

Short report

**NanoPASS: an easy-to-use user interface for nanoparticle
dosimetry with the 3DSDD model**

--- NanoPASS installation guide ---

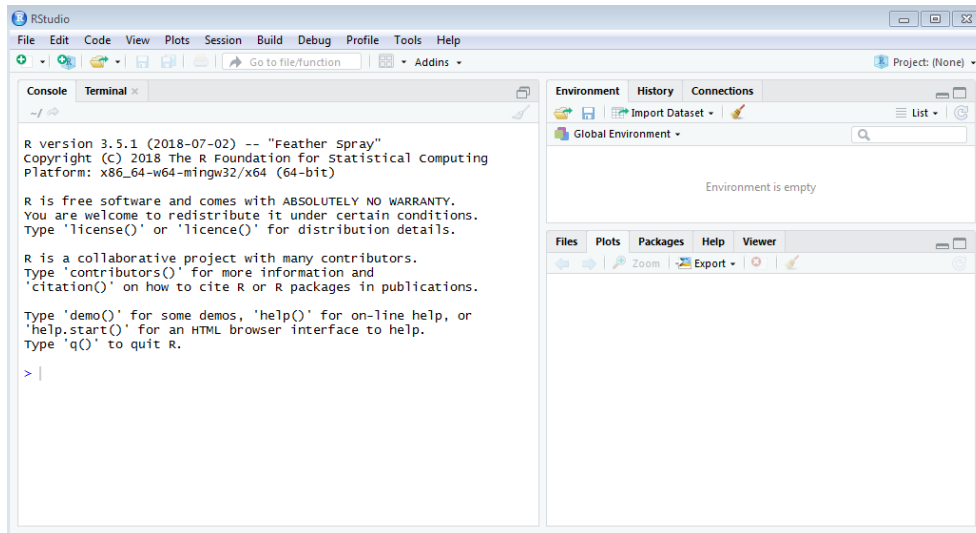
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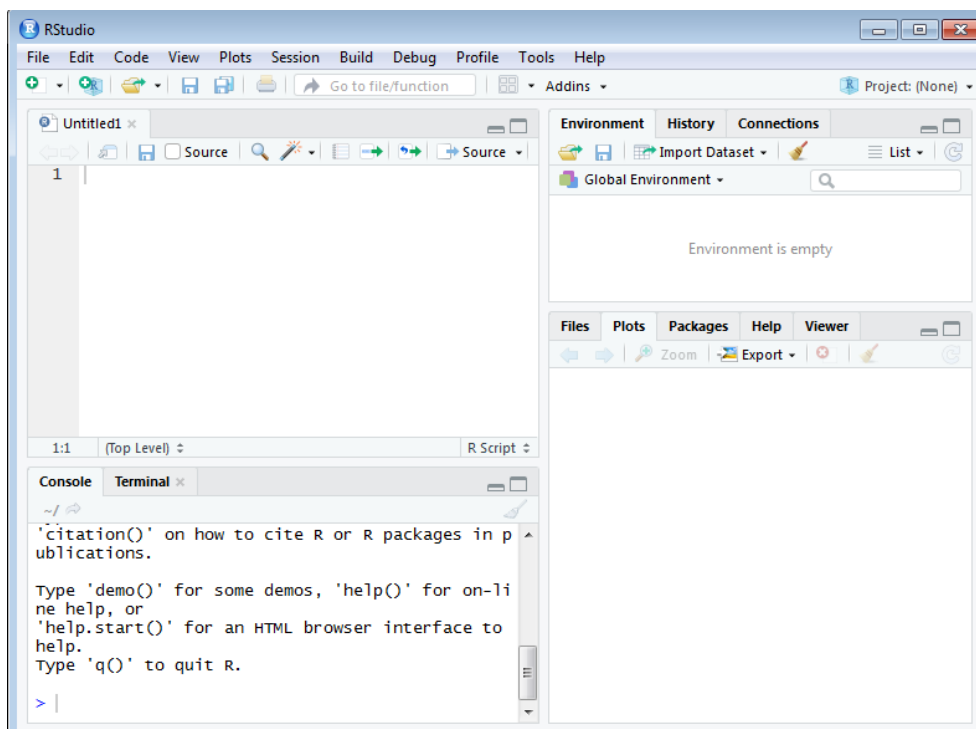
² Otto-von-Guericke University Magdeburg, Chair of Process Systems Engineering, Universitätsplatz 2, 39016 Magdeburg, Germany

Install R and RStudio:

- first install R on your computer (information on how this works for your operating system can be found under <https://cran.r-project.org/>)
- after installing R, download and install RStudio (<https://www.rstudio.com/>)
- open RStudio (icon for RStudio should be on your desktop when using recommended installation method)

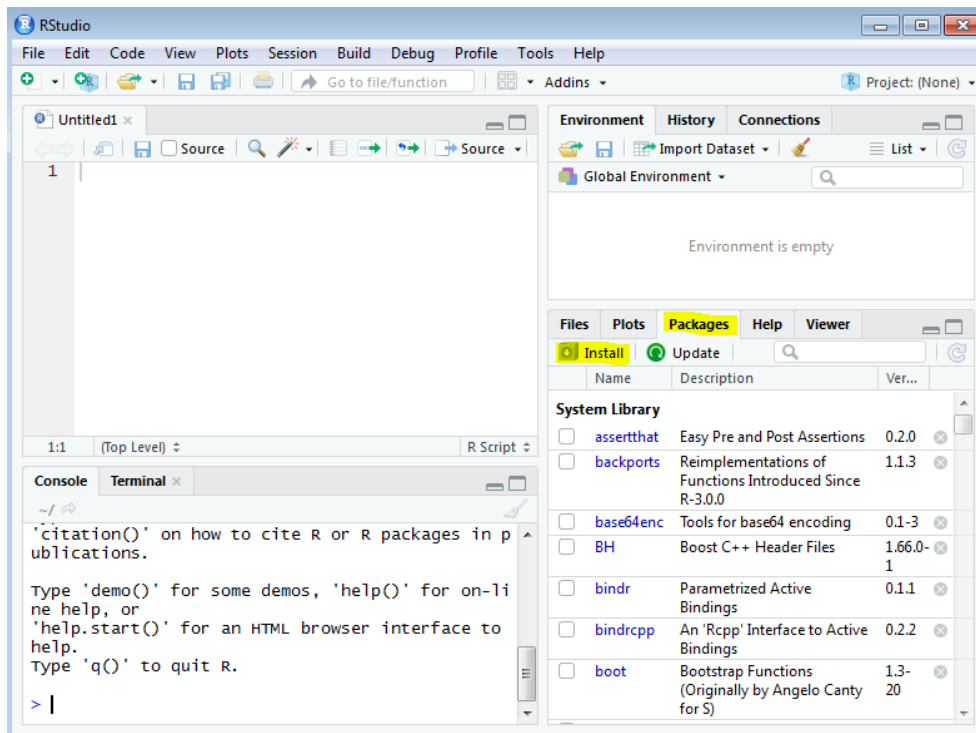


- then you should find the following panel in your RStudio IDE:
 - top right side: global environment (here stored R objects like variables and dataframes are shown);
 - (optional) top left side: script (here you can create a draft of your code);
 - bottom left side: console (here you can type your code directly);
 - bottom right side: (here you can install packages and show plots)

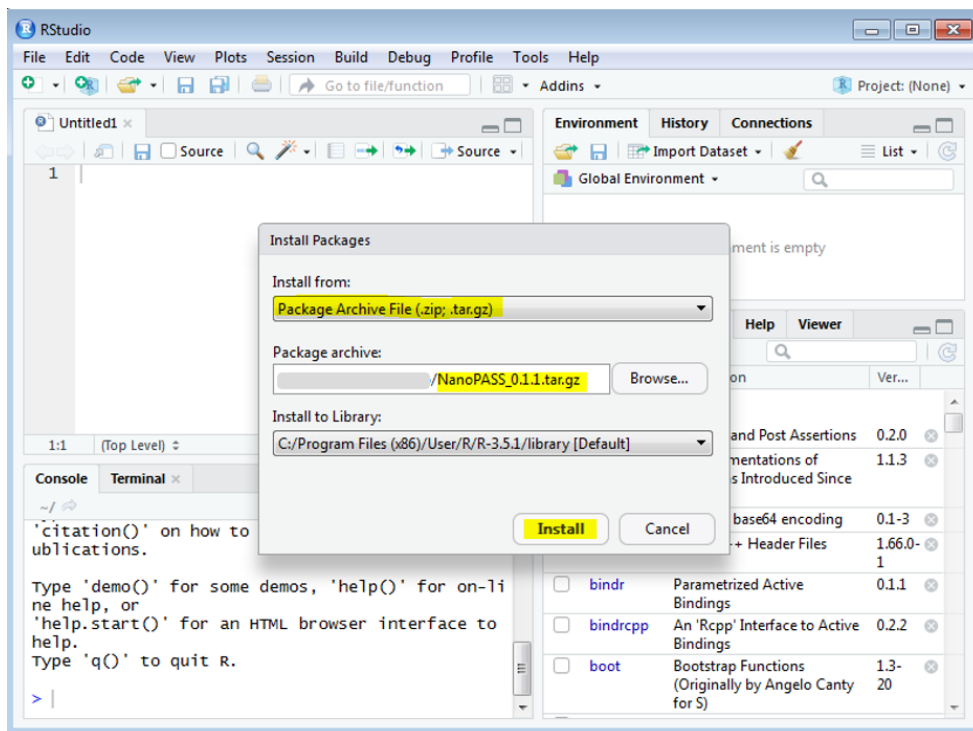


Install 3DSDD user interface NanoPASS:

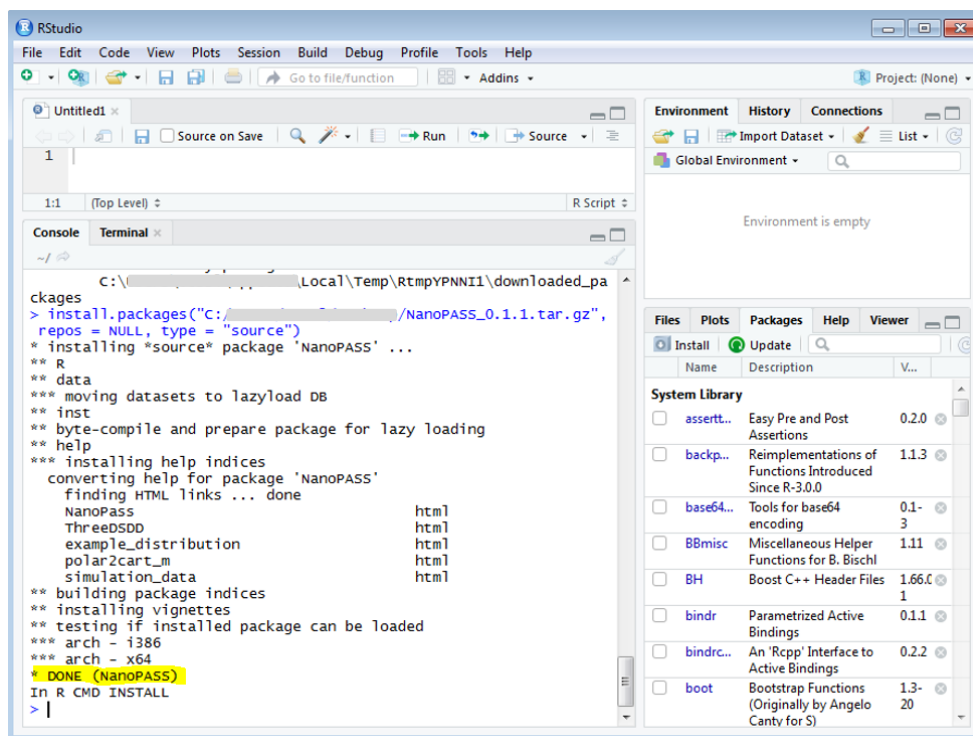
- install NanoPASS: download NanoPASS from GitHub (<https://github.com/falfren/NanoPASS>) or the additional file 2 of the paper to your computer
- in RStudio: click on “Packages” and then on “Install” (marked in yellow)



- an additional window opens; change at “Install from” to “Package Archive File”, browse for the NanoPASS-File on your computer and select the recently downloaded package file; click “install”



➤ there should be no error in the console.



Starting with R 4.0.0 (released April 2020), R for Windows uses a new toolchain bundle for compiling R-packages

- if this additional installation is needed, following error occurs:

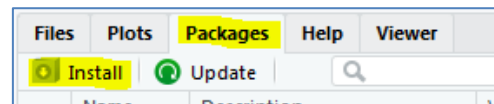
```

RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function Addins
Console Terminal Jobs
> install.packages("C:/Users/.../NanoPASS.zip", repos = NULL, type = "win.binary")
WARNING: Rtools is required to build R packages but is not currently installed. Please download and install the
appropriate version of Rtools before proceeding:
https://cran.rstudio.com/bin/windows/Rtools/
Installing package into 'C:/Users/.../R/win-library/4.0'
(as 'lib' is unspecified)
warning in install.packages :
  kann komprimierte Datei 'NanoPASS/DESCRIPTION' nicht öffnen. Grund evtl. 'No such file or directory'
Error in install.packages : kann Verbindung nicht öffnen
> |

```

- then you need to follow the instructions marked in **yellow** and on <https://cran.r-project.org/bin/windows/Rtools/>

- despite the NanoPASS package setting that all dependencies should be installed during the installation process: if an error occurs because of missing dependencies packages are not installed (as shown in the following picture in **yellow**), go again to Packages → Install



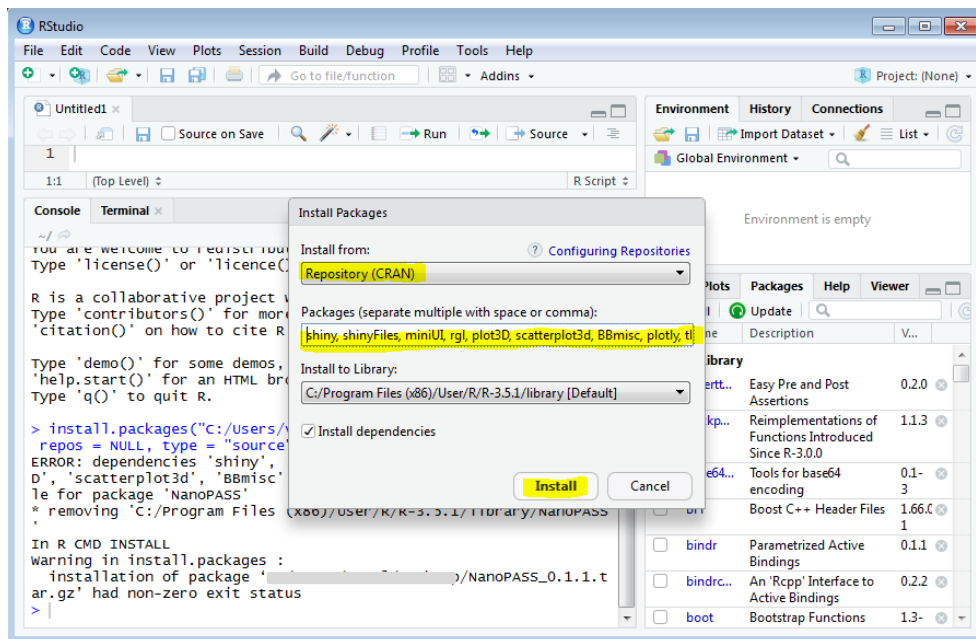
```

RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function Addins
Untitled1
1
1:1 (Top Level) R Script
Console Terminal
R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publication
s.
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.
> install.packages("C:/Users/.../NanoPASS_0.1.1.tar.gz", repos = NULL, type = "source")
ERROR: dependencies 'shiny', 'shinyFiles', 'miniUI', 'rgl',
'plot3D', 'scatterplot3d', 'BBmisc', 'plotly', 'threejs'
are not available for package 'NanoPASS'
* removing 'C:/Program Files (x86)/User/R/R-3.5.1/library/
NanoPASS'
In R CMD INSTALL
warning in install.packages :
  installation of package 'C:/Users/.../NanoPASS_0.1.1.tar.gz' had non-zero exit status
> |

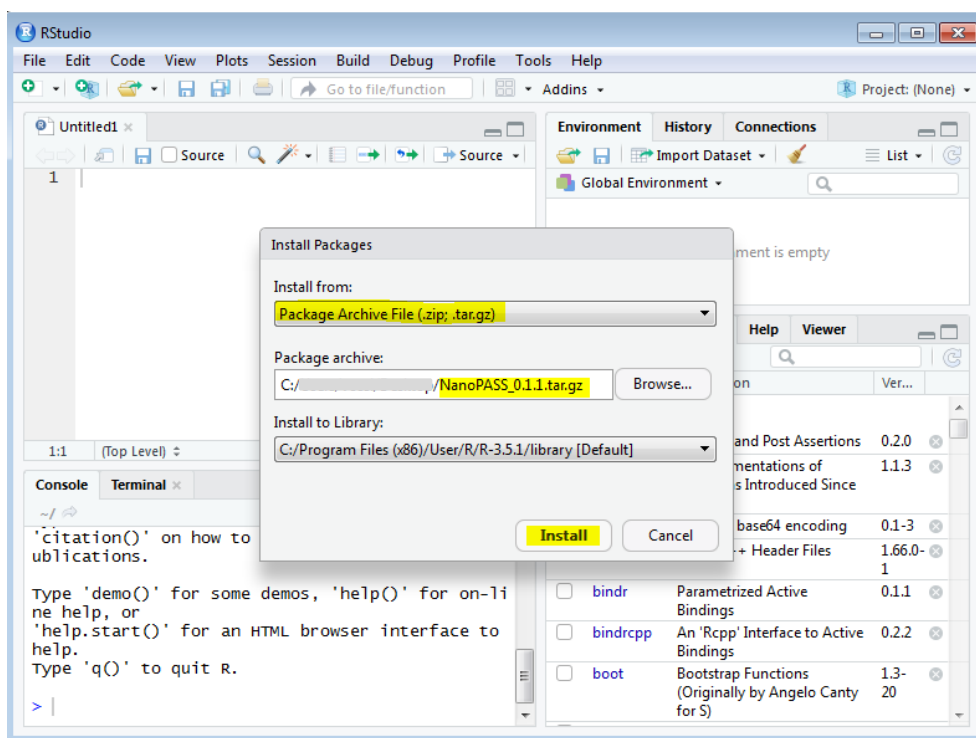
```

Name	Description	V...
asser...	Easy Pre and Post Assertions	0.2.0
back...	Reimplementations of Functions Introduced Since R-3.0.0	1.1.3
base...	Tools for base64 encoding	0.1-3
BH	Boost C++ Header Files	1.66.1
bindr	Parametrized Active Bindings	0.1.1
bind...	An 'Rcpp' Interface to Active Bindings	0.2.2
boot	Rentran	1.2-

- change at "Install from" to "Repository (CRAN)"; enter missing packages (shown in console in ' ') in the packages search bar (separated by ","); make sure to check the option "Install dependencies" and click on the "Install" button



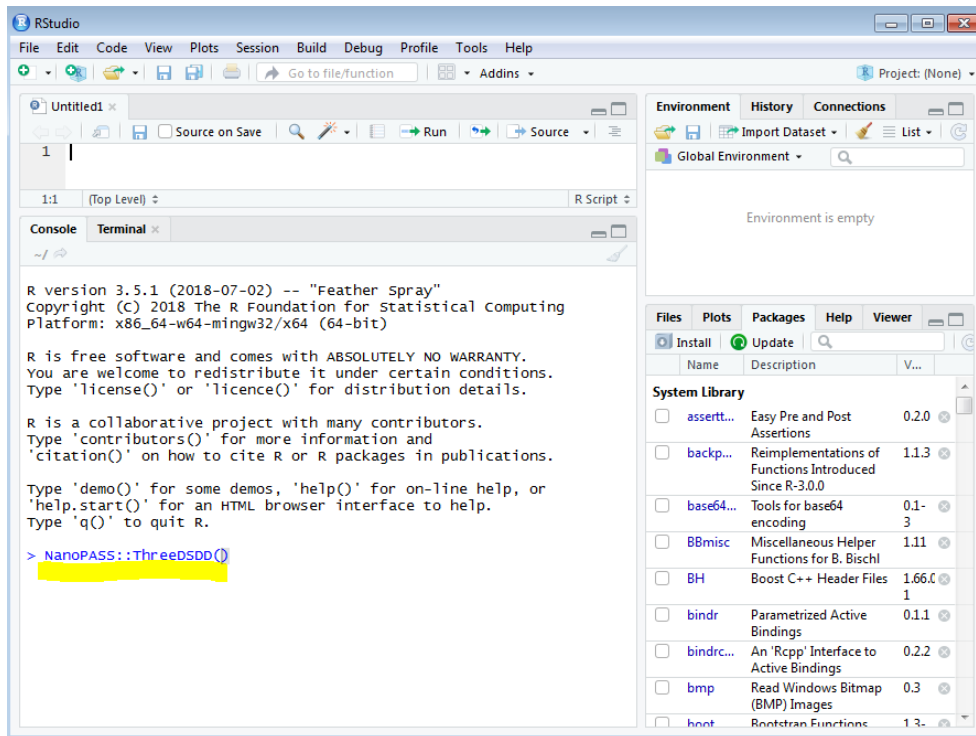
- then repeat the installation of NanoPASS



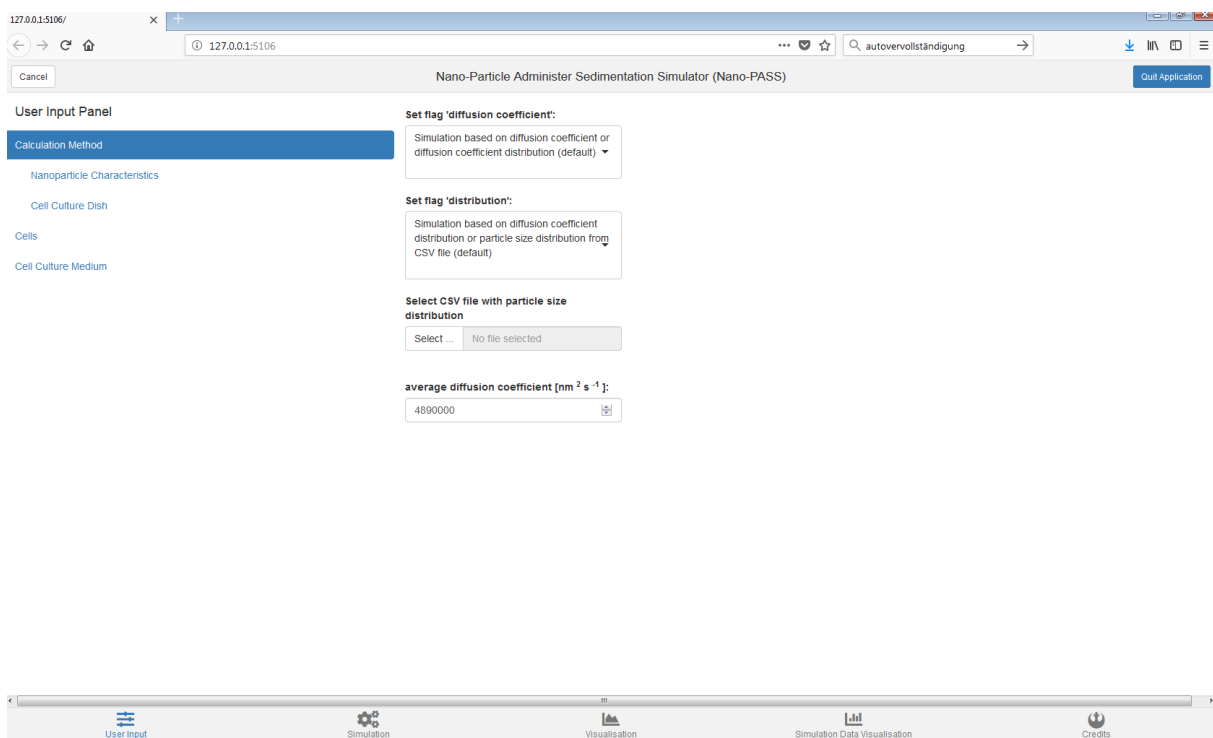
- from now on, NanoPASS is installed in R and you do not have to install it again when opening RStudio the next time; you can just start at the next slide
- in order to check whether the installation process was successful, NanoPASS shall be listed in the panel "Packages" in the bottom right panel

starting NanoPASS:

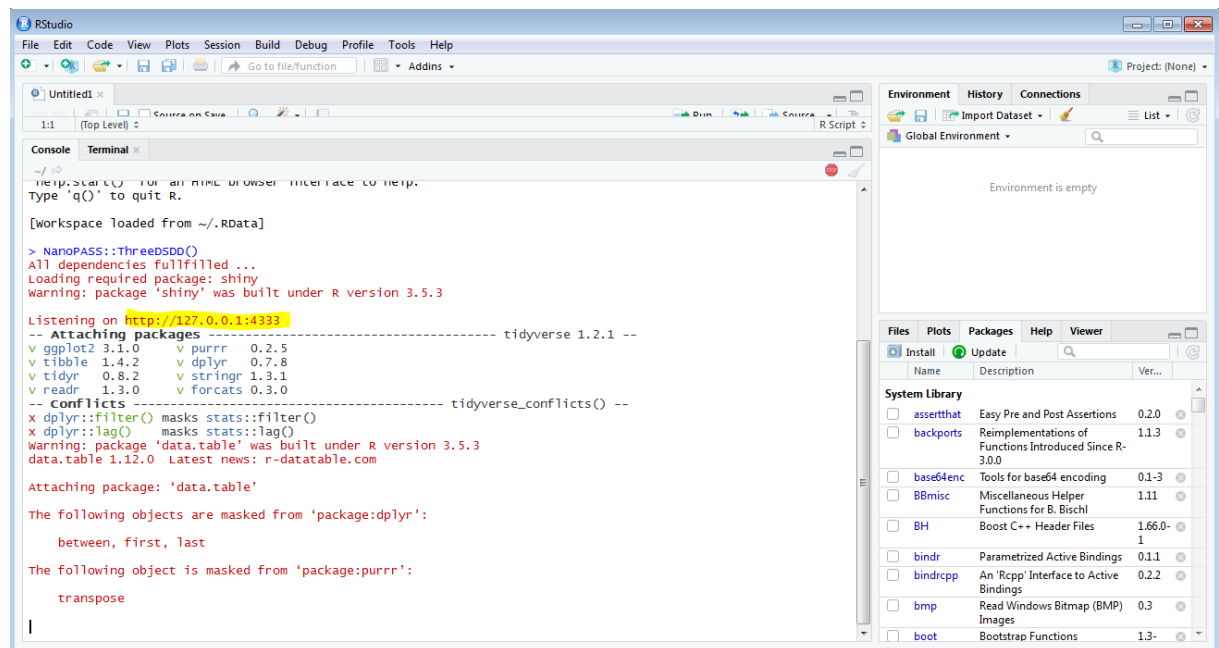
- open RStudio, enter "NanoPASS::ThreeDSDD()" in the console, Click ENTER; NanoPASS will open in your browser



➤ in your web browser, you should see this:



➤ if not, go back to your R-window, here you can find the link as well. Copy that in your browser and you will get to NanoPASS



- now you can start to use 3DSDD model with the NanoPASS user interface

To quit NanoPASS:

- when you are done in your browser, go back to RStudio and Stop the command by clicking on “Stop”; the “>” appears, you can now go on