

Julia is a program that can be used for the efficient NMR calculations with the full quantum mechanical formalism.

Burkhard Luy's advice from 28/08/2023 is below.

Packages, that are being used in the programs with the "using" command, need to be installed before you can use them. This is usually very easily done in one of the following ways.

- You can enter the pkg-mode in Julia by typing the right-hand square-bracket] into the Julia command line, something like
Julia >]
then the pkg-mode will be entered, visible by the changed command line. You can now simply add the Package "Package_Name" by typing
...pkg > add Package_Name
be sure that you write the Package name exactly the way it is written in the programs, as Julia is case-sensitive in all variables and names.
- You also can directly use the commands
Julia > using Pkg
Julia > Pkg.add("Package_Name")
to install the package.
- Maybe a hint: Pkg itself is a package that is already pre-installed with Julia. However, it might be necessary to load it into the Julia session with "using Pkg" as in the example above.

I should also point out that in the attached Julia programs the appearance of the plot command varies depending on where you run Julia. If you run it in the visual studio code editor as I did, only the last plot command will be visible within the editor. You can put the plot to a variable (like: plot1 = plot(...)) and then type "display(plot1)" into Julia to get a specific plot-window.

If you are interested in continuing with Julia, the documentation is quite good: <https://docs.julialang.org/en/v1/>

And on 28/08/2023:

Some more files are necessary to run the offset dependencies of shaped pulses using the Julia program.

The read_brucker_wave.jl file enables the readout for bruker shaped pulse files in the old format, where all lines starting with # can be ignored and otherwise pulse amplitudes in percent and pulse phases in degrees are read in. For the simulations, the maximum rf-amplitude (corresponding to 100%) must be specified in the offset_xy_z_rho.jl file (rfmax) as well as the length of the shape (tpulse, where 2000/1000000 means 2000 microseconds). Make sure that the path is changed to the ones on your own computer for the filename variable!

There is a relation between the 90° pulse length and the rf-amplitude: e.g. an rf-amplitude of 10000 Hz means, that at this field strength 10000 rotations around e.g. the x-axis (on-resonance) are performed. This implies, that a single rotation takes $1/10000 \text{ Hz} = 100 \mu\text{s}$ (=360°), which in turn results in $25 \mu\text{s}$ for a 90° pulse.