R packages mentioned before

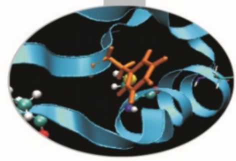
qsub jobs: examples (1)



- PBS Interactive job:

```
qsub -A cin_staff  -I -l select=1:ncpus=10:mpiprocs=10:mem=15GB -q parallel -- /bin/bash
module load autoload profile/advanced
module load autoload r
module load autoload openmpi
R --vanilla < kmeans_distMem_kddcup.R
```

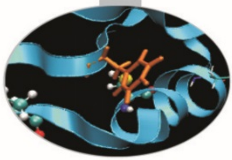
qsub jobs: examples (2)



- PBS Batch job:

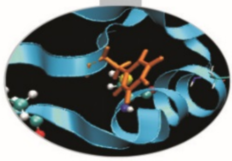
```
#!/bin/bash
#PBS -A cin_staff
#PBS -l walltime=1:00:00
#PBS -l select=1:ncpus=10:mpiprocs=10:mem=15GB
#PBS -o job.out
#PBS -e job.err
#PBS -q parallel
module load profile/advanced
module load autoload openmpi
module  load autoload r
R --vanilla < kmeans_distMem_kddcup.R > kmeans_kddcup_output.txt
```

PBS keywords



- #PBS -N jobname **# name of the job**
- #PBS -o job.out **# redirect stdout (output file)**
- #PBS -e job.err **# redirect stderr (error file)**
- #PBS -l walltime=1:00:00 **# hh:mm:ss**
- #PBS -q <queue-name> **# chosen queue**
- #PBS -A <my_account> **# name of the account**
- #PBS -l select=1:ncpus=10:mem=15gb:mpiprocs=10
  - **select** = number of chunks requested
  - **ncpus** = number of cpus per chunk requested
  - **mpiprocs** = number of mpi processes
  - **mem** = RAM memory per chunk

PICO login



- Via SSH client:
  - Open a SSH client
  - Press ENTER
  - Connect to Remote Host:
    - Host Name: **login.pico.cineca.it**
    - User Name: **the personal User Name**
    - Port Number: **the default one**
    - Authentication Method: **<Profile Settings>**
  - Enter the given Password
- Via SSH connection (Unix only!):
  - **ssh <username>@login.pico.cineca.it**
  - Enter the given password
- Via Secure Shell Plugin for Google Chrome