



Leibniz Supercomputing Centre  
of the Bavarian Academy of Sciences and Humanities

The background of the slide is a photograph of a modern, multi-story building with a glass and metal facade, likely the LRZ building. The image is overlaid with a semi-transparent blue filter. The building has several windows and a prominent vertical structure on the right side.

# High Performance Data Analytics Using R at LRZ – Part 1

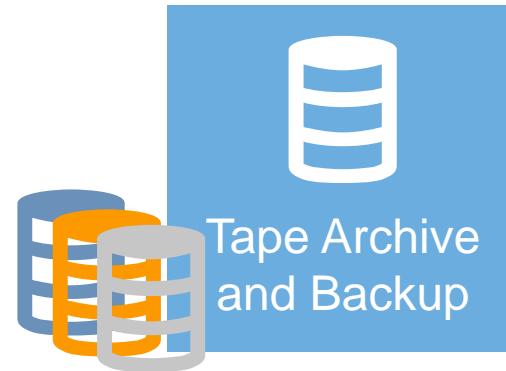
2021-10-15

# Course Information

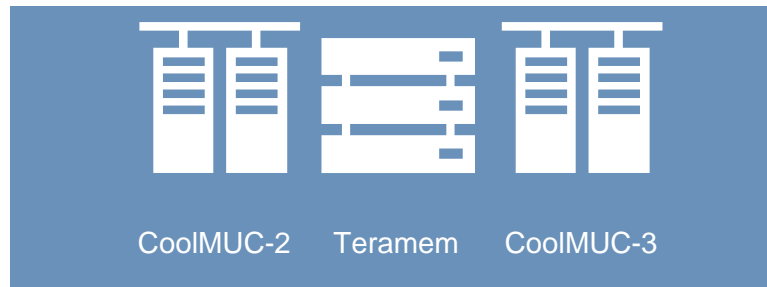
- The aim of this course is to demonstrate the different ways of using R efficiently and productively on LRZ systems with a focus on parallelization mechanisms and data analytics/machine learning tasks
- It is not an introduction to R itself
- Many of the topics covered in this course are based on issues encountered by users, for which they created tickets at the LRZ Servicedesk
- Also, it assumes you have some prior knowledge and experience in using GNU/Linux and SSH, as well as a good understanding of the LRZ HPC and AI Infrastructure (if you attended this week's courses, you are fine)



# HPC & BDAI Systems for Bavarian Universities



Data Science Storage  
(DSS)

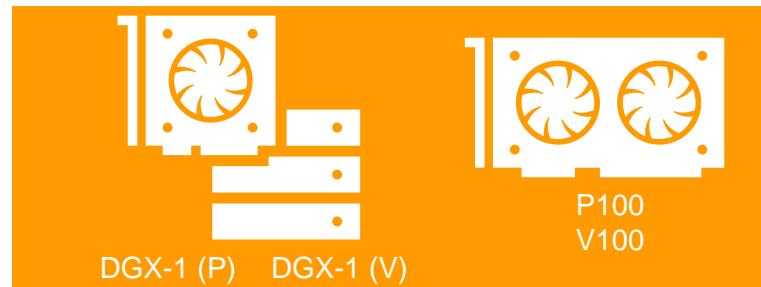


CoolMUC-2 Teramem CoolMUC-3

[lxlogin8.lrz.de](https://lxlogin8.lrz.de)

[lxlogin\[1-4\].lrz.de](https://lxlogin[1-4].lrz.de)

(<https://www.rstudio.lrz.de>)

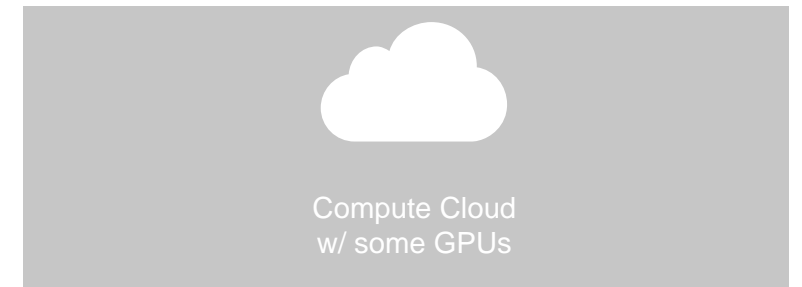


DGX-1 (P) DGX-1 (V)

P100  
V100

[datalab2.srv.lrz.de](https://datalab2.srv.lrz.de)

<https://datalab3.srv.lrz.de>



Compute Cloud  
w/ some GPUs

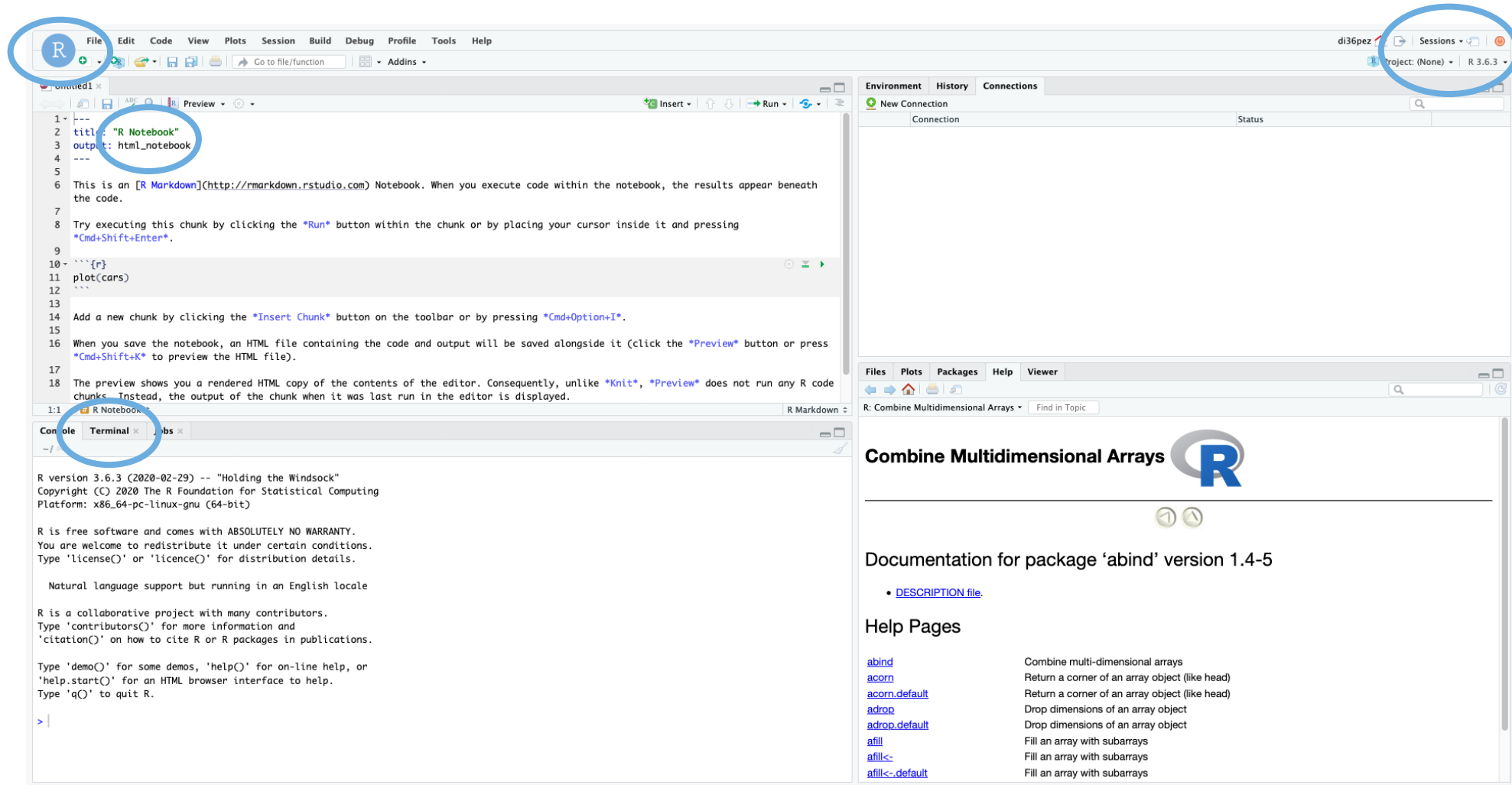
<https://cc.lrz.de>



# RStudio Server



- Web-based RStudio frontend
- Cluster of multiple nodes, each with
  - 40 cores (please do not use more than 20 individually!) and
  - 360 GB RAM
- Integrates with the Linux Cluster:
  - Directly access the data in your DSS-backed Linux Cluster home directory (\$HOME)
  - Allows to access any DSS-based storage container (NFS-export has to be set up by data curator)
  - Use the built-in Terminal to submit jobs to the Linux Cluster's batch queues via the Slurm Workload Manager
- For further details, see <https://doku.lrz.de/x/zQWVAg>
- **EOL: 30. November 2021 – use LRZ AI Systems instead!**  
**Contact us if you encounter any (migration) issues!**



The screenshot shows the RStudio Server interface with several elements circled in blue:

- The R logo in the top-left corner of the menu bar.
- The "R Notebook" title in the editor's title bar.
- The "Terminal" tab in the bottom-left pane.
- The "Sessions" button in the top-right corner of the window.

The editor displays R Markdown code for a notebook. The code includes a title, output format, and a chunk of R code:

```
1 ---  
2 title: "R Notebook"  
3 output: html_notebook  
4 ---  
5  
6 This is an [R Markdown](http://rmarkdown.rstudio.com) Notebook. When you execute code within the notebook, the results appear beneath  
7 the code.  
8 Try executing this chunk by clicking the *Run* button within the chunk or by placing your cursor inside it and pressing  
9 *Cmd+Shift+Enter*.  
10  
11 ```{r}  
12 plot(cars)  
13 ```  
14 Add a new chunk by clicking the *Insert Chunk* button on the toolbar or by pressing *Cmd+Option+I*.  
15  
16 When you save the notebook, an HTML file containing the code and output will be saved alongside it (click the *Preview* button or press  
17 *Cmd+Shift+K* to preview the HTML file).  
18  
19 The preview shows you a rendered HTML copy of the contents of the editor. Consequently, unlike *Knit*, *Preview* does not run any R code  
20 chunks. Instead, the output of the chunk when it was last run in the editor is displayed.
```

The terminal pane shows the R version and copyright information:

```
R version 3.6.3 (2020-02-29) -- "Holding the Windsock"  
Copyright (C) 2020 The R Foundation for Statistical Computing  
Platform: x86_64-pc-linux-gnu (64-bit)  
  
R is free software and comes with ABSOLUTELY NO WARRANTY.  
You are welcome to redistribute it under certain conditions.  
Type 'license()' or 'licence()' for distribution details.  
  
Natural language support but running in an English locale  
  
R is a collaborative project with many contributors.  
Type 'contributors()' for more information and  
'citation()' on how to cite R or R packages in publications.  
  
Type 'demo()' for some demos, 'help()' for on-line help, or  
'help.start()' for an HTML browser interface to help.  
Type 'q()' to quit R.  
  
> |
```

The right-hand pane displays the documentation for the 'abind' package version 1.4-5, including a list of help pages:

### Combine Multidimensional Arrays

Documentation for package 'abind' version 1.4-5

- [DESCRIPTION file.](#)

### Help Pages

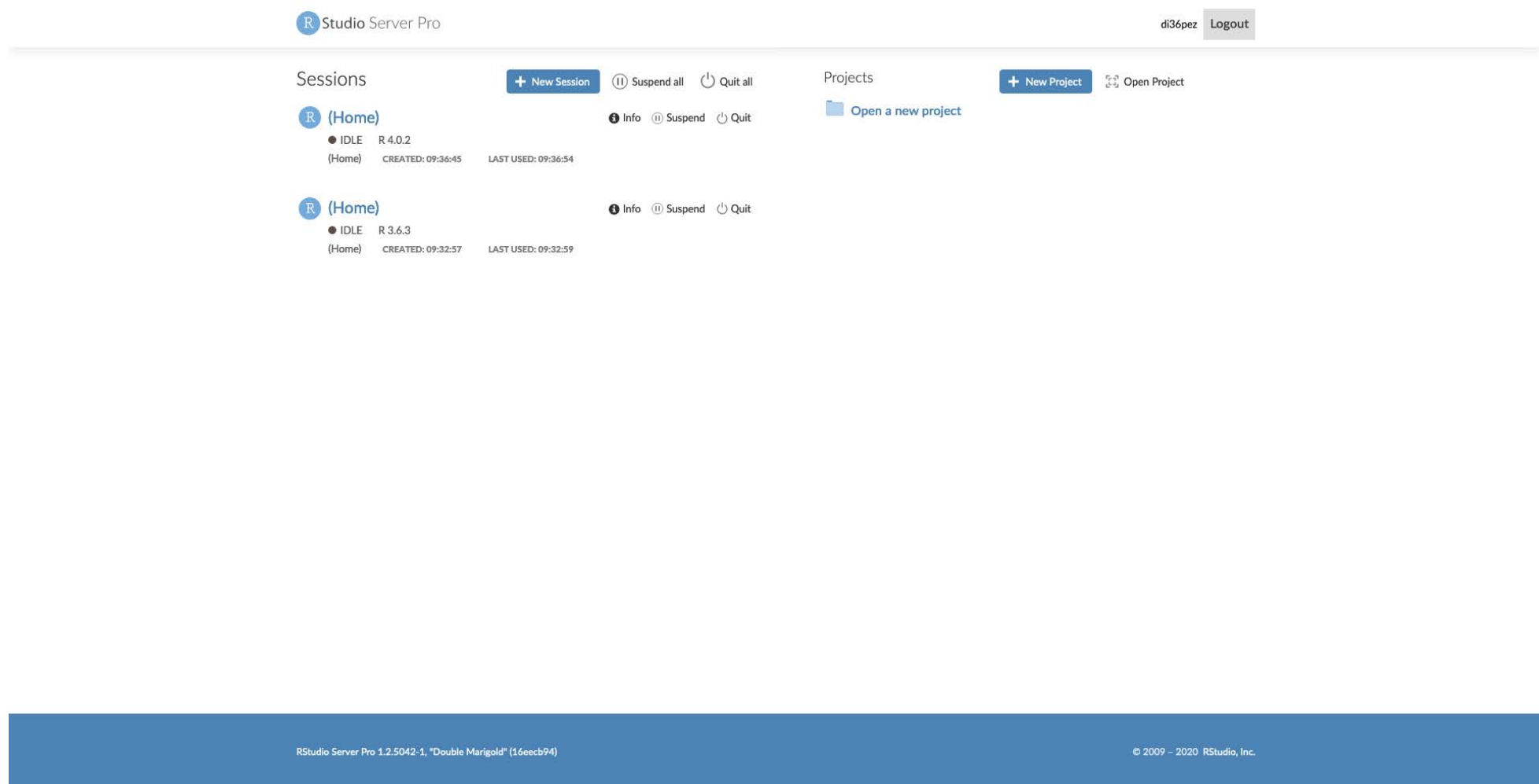
<a href="#">abind</a>	Combine multi-dimensional arrays
<a href="#">acorn</a>	Return a corner of an array object (like head)
<a href="#">acorn.default</a>	Return a corner of an array object (like head)
<a href="#">adrop</a>	Drop dimensions of an array object
<a href="#">adrop.default</a>	Drop dimensions of an array object
<a href="#">afill</a>	Fill an array with subarrays
<a href="#">afill&lt;-</a>	Fill an array with subarrays
<a href="#">afill&lt;- .default</a>	Fill an array with subarrays

- R Notebooks:  
R Markdown documents with code chunks that can be executed independently and interactively, with output visible immediately beneath the input

- Integrated Terminal:  
Provides access to the system shell from within Rstudio
- Can be used to submit jobs to the Slurm workload manager of CoolMUC-2



- You can open multiple concurrent sessions (please don't use more than 5 at any given time!)
- This can be used to work on multiple analyses in parallel (using different versions of R if needed) and they can be kept open (almost) indefinitely



The screenshot shows the RStudio Server Pro interface. At the top left, it says "R Studio Server Pro". At the top right, the user "di36pez" is logged in, with a "Logout" button. The main area is divided into two sections: "Sessions" and "Projects".

**Sessions:**

- Buttons: + New Session, || Suspend all, ⏻ Quit all
- Session 1: (Home) R 4.0.2, IDLE, (Home) CREATED: 09:36:45, LAST USED: 09:36:54. Actions: Info, || Suspend, ⏻ Quit.
- Session 2: (Home) R 3.6.3, IDLE, (Home) CREATED: 09:32:57, LAST USED: 09:32:59. Actions: Info, || Suspend, ⏻ Quit.

**Projects:**

- Buttons: + New Project, 📁 Open Project
- Action: 📁 Open a new project

At the bottom of the interface, there is a blue footer bar containing the text: "RStudio Server Pro 1.2.5042-1, 'Double Marigold' (16eeeb94)" on the left and "© 2009 - 2020 RStudio, Inc." on the right.



- Connect to the CoolMUC-2 segment of the Linux Cluster
- From a terminal application:  
`$ ssh <user>@lxlogin1.lrz.de`
- Alternatives would be  
lxlogin[2-4].lrz.de for CoolMUC-2 or  
lxlogin8.lrz.de for CoolMUC-3

- R is not accessible on the Linux Cluster by default (try: `$ which R`)
- Environment modules allow for the dynamic modification of environment variables
- A (minimal) set of default modules is active after login:  
`$ module list`
- Use the module system to search for different R versions:  
`$ module available r` (or `module av r`)

```
di36pez@ivy-login: ~
Datei Bearbeiten Ansicht Suchen Terminal Hilfe
di36pez@ivy-login:~$ which R
which: no R in (/lrz/sys/intel/studio2017_u6/mpi/2017.4.256/lrzbin:/lrz/sys/intel/studio2017_u6/mpi/2017.4.256/bin64:/lrz/sys/intel/studio2017_u6/compilers_and_libraries_2017.6.256/linux/bin/intel64:/lrz/sys/share/modules/bin:/lrz/sys/bin:/usr/local/bin:/usr/bin:/bin:/usr/bin/X11:/usr/games:/opt/ibutils/bin:/lrz/sys/tools/slurm_utils/bin)
di36pez@ivy-login:~$ module list
Currently Loaded Modulefiles:
 1) admin/1.0          3) intel/17.0        5) mpi.intel/2017      7) lrz/default
 2) tempdir/1.0       4) mkl/2017          6) spack/release/18.2
di36pez@ivy-login:~$ module av r
----- /lrz/sys/share/modules/files/graphics -----
rvsvnc/1.0(default)
----- /lrz/sys/share/modules/files/libraries -----
root/6.12(default)
----- /lrz/sys/share/modules/files/tools -----
redis/3.2.5(default)
----- /lrz/sys/spack/18.2/modules/x86_avx/linux-sles12-x86_64 -----
r/3.4.4-X11          r/3.5.0-X11          readline/7.0
r/3.4.4-X11-mkl     r/3.5.0-X11-mkl     renderproto/0.11.1
di36pez@ivy-login:~$
```

- (The current default version of) R can be loaded using `$ module load r`
- If you need a different version, you have to specify the full name of the module, e.g. “r/3.4.4-gcc8-mkl”

```
di36pez@ivy-login: ~  
Datei Bearbeiten Ansicht Suchen Terminal Hilfe  
di36pez@ivy-login:~$ module load r  
di36pez@ivy-login:~$ which R  
/lrz/mnt/sys.x86_sles12/spack/18.2/opt/x86_avx/r/3.5.0-gcc-pzdtq2a/bin/R  
di36pez@ivy-login:~$
```

- We are using the package manager Spack (<https://spack.io>) to provide applications/modules
- Spack “meta modules” make the (additional) module path(s) available
- By default, the latest LRZ release of Spack is loaded (cf. `$ module list`)
- Going forward, there might be newer (pre-release) versions of the Spack software stack available (e.g. `spack/staging/20.2`, `spack/develop`) which might then also provide newer versions of R
- If in doubt, stick to the final releases set as default (i.e. `spack/release/YY.X`)!

- All R packages are installed into libraries – these are (just) directories in the file system with subdirectories for each installed package
- The default installation of R comes with a single library (`R_HOME/library`) usually containing the standard and recommended packages (in RStudio, this is called the System Library)
- On a multiuser system, regular users may not add/install packages directly into this library (but administrators can)
- For the latest versions of R on the Linux Cluster we only provide the standard set of base packages in this central location



- Individual users can have (one or more) additional, personal libraries (called User Library in RStudio)
- The path for this library directory can be specified by the environment variable `$R_LIBS_USER` (amongst others)
- If this is not defined, R will ask you to create a personal package library when installing packages for the first time...

```
di36pez@ivy-login: ~  
Datei Bearbeiten Ansicht Suchen Terminal Hilfe  
R version 3.5.0 (2018-04-23) -- "Joy in Playing"  
Copyright (C) 2018 The R Foundation for Statistical Computing  
Platform: x86_64-pc-linux-gnu (64-bit)  
  
R ist freie Software und kommt OHNE JEGLICHE GARANTIE.  
Sie sind eingeladen, es unter bestimmten Bedingungen weiter zu verbreiten.  
Tippen Sie 'license()' or 'licence()' für Details dazu.  
  
R ist ein Gemeinschaftsprojekt mit vielen Beitragenden.  
Tippen Sie 'contributors()' für mehr Information und 'citation()',  
um zu erfahren, wie R oder R packages in Publikationen zitiert werden können.  
  
Tippen Sie 'demo()' für einige Demos, 'help()' für on-line Hilfe, oder  
'help.start()' für eine HTML Browserschnittstelle zur Hilfe.  
Tippen Sie 'q()', um R zu verlassen.  
  
> install.packages("ggplot2")  
Warnung in install.packages("ggplot2")  
  'lib = "/lrz/mnt/sys.x86_sles12/spack/18.2/opt/x86_avx/r/3.5.0-gcc-pzdtq2a/rli  
b/R/library" ist nicht schreibbar  
Would you like to use a personal library instead? (yes/No/cancel) yes  
Would you like to create a personal library  
'~/R/x86_64-pc-linux-gnu-library/3.5'  
to install packages into? (yes/No/cancel) █
```

- Notice the suggested path – it is specific to the (minor) version of R!
- You can use the `.libPaths()` function within R to check the current library directories...

```
di36pez@ivy-login: ~
Datei Bearbeiten Ansicht Suchen Terminal Hilfe
di36pez@ivy-login:~$ R
R version 3.5.0 (2018-04-23) -- "Joy in Playing"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R ist freie Software und kommt OHNE JEGLICHE GARANTIE.
Sie sind eingeladen, es unter bestimmten Bedingungen weiter zu verbreiten.
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Tippen Sie 'demo()' für einige Demos, 'help()' für on-line Hilfe, oder
'help.start()' für eine HTML Browserschnittstelle zur Hilfe.
Tippen Sie 'q()', um R zu verlassen.

> .libPaths()
[1] "/home/hpc/pr28fa/di36pez/R/x86_64-pc-linux-gnu-library/3.5"
[2] "/lrz/mnt/sys.x86_sles12/spack/18.2/opt/x86_avx/r/3.5.0-gcc-pzdtq2a/rlib/R/library"
>
```

- So, subject to the system/cluster segment and R version you're using, you will depend on different system and user libraries
- You can always control the R packages you use (and their versions) by maintaining your user library...
- ... it might even be beneficial to do this in a project-specific manner.

- A challenge: on GNU/Linux (most) „add-on“ R packages will be compiled from source
- This requires compilers, tools and additional dependencies available on the system
- For general compatibility use (a recent version) of the GNU Compiler Collection GCC to compile add-on packages:

```
module unload intel-mpi  
module unload intel  
module load gcc  
module load r
```

- If you miss any dependencies, make sure to check the available modules!
- And, as always: if you encounter any problems, please talk to us!

- Optional:  
there are package managers which can be run as user applications and may provide additional dependency requirements
- They manage R and (many of) its packages „from the outside“
- You could take a look at Spack (<https://spack.io>), conda (<https://conda.io>) or Homebrew (<https://brew.sh>)

- Slurm is a job scheduler:
  - Allocates access to resources (time, memory, nodes/cores)
  - Provides framework for starting, executing, and monitoring work
  - Manages queue of pending jobs (enforcing “fair share” policy)
- Use the `sinfo` command to get information about the available clusters

```
$ sinfo --clusters=all or, shortened:
```

```
$ sinfo -M all
```



```
di36pez@mpp2-login5: ~
Datei Bearbeiten Ansicht Suchen Terminal Hilfe
di36pez@mpp2-login5:~$ sinfo -M all
CLUSTER: bsbslurm
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
bsb_konvert* up    infinite    1      mix hbsbr09c05s02
bsb_konvert* up    infinite    1      alloc hbsbr09c05s01
bsb_konvert* up    infinite    4      idle hbsbr09c05s[03-06]

CLUSTER: hm_mech
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
hm_mech_batch* up 14-00:00:0 12      alloc hhmkr09c04s[01-12]

CLUSTER: httf
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
httf_batch* up 3-00:00:00 5        resv httfr05c05s[01-05]

CLUSTER: htus
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
htus_batch* up 3-00:00:00 2        idle htusr05c04s[05-06]

CLUSTER: inter
PARTITION   AVAIL  TIMELIMIT  NODES  STATE NODELIST
mpp3_inter* up    2:00:00    1      alloc mpp3r03c05s03
mpp3_inter* up    2:00:00    2      idle mpp3r03c05s[01-02]
teramem_inter up 4-00:00:00 1        mix teramem1
```

- Look for the cluster segments
  - inter (allows for interactive usage)
  - cm2 (the main CoolMUC-2 cluster)
  - serial (shared nodes for serial jobs)
- What is their current status?
- Get information about a specific cluster segment, e.g.  
`$ sinfo -M inter` or  
`$ sinfo -M cm2`

# CoolMUC-2 Overview



Slurm Cluster	Slurm Partition	Node Range	Slurm Job Settings
cm2	cm2_large	25-64	--clusters=cm2 --partition=cm2_large --qos=cm2_large
	cm2_std	3-24	--clusters=cm2 --partition=cm2_std --qos=cm2_std
cm2_tiny	cm2_tiny	1-4	--clusters=cm2_tiny
serial	serial_std	1	--clusters=serial --partition=serial_std --mem=<memory_per_node>MB
	serial_long	1	--clusters=serial --partition=serial_long --mem=<memory_per_node>MB
inter	cm2_inter	1-4	--clusters=inter --partition=cm2_inter
	teramem_inter	1	--clusters=inter --partition=teramem_inter

For additional details see <https://doku.lrz.de/display/PUBLIC/Job+Processing+on+the+Linux-Cluster>



- The inter cluster can be used for interactive resource allocation:  
`$ salloc -p cm2_inter -N 1`
- Using this shell, you can e.g. run R interactively on this node (if the R module is loaded):  
`$ R`

# Interactive R Session



```
user@cm2login1:~$ salloc -p cm2_inter -N 1
salloc: Granted job allocation 159945
user@i22r07c05s11:~$ module load r
user@i22r07c05s11:~$ R
```

```
R version 3.6.3 (2020-02-29) -- "Holding the Windsock"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
```

```
[...]
```

```
> library(parallel)
> detectCores()
[1] 56
>
```

- For production jobs, you want to prepare and submit batch scripts
- They tell Slurm about the resources you need and the scripts/programs you want to run...

```
#!/bin/bash
#SBATCH --clusters=cm2_tiny
#SBATCH --nodes=1

module load slurm_setup

module load r

Rscript myscript.R
```

- A very minimal example of a job script (not necessarily recommended, but working in some cases), requesting
  - a single, exclusive node (with 28 cores)
  - of the cm2\_tiny partition/cluster, part of
  - the CoolMUC-2 system
- Submit this job script to the queue:  
\$ sbatch <myjob.sh>

```
#!/bin/bash
#SBATCH -o /dss/dsshhome1/.../.../myjob.%j.%N.out
#SBATCH -D /dss/dsshhome1/.../.../workdir
#SBATCH -J jobname
#SBATCH --get-user-env
#SBATCH --clusters=cm2
#SBATCH --partition=cm2_std
#SBATCH --nodes=3
#SBATCH --mail-type=end
#SBATCH --mail-user=xyz@xyz.de
#SBATCH --export=NONE
#SBATCH --time=08:00:00

module load slurm_setup
module unload intel-mpi
module load openmpi

module load r

mpirun R -f myscript.R
```

- A more practical example...
  - defining custom output file(s)
  - setting a working directory
  - assigning a job name
  - configuring mail notifications
  - managing the environment
  - limiting walltime explicitly
- See documentation for more details:

<https://doku.lrz.de/x/AgaVAg>

- Submit a job:  
`$ sbatch myjob.sh`
- Query status of your jobs:  
`$ squeue -M <cluster> -u <user>`
- Approximate start time of pending jobs:  
`$ squeue -M <cluster> -u <user> --start`
- Abort a job:  
`$ scancel -M <cluster> <jobid>`
- Get accounting data for (past) jobs:  
`$ sacct -X -M <cluster> [-S <YYYY-MM-DD>] -u <user>`

- Jobs get aborted (by Slurm) if they use more resources than specified
  - > you need to estimate memory and runtime requirements
    - Estimate memory requirements from a (single, local) serial run, extrapolate if needed (use e.g. your system monitor or the “top” command line tool)
    - Provide some “buffer” for runtime
- Queuing times can be long
  - Use “sinfo” to find less busy cluster segments
  - Smaller, less demanding jobs generally start faster
    - > you can benefit from accurate resource estimation

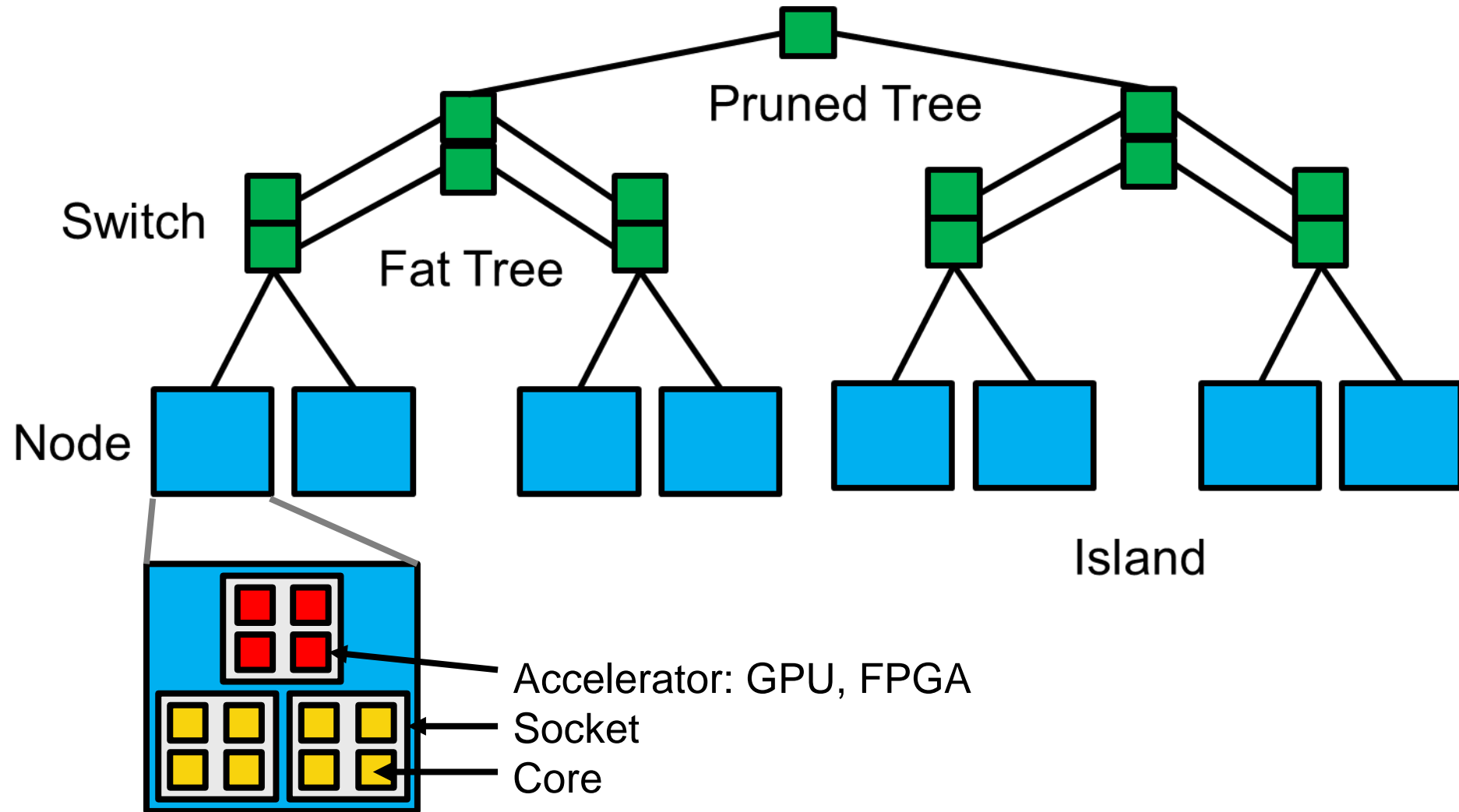
- Debugging can be inconvenient
- The time interval between changes in the R code and seeing results/getting feedback is longer than usual
- The compute environment (compute nodes of the cluster) and the development/test environments (local, login or interactive nodes) are usually not exactly the same
  - Debug as much as possible in a serial fashion
  - Prepare small jobs and test them interactively (using “salloc”/”srun”)



The background of the slide is a photograph of a modern, multi-story building with a glass and metal facade, likely the LRZ building. The image is overlaid with a semi-transparent blue filter. The building has several windows and a prominent vertical structure on the right side.

# High Performance Data Analytics Using R at LRZ – Part 2

2021-10-15



# Parallelization

Motivation:

- You have a lot of (more or less) independent tasks or
- You want to accelerate a single complex task -> it might be possible to turn the single complex task into many (more or less) independent tasks

...and you have access to a (massively parallel) supercomputer!



# Parallelization Scenario: Embarrassingly/Pleasingly Parallel



- many independent processes (10 - 100.000)
- individual task (list) for each process
- private memory for each process
- no communication between processes
- results are stored separately on a (large) storage medium

# Parallelization Scenario: Worker Queue



- many independent processes (10 - 100.000)
- central task scheduler (database)
- private memory for each process
- results are sent back to task scheduler
- re-scheduling of failed tasks possible

# Parallelization Scenario: Shared Memory

- a few processes working closely together (10-100)
- single task list (script/program)
- shared memory (cache coherent non-uniform memory architecture aka ccNUMA)
- results are kept in shared memory



# Parallelization Scenario: Message Passing

- many independent processes (10 - 100.000)
- one task list (script/program) for all processes
- each process can (in principle) talk to every other process
- private memory
- needs communication strategy in order to scale (area of optimization, e.g. nearest neighbor communication)
- beware of deadlocks!



# CRAN Task View: High-Performance and Parallel Computing



## CRAN Task View: High-Performance and Parallel Computing with R

**Maintainer:** Dirk Eddelbuettel  
**Contact:** Dirk.Eddelbuettel at R-project.org  
**Version:** 2018-08-27  
**URL:** <https://CRAN.R-project.org/view=HighPerformanceComputing>

This CRAN task view contains a list of packages, grouped by topic, that are useful for high-performance computing (HPC) with R. In this context, we are defining 'high-performance computing' rather loosely as just about anything related to pushing R a little further: using compiled code, parallel computing (in both explicit and implicit modes), working with large objects as well as profiling.

Unless otherwise mentioned, all packages presented with hyperlinks are available from CRAN, the Comprehensive R Archive Network.

Several of the areas discussed in this Task View are undergoing rapid change. Please send suggestions for additions and extensions for this task view to the [task view maintainer](#).

Suggestions and corrections by Achim Zeileis, Markus Schmidberger, Martin Morgan, Max Kuhn, Tomas Radivoyevitch, Jochen Knaus, Tobias Verbeke, Hao Yu, David Rosenberg, Marco Enea, Ivo Welch, Jay Emerson, Wei-Chen Chen, Bill Cleveland, Ross Boylan, Ramon Diaz-Uriarte, Mark Zeligman, Kevin Ushey, Graham Jeffries, Will Landau, Tim Flutre, Reza Mohammadi, Ralf Stubner, and Bob Jansen (as well as others I may have forgotten to add here) are gratefully acknowledged.

Contributions are always welcome, and encouraged. Since the start of this CRAN task view in October 2008, most contributions have arrived as email suggestions. The source file for this particular task view file now also reside in a GitHub repository (see below) so that pull requests are also possible.

The `ctv` package supports these Task Views. Its functions `install.views` and `update.views` allow, respectively, installation or update of packages from a given Task View; the option `coreOnly` can restrict operations to packages labeled as `core` below.

**Direct support in R started with release 2.14.0** which includes a new package **parallel** incorporating (slightly revised) copies of packages **multicore** and **snow**. Some types of clusters are not handled directly by the base package 'parallel'. However, and as explained in the package

### Parallel computing: Explicit parallelism

- Several packages provide the communications layer required for parallel computing. The first package in this area was `rpvm` by Li and Rossini which uses the PVM (Parallel Virtual Machine) standard and libraries. `rpvm` is no longer actively maintained, but available from its CRAN archive directory.
- In recent years, the alternative MPI (Message Passing Interface) standard has become the de facto standard in parallel computing. It is supported in R via the `Rmpi` by Yu. `Rmpi` package is mature yet actively maintained and offers access to numerous functions from the MPI API, as well as number of R-specific extensions. `Rmpi` can be used with the LAM/MPI, MPICH / MPICH2, Open MPI, and Deino MPI implementations. It should be noted that LAM/MPI is now in maintenance mode, and new development is focused on Open MPI.
- The `pbdMPI` package provides S4 classes to directly interface MPI in order to support the Single Program/Multiple Data (SPMD) parallel programming style which is particularly useful for batch parallel execution. The `pbdSLAP` builds on this and uses scalable linear algebra packages (namely BLACS, PBLAS, and ScaLAPACK) in double precision based on ScaLAPACK version 2.0.2. The `pbdBASE` builds on these and provides the core classes and methods for distributed data types upon which the `pbdDMAT` builds to provide distributed dense matrices for "Programming with Big Data". The `pbdNCDF4` package permits multiple processes to write to the same file (without manual synchronization) and supports terabyte-sized files. The `pbdDEMO` package provides examples for these packages, and a detailed vignette. The `pbdPROF` package profiles MPI communication SPMD code via MPI profiling libraries, such as `fpmpi`, `mpiP`, or `TAU`.
- An alternative is provided by the `nws` (NetWorkSpaces) packages from REvolution Computing. It is the successor to the earlier LindaSpaces approach to parallel computing, and is implemented on top of the Twisted networking toolkit for Python.
- The `snow` (Simple Network of Workstations) package by Tierney et al. can use PVM, MPI, NWS as well as direct networking sockets. It provides an abstraction layer by hiding the communications details. The `snowFT` package provides fault-tolerance extensions to `snow`.
- The `snowfall` package by Knaus provides a more recent alternative to `snow`. Functions can be used in sequential or parallel mode.

The **foreach** package allows general iteration over elements in a collection without the use of an explicit loop counter.

- The `Rborist` package employs OpenMP pragmas to exploit predictor-level parallelism in the Random Forest algorithm which promotes efficient use of multicore hardware in restaging data and in determining splitting criteria, both of which are performance bottlenecks in the algorithm.
- The `h2o` package connects to the h2o open source machine learning environment which has scalable implementations of random forests, GBM, GLM (with elastic net regularization), and deep learning.
- The `randomForestSRC` package can use both OpenMP as well as MPI for random forest extensions suitable for survival analysis, competing risks analysis, classification as well as regression
- The `parSim` package can perform simulation studies using one or multiple cores, both locally and on HPC clusters.
- The `qsub` package can submit commands to run on gridengine clusters.

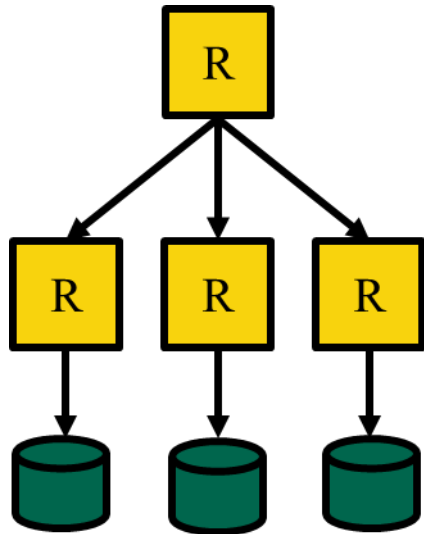


# (Explicit) Parallelization Using R



- Embarrassingly/pleasingly parallel (independent processes):
  - basic approach: start as many R processes as you need in the shell with different scripts

# Parallelization Using R: Embarrassingly/Pleasingly Parallel



Embarrassingly/Pleasingly  
Parallel

```
$ R -f script.R &
```

# Parallelization Using R: Embarrassingly/Pleasingly Parallel



- Use the command line to start your R process (in the background):  
`$ Rscript script0.R &`
- If you do this repeatedly, the resulting R processes will be distributed by the OS to different cores (subject to availability):  
`$ Rscript script1.R &`  
`$ Rscript script2.R &`  
`$ Rscript script3.R & ...`
- To further automate this procedure, you could write a bash script (`run_all_R_scripts.sh`) containing these commands and then run this single script:  
`$ bash run_all_R_scripts.sh &`
- Typically, do not start more processes than cores!
- Do not use the (cluster) login nodes for this (e.g. request an interactive shell instead)!

There is, of course, also a R package to achieve this: callr

- “It is sometimes useful to perform a computation in a separate R process, without affecting the current R process at all. This package does exactly that.”
- Use `r()` to run an R function in a new R process.

```
library(callr)  
r(function() var(iris[, 1:4]))
```

```
#>          Sepal.Length Sepal.Width Petal.Length Petal.Width  
#> Sepal.Length      0.6856935 -0.0424340      1.2743154      0.5162707  
#> Sepal.Width      -0.0424340  0.1899794     -0.3296564     -0.1216394  
#> Petal.Length      1.2743154 -0.3296564      3.1162779      1.2956094  
#> Petal.Width       0.5162707 -0.1216394      1.2956094      0.5810063
```

# Parallelization Using R: Embarrassingly/Pleasingly Parallel



- Let's look at a toy problem:

```
for(i in 1:20) sum(sort(runif(1e7)))
```

- Add a time measurement:

```
system.time(for(i in 1:20) sum(sort(runif(1e7))))
```

- You might also be familiar with alternatives like the following:

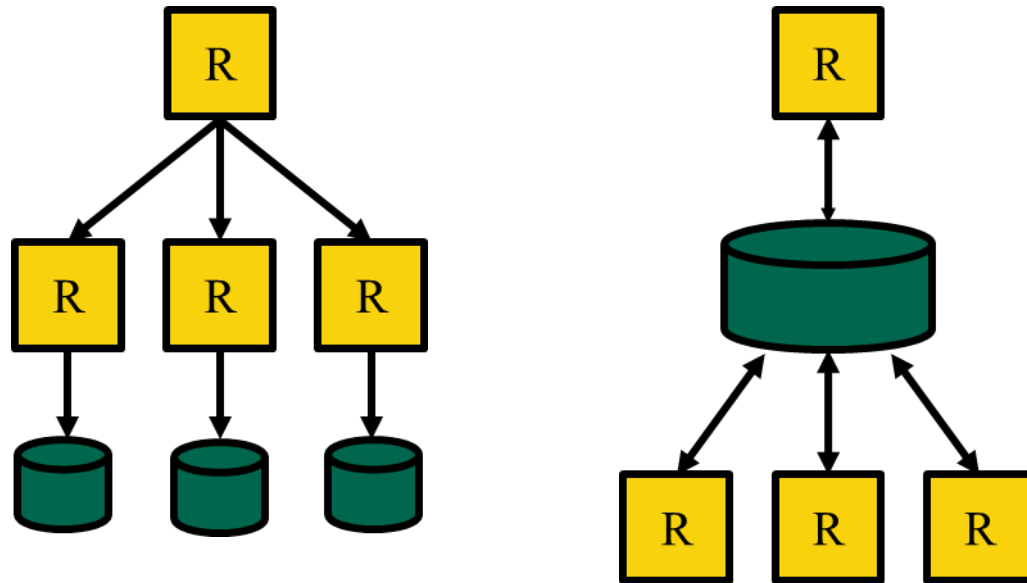
```
lapply(1:20, function(x) sum(sort(runif(1e7))))
```

# (Explicit) Parallelization Using R



- Embarrassingly/pleasingly parallel (independent processes):
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- Worker Queue (weak coupling, shared file system or database):
  - a main process (with access to a database/shared file system) coordinates several R processes, potentially on different compute nodes (e.g. batchtools, rredis/doRedis)

# Parallelization Using R: Worker Queue



Embarrassingly/Pleasingly  
Parallel

```
$ R -f script.R &
```

Shared file system or  
database  
rredis/doRedis,  
batchtools, clustermq

# Parallelization Using R: rredis/doRedis



Redis is an open source, fast, persistent, networked database with many features, among them a blocking queue-like data structure (Redis “lists”). This feature makes Redis useful as a lightweight back end for parallel computing.

A Redis server has to be set up as part of the cluster (e.g. on a login node) or even somewhere else, containing the problem description(s). Worker processes connect to this server and tasks are assigned to them.

This is a very flexible and dynamic approach, as workers can basically run wherever you want (as long as they can connect to the server). When running on the cluster, you have to deal with resource allocation separately (via the Slurm workload manager) and potential firewall access restrictions.



## Parallelization Using R: batchtools



“batchtools provides a parallel implementation of Map for high performance computing systems managed by schedulers like Slurm, ...

- all relevant batch system operations (submitting, listing, killing) are either handled internally or abstracted via simple R functions
- with a well-defined interface, the source is independent from the underlying batch system - prototype locally, deploy on any high performance cluster”

i.e. a (interactive) R process is used in combination with the shared file system and the workload manager of the cluster to distribute workloads across nodes

## Parallelization Using R: clustermq

- Allows to send function calls as jobs on a computing cluster with a minimal interface provided by the `Q()` function

```
library(clustermq)
fx = function(x) x * 2
```

```
Q(fx, x=1:3, n_jobs=1)
```

- All calculations are load-balanced, i.e. workers that get their jobs done faster will also receive more function calls to work on
- Computations are done entirely on the network and without any temporary files on network-mounted storage

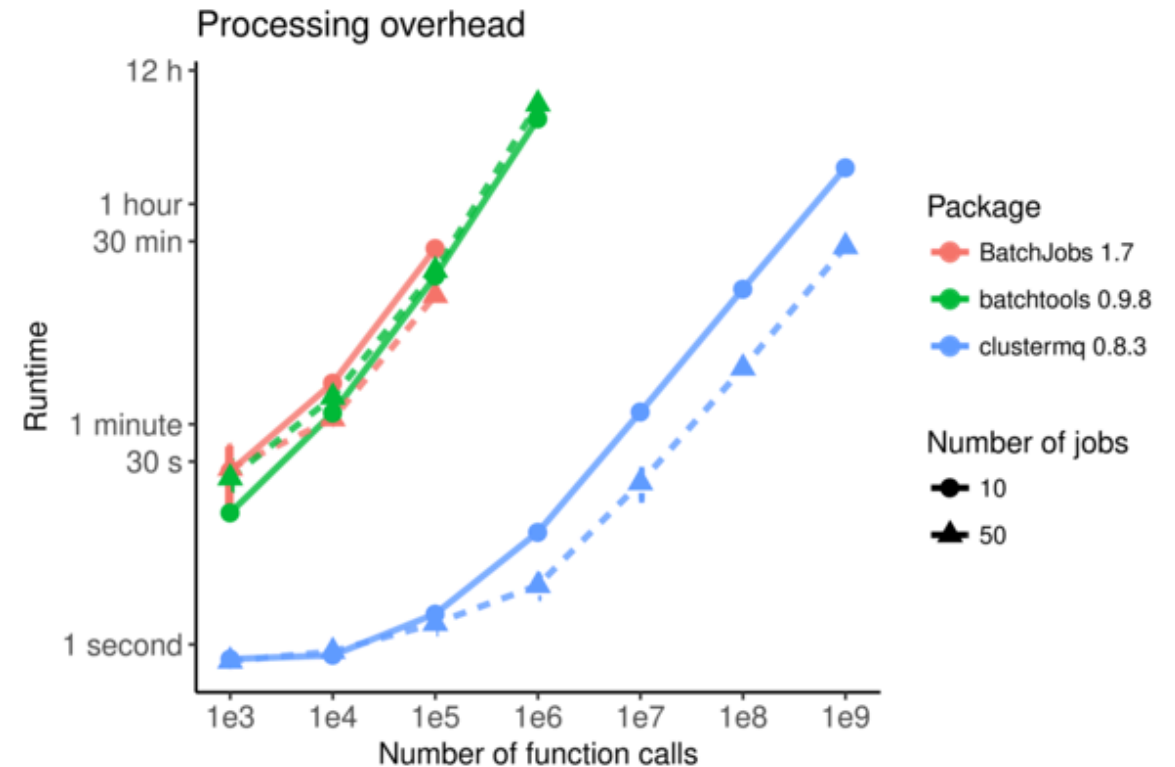
# Parallelization Using R: clustermq

Use clustermq if you want:

- a one-line solution to run cluster jobs with minimal setup
- access cluster functions from your local machine (e.g. using RStudio) via SSH
- fast processing of many function calls without network storage I/O

Use batchtools if you:

- want to use a mature and well-tested package
- don't mind that arguments to every call are written to/read from disc
- don't mind there's no load-balancing at run-time

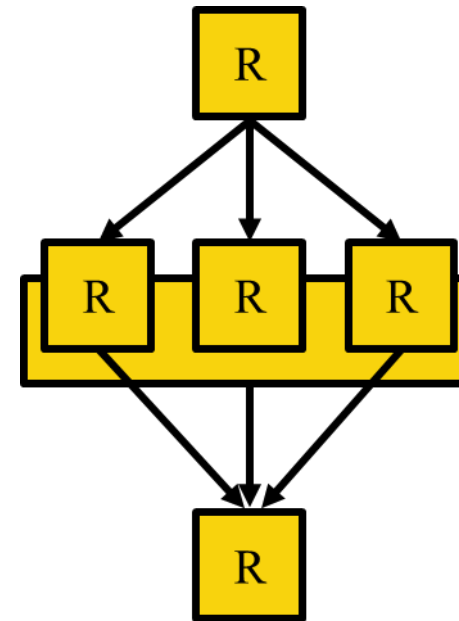
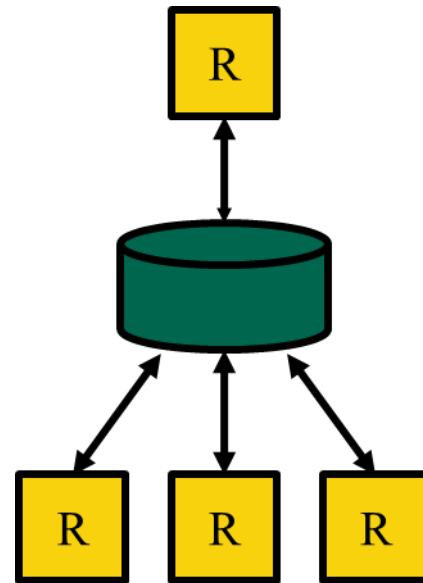
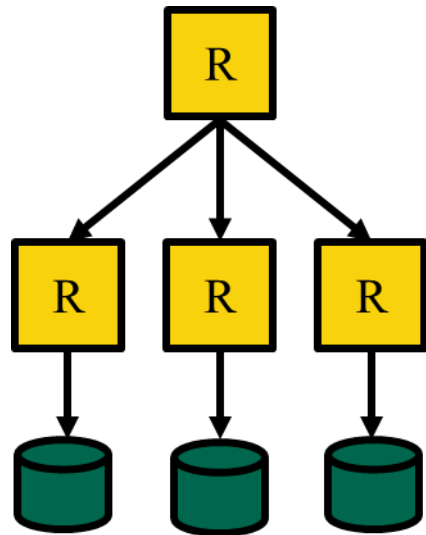


# (Explicit) Parallelization Using R



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- Worker Queue (weak coupling, shared file system or database):
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- Shared Memory (strong coupling):
  - one R process spawns sub-processes on a single node with many cores (e.g. parallel/doParallel; formerly multicore/doMC, snow/doSNOW)

# Parallelization Using R: Shared Memory



Embarrassingly/Pleasingly Parallel

```
$ R -f script.R &
```

Shared file system or database  
rredis/doRedis,  
batchtools, clustermq

Shared memory

```
parallel/doParallel
```

- As seen earlier, the for loop construct in R:  

```
for(i in 1:20) sum(sort(runif(1e7)))  
# serial execution/single thread
```
- “The foreach package provides a new looping construct for executing R code repeatedly. [...] it supports parallel execution, that is, it can execute those repeated operations on multiple processors/cores on your computer, or on multiple nodes of a cluster.”

```
library(foreach)  
foreach(i = 1:20) %do% sum(sort(runif(1e7))) # serial execution
```

```
foreach(i = 1:20) %dopar% sum(sort(runif(1e7)))  
# multithread execution (?)
```

- This is where the “do-back ends” (e.g. doParallel) come into play...
- By creating/registering a cluster, foreach’s %dopar% operator can rely on these parallel resources, e.g. using parallel’s multicore-like functionality (“forking”):

```
library(foreach)
library(doParallel)
registerDoParallel(cores=4)
  # define number of cores, this enables multicore-functionality
  # (preferred on GNU/Linux, but won't work on Windows)
foreach(i = 1:20) %dopar% sum(sort(runif(1e7)))
```

- The procedure is similar for snow-like functionality:

```
library(foreach)
library(doParallel)
cluster.object <- makePSOCKcluster(4)
registerDoParallel(cluster.object)
foreach(i = 1:20) %dopar% sum(sort(runif(1e7)))
stopCluster(cluster.object)
```

- This uses Rscript to launch further copies of R (on the same host or optionally elsewhere; in the latter case, hostnames need to be provided)
- [parallel, by relying on snow, also allows to create MPI-clusters (makeMPIcluster()-function) but Rmpi/doMPI is usually recommended to be used instead]

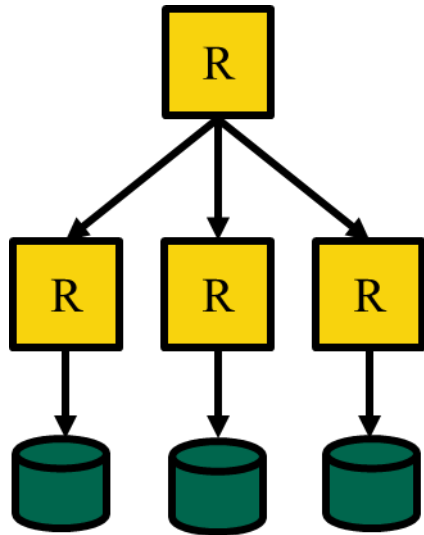


# (Explicit) Parallelization Using R



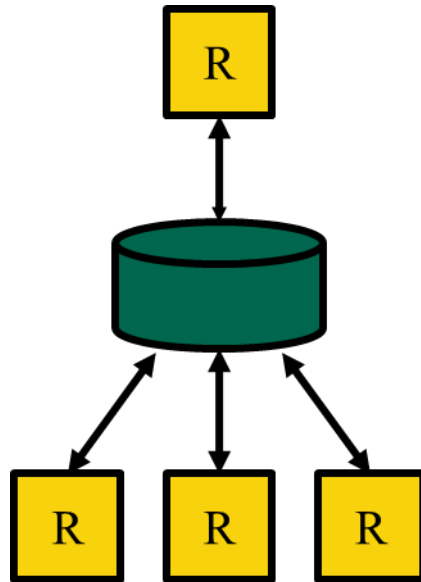
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- Shared Memory (strong coupling):
  - one R process spawns sub-processes on a single node with many cores (e.g. parallel/doParallel; formerly multicore/doMC, snow/doSNOW)
- Message Passing (strong coupling):
  - several R processes talk to each other (across different nodes) by passing messages (e.g. Rmpi/doMPI), this also allows for a (single) main and (multiple) workers model

# Parallelization Using R: Message Passing

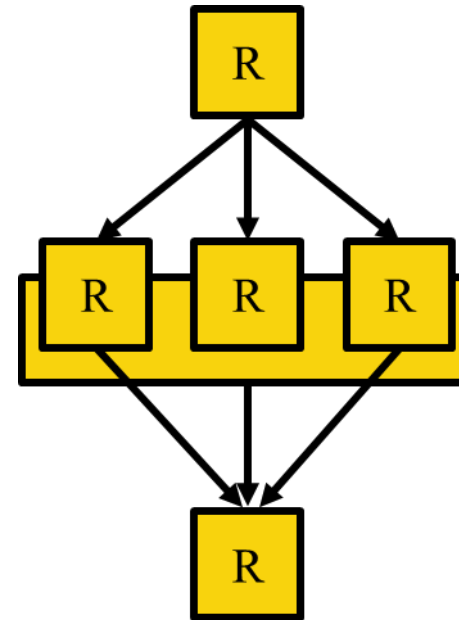


Embarrassingly/Pleasingly Parallel

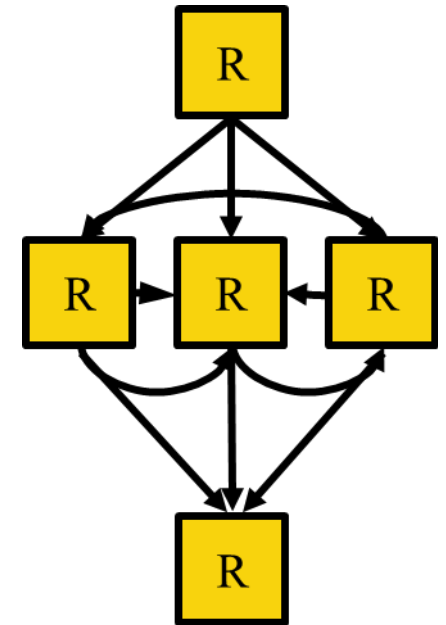
```
$ R -f script.R &
```



Shared file system or database  
rredis/doRedis,  
batchtools, clustermq



Shared memory  
parallel/doParallel



Message Passing  
Rmpi/doMPI

- To execute a doMPI script on multiple compute nodes a “message passing environment” needs to be set up, i.e. the R interpreter needs to be executed using a command such as `mpirun` (i.e. `mpirun R -f script.R`)
- Then, the already familiar „do-back end“-pattern is put to use within R:

```
library(foreach)
library(doMPI)
cluster.object <- startMPIcluster()
registerDoMPI(cluster.object)
foreach(i = 1:20) %dopar% sum(sort(runif(1e7)))
closeCluster(cluster.object)
```

# More on foreach()



- `clustermq::register_dopar_cmq(...)` registers `clustermq` as `foreach` parallel handler
- use `times()` for simple repetitions:  

```
times(10) %do% sum(sort(runif(1e7)))
```
- `foreach` is a function with several arguments...  

```
foreach(i = 1:10, .combine = c, ...) %do% sth() # process results  
as they get generated, e.g. c(), cbind(), list(), sum(), ...
```
- ... evaluates iterators...  

```
foreach(i = iter(input)) %do% sth() # see package iterators  
foreach(i = irnorm(100)) %do% sth()
```
- ... and provides additional operators:  

```
foreach(i = 1:10) %:% when(cond) %do% sth() # nesting operator  
and condition cf. Python's list comprehensions
```

- parallel provides parallel replacements of lapply and related functions (as have snow and multicore):
  - multicore-like: e.g. `mclapply(1:10, function(x) sum(sort(runif(1e7))))`,  
`mcmapply(x, FUN, ...)`, `mcMap(FUN, ...)`
  - snow-like: `clusterApply(cl, x, fun, ...)`, e.g. `parLapply(cl, x, FUN, ...)`

# Even More parallel: Futures/Promises



- Constructs for synchronizing program execution. Describe objects that act as proxies for a result, which is yet unknown (because the computation is incomplete)
- Send command to background and return handle:  
`handle <- mcpParallel(some_expensive_function)`
- Collect result at later point:  
`result <- mcCollect(handle)`

```
> system.time(sum(sort(runif(1e7))))
  user  system elapsed
1.581   0.112   1.700

> system.time(sapply(1:20, function(x) sum(sort(runif(1e7)))))
  user  system elapsed
28.875   2.998  31.883

> library(parallel)
> h <- mcpipeline(sapply(1:20, function(x) sum(sort(runif(1e7)))))
> mcollect(h, wait = FALSE)
NULL
# wait approx. 30 seconds for job to finish
> mcollect(h, wait = FALSE)
[1] 5000214 4999121 5001166 ...
```

## Futures/Promises

- Package future tries to unify the previous approaches:  
“The purpose of this package is to provide a lightweight and unified Future API for sequential and parallel processing of R expressions via futures. [...] Because of its unified API, there is no need to modify any code in order switch from sequential on the local machine to, say, distributed processing on a remote compute cluster.”
- **Implicit:**  

```
v %<-% { expr } # future assignment , creates a future and a  
           promise to its value (instead of regular assignment <-)
```
- **Explicit:**  

```
f <- future({ expr }) # creates a future  
v <- value(f) # gets the value of the future  
           (blocks if not yet resolved)
```



## Futures/Promises



- Function `plan()` allows the user to plan the future, i.e. it specifies how futures are resolved
- For example: `plan(sequential)` and more

```
> library("future")
> plan(sequential)
> v %<-% {
+   cat("Hello world!\n")
+   3.14
+ }
> v
Hello world!
[1] 3.14
```

## Futures/Promises

Name	OSes	Description
<i>synchronous:</i>		<i>non-parallel:</i>
sequential	all	sequentially and in the current R process
<i>asynchronous:</i>		<i>parallel:</i>
multisession	all	background R sessions (on current machine)
multicore	not Windows	forked R processes (on current machine)
cluster	all	external R sessions on current, local, and/or remote machines
remote	all	simple access to remote R sessions

- The `future.callr` package provides future backends that evaluates futures in a background R process utilizing the `callr` package - they work similarly to `multisession` futures but have a few advantages (e.g. more than 125 parallel R processes)
- Package `future.batchtools` provides an implementation of the Future API on top of the `batchtools` package, i.e. it allows to process futures (as defined by the `future` package) on HPC infrastructure

## doFuture: future and foreach

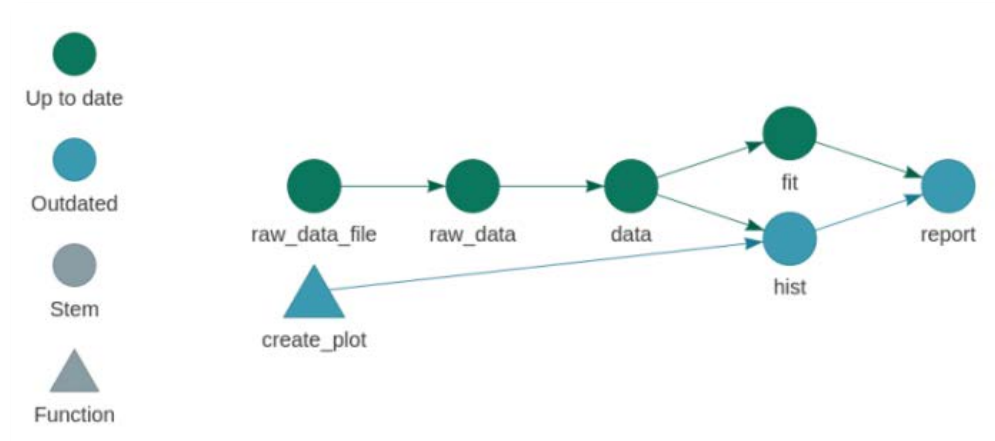


- Package doFuture provides a %dopar% adaptor for the foreach package such that any type of future (that is supported by the Future API of the future package) can be used for asynchronous (parallel/distributed) or synchronous (sequential) processing.
- Example:

```
library(doFuture)
registerDoFuture()
plan(multicore)
foreach(i = 1:20) %dopar% sum(sort(runif(1e7)))
```
- Look out for the use of foreach (and the possibility to register all these different back ends) in other R packages!

## ... and beyond: the targets package

- The targets package is a Make-like pipeline toolkit for statistics and data science in R
  - maintain a reproducible workflow without repeating yourself
  - skip costly runtime for tasks that are already up to date
  - run the necessary computation with implicit parallel computing
  - abstract files as R objects
- A fully up-to-date targets pipeline is tangible evidence that the output aligns with the code and data, which substantiates trust in the results



## The targets package



- targets supports high-performance computing with the `tar_make_clustermq()` and `tar_make_future()` functions (using the `future.batchtools` backend)
- These functions are like `tar_make()`, but they allow multiple targets to run simultaneously over parallel workers. Again, these workers can be processes on your local machine, or they can be jobs on a computing cluster.
- `tar_make_clustermq()` uses persistent workers. That means all the parallel processes launch together as soon as there is a target to build, and all the processes keep running until the pipeline winds down.
- `tar_make_future()` runs transient workers. That means each target gets its own worker which initializes when the target begins and terminates when the target ends.

# Conclusion

- Parallel programming is here to stay (for the foreseeable future).
- Know your hardware...
- ... and the possibilities of your software/programming environment.
- Applying proper (high level) abstractions (foreach, futures, targets...) to fully utilize the features of modern CPUs/GPUs and supercomputing infrastructure will allow you to write fast and scalable programs.

