
Scientific Programming ~~and Machine Learning~~ with Julia

Kick-off meeting

Antonello Lobianco

“A language that doesn't affect the way you think about programming is not worth knowing.”

-- Alan Perlis(American computer scientist)

Today's objectives

- What this course is about
- How this course is organised
- Who am I ? (Who are you ?)
- What is Julia ? (Why to bother with yet-an-other language ?)
- Let's set up the environment for the course !
 - diff, git, github
 - computational environment
- Let's start by learning to work with packages

This course

- A brief but solid introduction to the Julia Programming Language
 - General syntax and programming constructs (packages, data types, control flows, macros, I/O,...°
 - "scientific" programming: wrangling and visualising data, optimisation problems, statistics, ...
- The course follows the following references :
 - The book "Julia Quick Syntax Reference" (Apress 2019) for the Julia part (PDF available on the course site – to not redistribute, only for you !)
- Course on Arche: <https://arche.univ-lorraine.fr/course/view.php?id=53796>
- Course on GitHub: <https://github.com/sylvaticus/SPMLJ>

Course organisation

- This kick-off meeting
- 2 additional recorded video "lessons":
 - Basic Julia programming
 - Scientific programming with Julia
- ~~One Lesson == One week~~ One Lesson != One week
 - Videos and related exercises open each week and are due for the ending of the week (see calendar for details)
 - You can either watch the video or just play by yourself with the associated Julia script or study them in the "compiled form" online
- The computational environment
 - The best option: you install the computational environment on your own PC (one reason why we have a kick-off meeting)
 - The fallback: a server is available for you for this course
 - could be slow
 - documents will not remain available after the course end
 - Other online computational environments with Julia support: <https://cocalc.com>, <https://nextjournal.com>, <https://notebooks.gesis.org>, <https://codeocean.com>, <https://visualstudio.microsoft.com/services/github-codespaces> , <https://replit.com/languages/julia>

Let's present us

- I'm a research engineer in Forest and Environmental Economics at BETA (Bureau d'économie théorique et appliquée) Nancy (UMR AgroParisTech, INRAE, University of Lorraine, University of Strasbourg, CNRS)
- My work involves a lot of modelling and simulations
 - agent-based farm-level to regional simulations → [RegMAS](#) (Regional Multi Agent Simulator)
 - bio-economic models of the forest sector (forest dynamics, timber markets equilibrium, carbon cycle) → [FFSM](#) (French Forest Sector Model)
- My pathway with programming:
 - Commodore 16, Commodore64 Basic, DOS, VBA, Pascal, Perl, PHP, C++, Python, Julia
 - I have experience also with setting LAMP servers/middleware
 - What I used this for? [Everything](#) from management applications (including the students management office of my university), web sites, numerical utilities.. research
- And you ?
 - Which programming languages do you use (let me guess.. R ? Python? Maybe javascript or Matlab ?)
 - What's your background ?
 - Have you already used ML algorithms ?
 - What are you looking / expect from this course ?

JULIA

A comparative timeline of R, Python, Julia, LLVM

1991: Python announced

1993: R announced

1994: Python reaches v1.0

2000: R reaches v1.0

2003: LLVM announced (v1.0)

2012: Julia announced by a MIT team
to solve the "two languages problem"

2018: Julia reaches v1.0

JuPyteR notebooks

JIT compiled

- R: `compiler` library (JIT default in 3.4)
- Python: Numba, PyPy, ...
- Julia: natively, with type inference

Julia: multiple dispatch

- dispatch the call to a function to the most specific version ("method") based on the types of all the arguments
- is a generalisation of OO single argument dispatch `obj.foo(arg2, arg3) → foo(obj, arg2, arg3)`
- not to be confused with C++ -style polymorphism (at compile time)
- simplify code composition: as soon new types know how to handle low level functionalities, they can reuse high level one

- Julia libraries

- DataFrames:



- Flux:

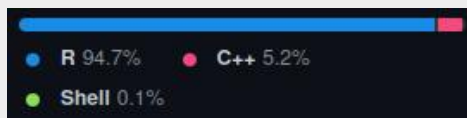


- BetaML:

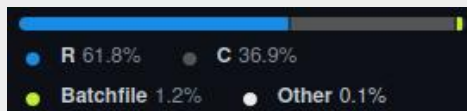


- R libraries

- Dplyr:

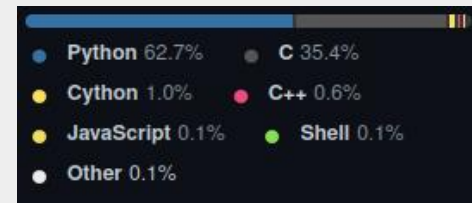


- data.table:

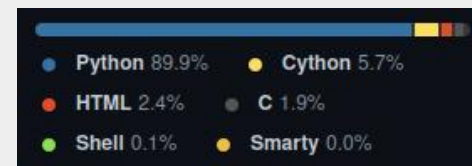


- Python libraries:

- Numpy:



- Pandas:



- Pytorch:



Multiple kinds of parallel computation

Hardware level SIMD (single instruction multiple data), GPU

- `@simd for i in ...`
- `CUDA.jl`

Multithreading

- `Threads.@threads for i in ...`

Multiprocessing

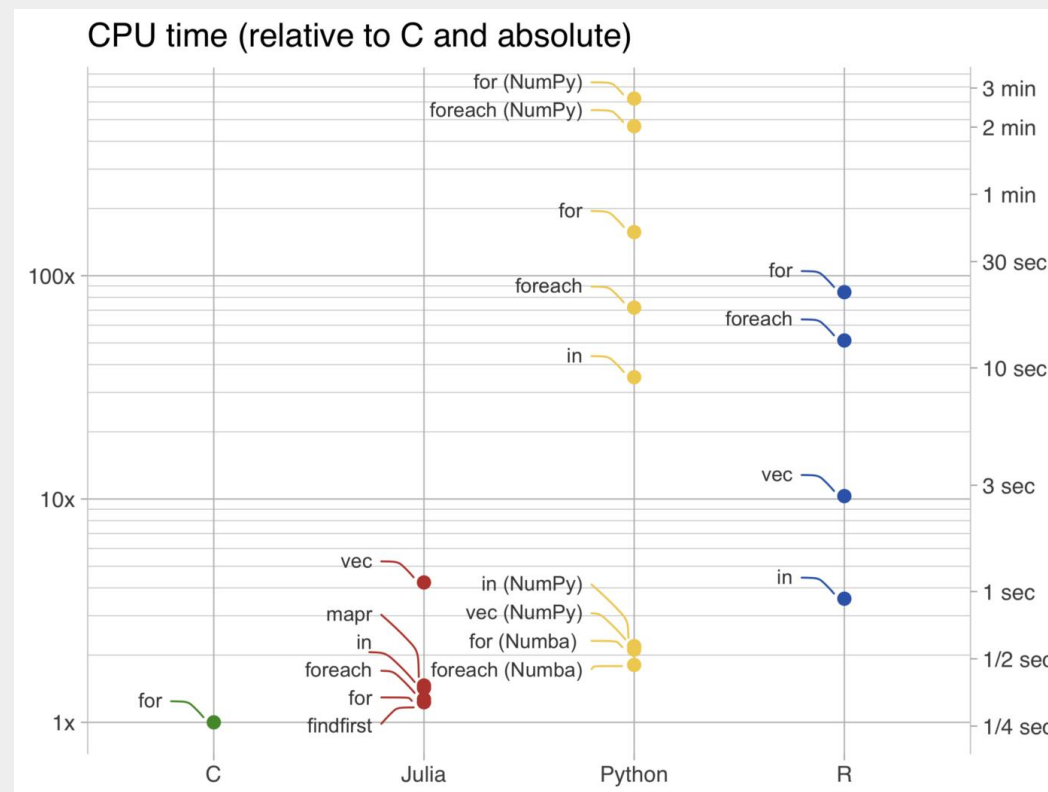
- `addprocs(n, ssh parameters)` same machine or other HPC nodes using SSH tunnelling
- `@everywhere function foo(arg) ...`
- `pmap(foo, data)`

Other characteristics of Julia for Scientific Programming

- Macro and meta-programming: at the level of the Abstract Syntax Tree
 - allow more flexible APIs (compare those of JuMP with the equivalent of PYOMO)
- Extended Unicode support on any identifier: `julia>  $\tilde{\sigma}^2 = 1$` `julia>  $\bar{x}_2 \in [1,2,n,e]$`
- Support to user-defined primitive type (need a Int24 type ??), even basic operators are extendible: `+(x,y::Int24) = ...`
- Linear algebra built in: `x' * Y^(-1)`
- Broadcasting support to any function (including user-defined): `foo.(args)` (note the dot)
- Direct interoperability with C/Fortran libraries `ccall(:foo,foolib,...)` and VERY easy integration with R and Python
- Modern testing and documentation facilities (Test module – in the st.lib -, Literate.jl, Documenter.jl, integration with GitHub actions and CodeCov)
- Light-wise git-based environments for easy replicability

When Julia is no (computational) advantage over R, Python, Matlab...

- when the bottleneck is given by some matrix operation (multiplication, inverse,...)
 - it resolves to the underlying BLAS/LAPACK library employed
 - still in Julia ≥ 1.7 very easy to switch to MLK if needed
- when the bottleneck of your code is in using some highly-optimised C/Fortran libraries with a R/Python wrapper (including vectorised ops with numpy)

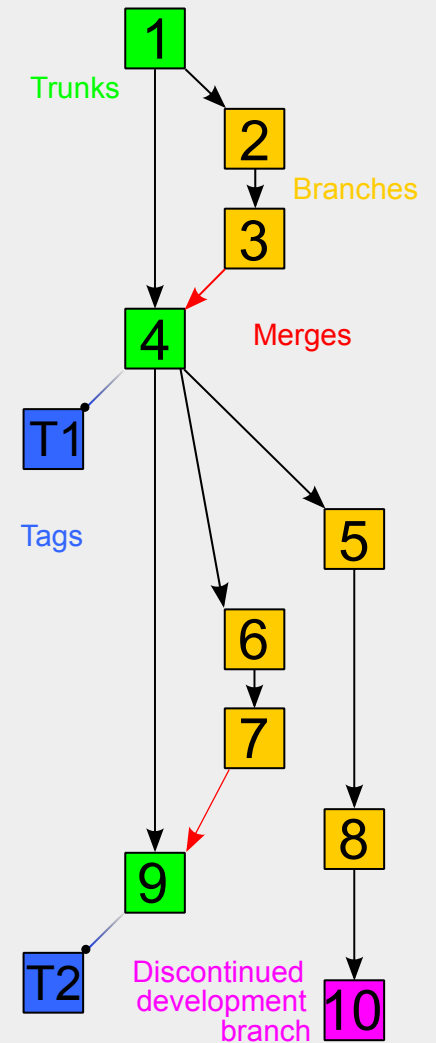


<https://towardsdatascience.com/r-vs-python-vs-julia-90456a2bcbab>

HANDS ON

Version control software

- Used to keep track of the development of a project and allow easy integration of multiple sub-projects or team contributions
- Typically they allow assigning a name/log entry to a given “screenshot in time” of project development, visualise diffs between them, create and merge branches of different development pathways, automatically manage or facilitate resolution of conflicts between versions,...
- First generation (CVS, SVN,...):
 - client-server model → the full project (history) is kept in a centralised server and individual users connect and keep in their pc one specific version
- Second generation (Git, Mercurial, Bazaar,...):
 - distributed model → each user has the whole copy (including history) of the project and exchanges its contribution with the other “remote” nodes
 - increases redundancy
 - decreases network load
 - faster operations (many operations – e.g. diff – can be fully done in local)



Set up the environment

- Create our first git repository
 - register or sign in on github.com
 - add new repository "testGit" (attention capital letters! no spaces!)
 - add readme, gitignore (Julia) and licence (MIT? GPL?)
- Install Julia (terminal): <https://julialang.org/> → download → 1.7 64 bit installer → run with the option "add julia to path"
- Install Git for Windows: <https://git-scm.com/download/win> Check the options !
- Install Visual Studio Code: <https://code.visualstudio.com/> → download → run with the options additional icons/other
- Install Julia extension:
 - search in extensions: "julia" (not "julia insider")
 - try it is working: new file -> select a language -> julia -> println("Hello World!") SHIFT+ENTER

In case of impossibility to set up the environment on your own pc an account on the lab server at <https://lef-nancy.org> has been set for you (username: your surname all in lower letters, psw [XXXXXX])

Help: this course forum (for those with access to it), <https://discourse.julialang.org/> , [StackOverflow](#) (using the "julia" tag)

Essential git workflow

- Clone an existing repositories or start a new one: `git clone [url]` or `git init`
- ..work on your project..
- Add files: `git add [file]`
- Commit your work: `git commit -a -m "[message]"`
- See branches: `git branch`
- Create branch: `git branch [branchname]`
- Switch to branch: `git checkout [branchname]`
- Merge a branch: `git merge [branchname]`
- Delete a local branch: `git branch -d [branchname]`
- Fetch a remote repository (without attempt to update the local repository): `git fetch`
- Fetch and try to merge from a remote repository: `git pull`
- Push your data to a remote repository: `git push`
- List all the remote repositories: `git remote`
- Get current repository status: `git status`
- Get git logs: `git log`
- See diff with HEAD: `git diff`
- See diff between any commit(s): `git diff [commithash1] [commithash2]`

Further resources

Git tutorials (shorts):

- <https://git-scm.com/docs/gittutorial>
- <https://thenewstack.io/tutorial-git-for-absolutely-everyone>

Git book (long):

- <https://git-scm.com/book>

A first look on git(hub)

- retrieve the repository locally

- Clone the repository locally using Visual Code Studio
 - Automatic way
 - CTRL+SHIFT+P to open the command palette and search for git:clone
 - Clone from github
 - Authorise
 - Choose the repository to clone
 - Open in new file
 - Manual way
 - open a new "git bash" terminal using "new terminal" and then the "plus"
 - `git clone https://github.com/[YOUR GITHUB USERNAME]/testGit.git`
 - open folder This PC > OS (C:) > Users > Your name > testGit

A first look on git(hub)

- work, commit & push

- Add a file "test.jl" → `println("Hello World!")` → CTRL+ENTER → save
- Edit the README.md file
- `git status`
- `git add test.jl`
- `git status`
- `git config --global user.email "you@example.com"`
- `git config --global user.name "Your Name"`
- `git commit -a` → add a message → CTR+X → Y
- `git push` → follow online instruction to authorise
- => changes are back to github

A first look on git(hub)

- working with branches

- Edit file "test.jl" to add text on lines 4, 7 and 9, save and commit
- Open a git bash terminal
- git branch temp
- git checkout temp
- Edit test.jl on line 9, save and commit
- git checkout main
- Edit test.jl on line 5, save and commit
- git diff main temp
- git branch
- git merge temp
- git log
- git push
- git branch -d temp

Modules and packages

Structure of a module:

```
module ModuleName
export myObjects # functions, structs, and other objects that will be directly available once `using
ModuleName` is typed
[...module code...]
end
```

- `using pkgOrModule`
- `import pkgOrModule: X,Y,Z`
- Module names are customary starting with a capital letter and the module content is usually not indented. Modules can be entered in the REPL as normal Julia code or in a script that is imported with `include("file.jl")`.
- There is no connection between a given file and a given module as in other languages, so the logical structure of a program can be decoupled from its actual division in files. For example, one file could contain multiple modules.
- A more common way to use modules is by loading a package that will consists, at least, of a module with the same name of the package.
- All modules are children of the module `Main`, the default module for global objects in Julia, and each module defines its own set of global names.
- Note: `using` and `import`, when they are followed with either `Main.x` or `.x`, look for a module already loaded and bring it and its exported objects into scope (for `import` only those explicitly specified). Otherwise, they do a completely different job: they expects a *package*, and the package system lookups the correct version of the module `x` embedded inside package `x`, it loads it, and it bring it and its exported objects into scope (again, for `import x` only those explicitly specified).

<https://syll.gitbook.io/julia-language-a-concise-tutorial/language-core/11-developing-julia-packages>

The integrated Pkg manager

```
julia> using Pkg

julia> Pkg.add("DataFrames")
  Resolving package versions...
  No Changes to `~/julia/environments/v1.6/Project.toml`
  No Changes to `~/julia/environments/v1.6/Manifest.toml`

julia> █
```

```
(@v1.6) pkg> add DataFrames
  Updating registry at `~/julia/registries/General`
  Resolving package versions...
  No Changes to `~/julia/environments/v1.6/Project.toml`
  No Changes to `~/julia/environments/v1.6/Manifest.toml`
  Progress [=====] 3/3
  3 dependencies successfully precompiled in 44 seconds (366 already precompiled)

(@v1.6) pkg> █
```

Some useful package commands:

- `status` Retrieves a list with name and versions of locally installed packages
- `update` Updates your local index of packages and all your local packages to the latest version
- `add myPkg` Automatically downloads and installs a package
- `rm myPkg` Removes a package and all its dependent packages that has been installed automatically only for it
- `add pkgName#master` Checkouts the master branch of a package (and `free pkgName` returns to the released version)
- `add pkgName#branchName` Checkout a specific branch
- `add git@github.com:userName/pkgName.jl.git` Checkout a non registered pkg
- `free pkgName` Return to the "standard" latest compatible released version of a package

<https://syl1.gitbook.io/julia-language-a-concise-tutorial/language-core/11-developing-julia-packages>

Julia environments

- Packages themselves are downloaded, "installed" (precompiled) and stored in a user common directory (e.g. /home/[username]/.julia in Linux)
- Each project can (should!) have its own "environment"
- This is really simple and "light", as it is a simple, automatically managed file ("Manifest.toml") that list all the packages and sub-packages used in the project and their versions
 - providing this file to the "customer"/book, together with the source code, the set of inputs and using a fixed seed for the random numbers at the beginning of the script(s) guarantee reproducible analysis/research
- `cd(@__DIR__)`
- `using Pkg`
- `Pkg.activate(".")`
- `Pkg.instantiate()`

An Example of Manifest file

```
1 # This file is machine-generated - editing it directly is not advised
2
3 [[ArgTools]]
4 uuid = "0dad84c5-d112-42e6-8d28-ef12dabb789f"
5
6 [[Artifacts]]
7 uuid = "56f22d72-fd6d-98f1-02f0-08ddc0907c33"
8
9 [[Base64]]
10 uuid = "2a0f44e3-6c83-55bd-87e4-b1978d98bd5f"
11
12 [[Compat]]
13 deps = ["Base64", "Dates", "DelimitedFiles", "Distributed", "InteractiveUtils",
14         "LibGit2", "Libdl", "LinearAlgebra", "Markdown", "Mmap", "Pkg", "Printf", "REPL",
15         "Random", "SHA", "Serialization", "SharedArrays", "Sockets", "SparseArrays",
16         "Statistics", "Test", "UUIDs", "Unicode"]
14 git-tree-sha1 = "727e463cfebd0c7b999bbf3e9e7e16f254b94193"
15 uuid = "34da2185-b29b-5c13-b0c7-acf172513d20"
16 version = "3.34.0"
17
18 [[Crayons]]
19 git-tree-sha1 = "3f71217b538d7aaee0b69ab47d9b7724ca8afa0d"
20 uuid = "a8cc5b0e-0ffa-5ad4-8c14-923d3ee1735f"
21 version = "4.0.4"
22
23 [[DataAPI]]
24 git-tree-sha1 = "ee400abb2298bd13bfc3df1c412ed228061a2385"
25 uuid = "9a962f9c-6df0-11e9-0e5d-c546b8b5ee8a"
26 version = "1.7.0"
27
28 [[DataFrames]]
29 deps = ["Compat", "DataAPI", "Future", "InvertedIndices",
30         "IteratorInterfaceExtensions", "LinearAlgebra", "Markdown", "Missings", "PooledArrays",
31         "PrettyTables", "Printf", "REPL", "Reexport", "SortingAlgorithms", "Statistics",
32         "TableTraits", "Tables", "Unicode"]
30 git-tree-sha1 = "d785f42445b63fc86caa08bb9a9351008be9b765"
31 uuid = "a93c6f00-e57d-5684-b7b6-d8193f3e46c0"
32 version = "1.2.2"
33
```