Learning Scientific computing with 

Semana de la Ciencia 2020

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uc3m

semana de la ciencia y la innovación
Un planeta, muchos mundos 2020

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- Scientific computing languages and Julia
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- Basics of VS Code and the Julia REPL
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- Fourth example: Now, show me the ship!
- Final project: The Lorenz attractor
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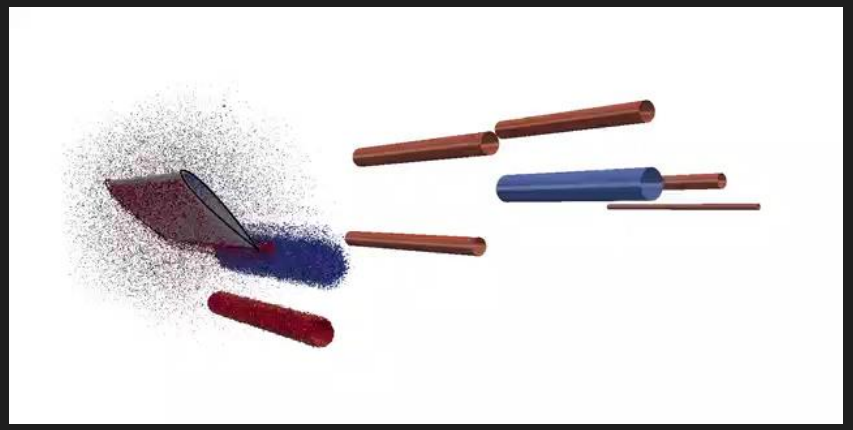
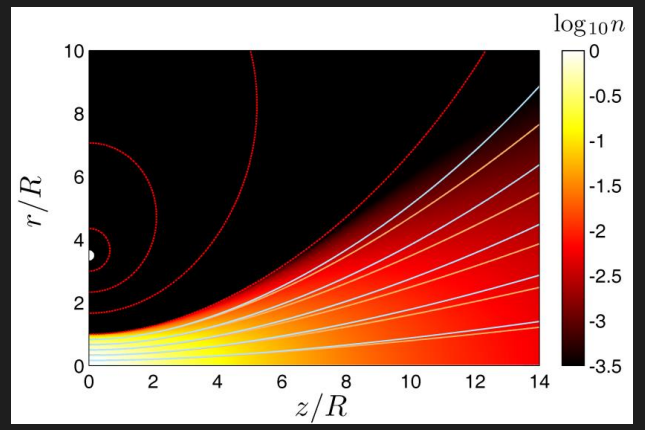
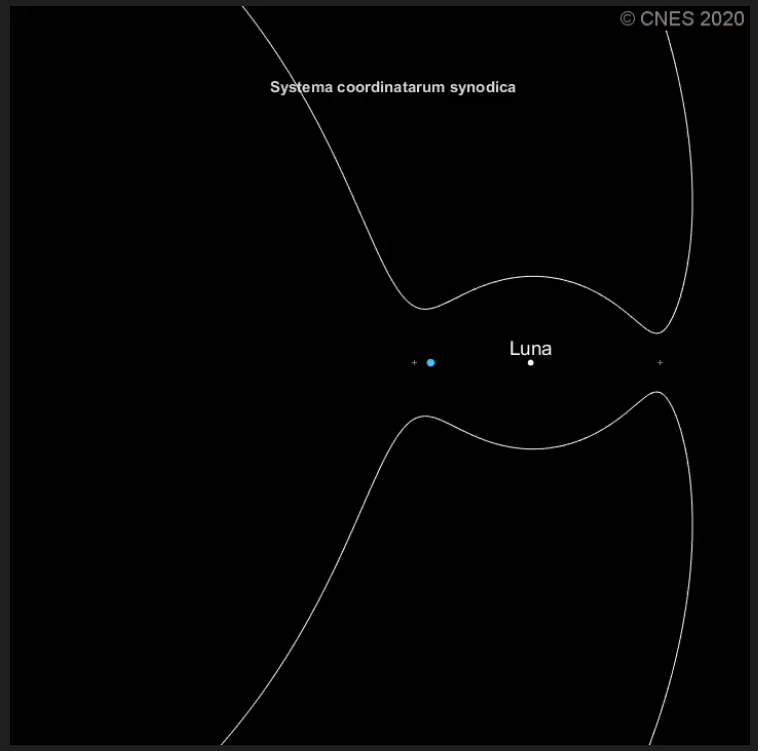
- List of other recommended packages & where to find help

Scientific computing languages

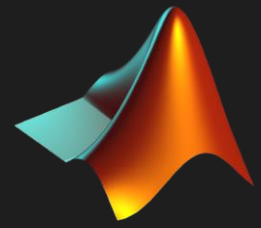
- Modeling, simulating, and visualizing real life is a big deal in science and engineering!







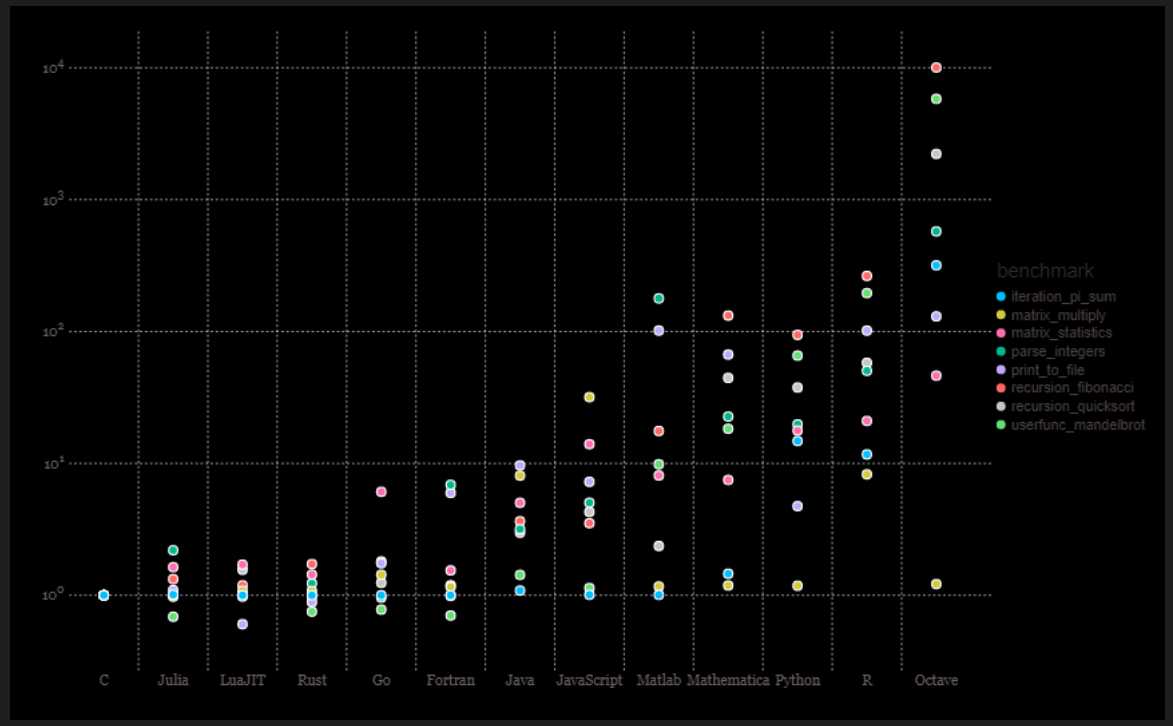
- Programming languages are divided into compiled and interpreted



julia

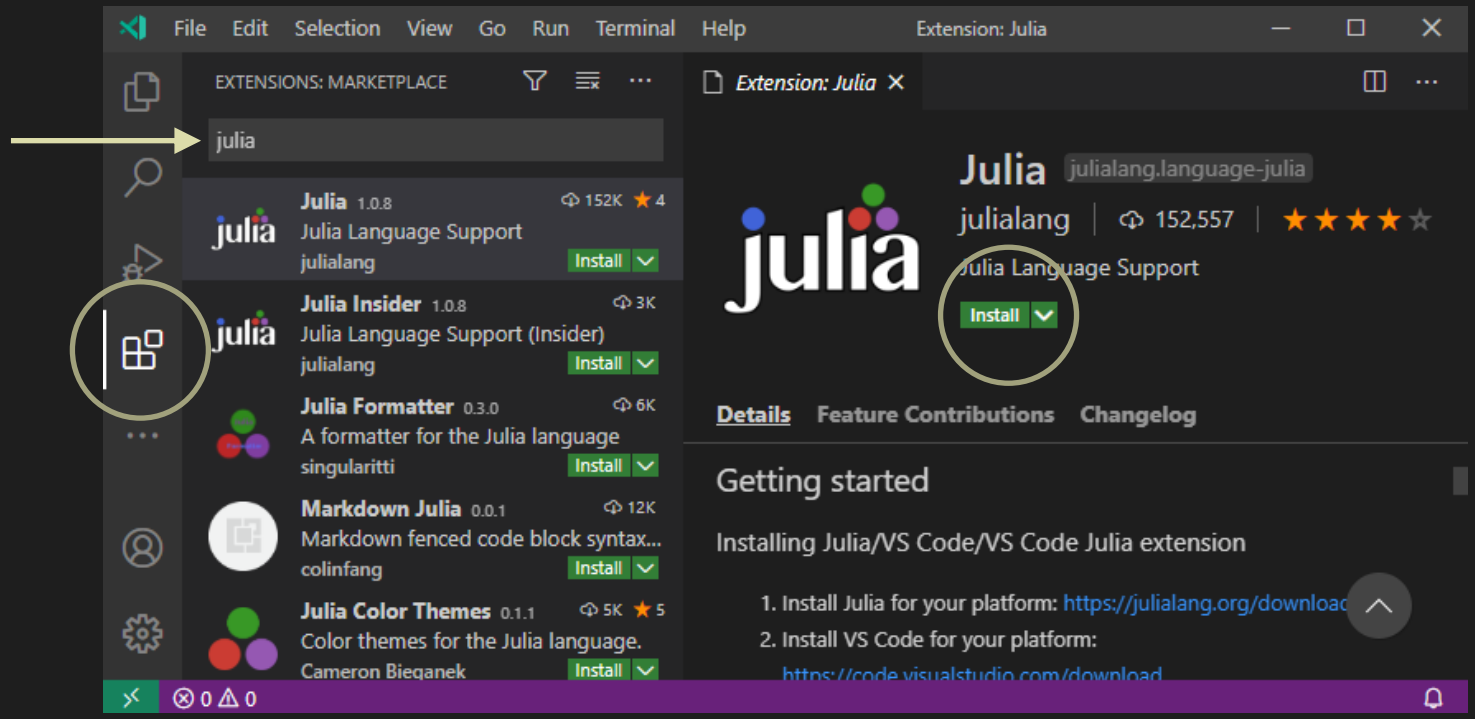
- Modern, dynamically-typed, great for fast prototyping and interaction
- Just in time compilation for high performance
- Designed for scientific computing, not as an afterthought
- Convenient syntax for maths and physics, similar to Matlab

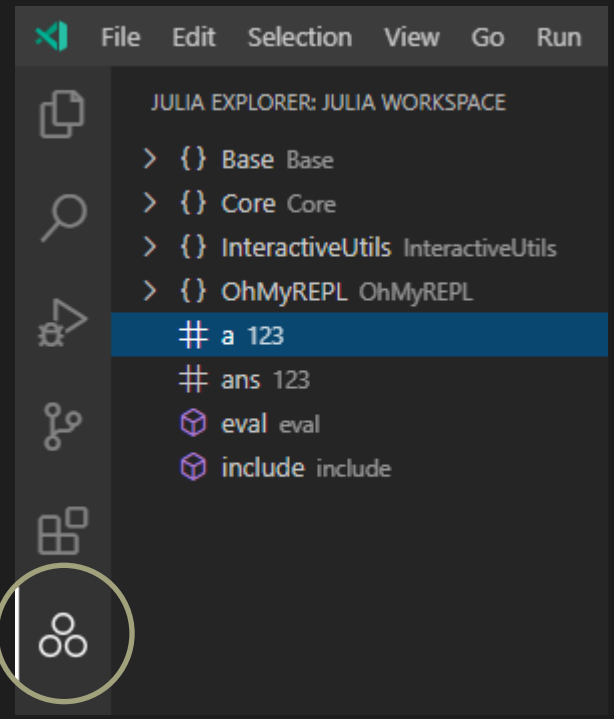
```
function myfactorial(n)
    fact = 1
    for m = 1:n
        fact = fact * m
    end
    return fact
end
```



Setting things up:

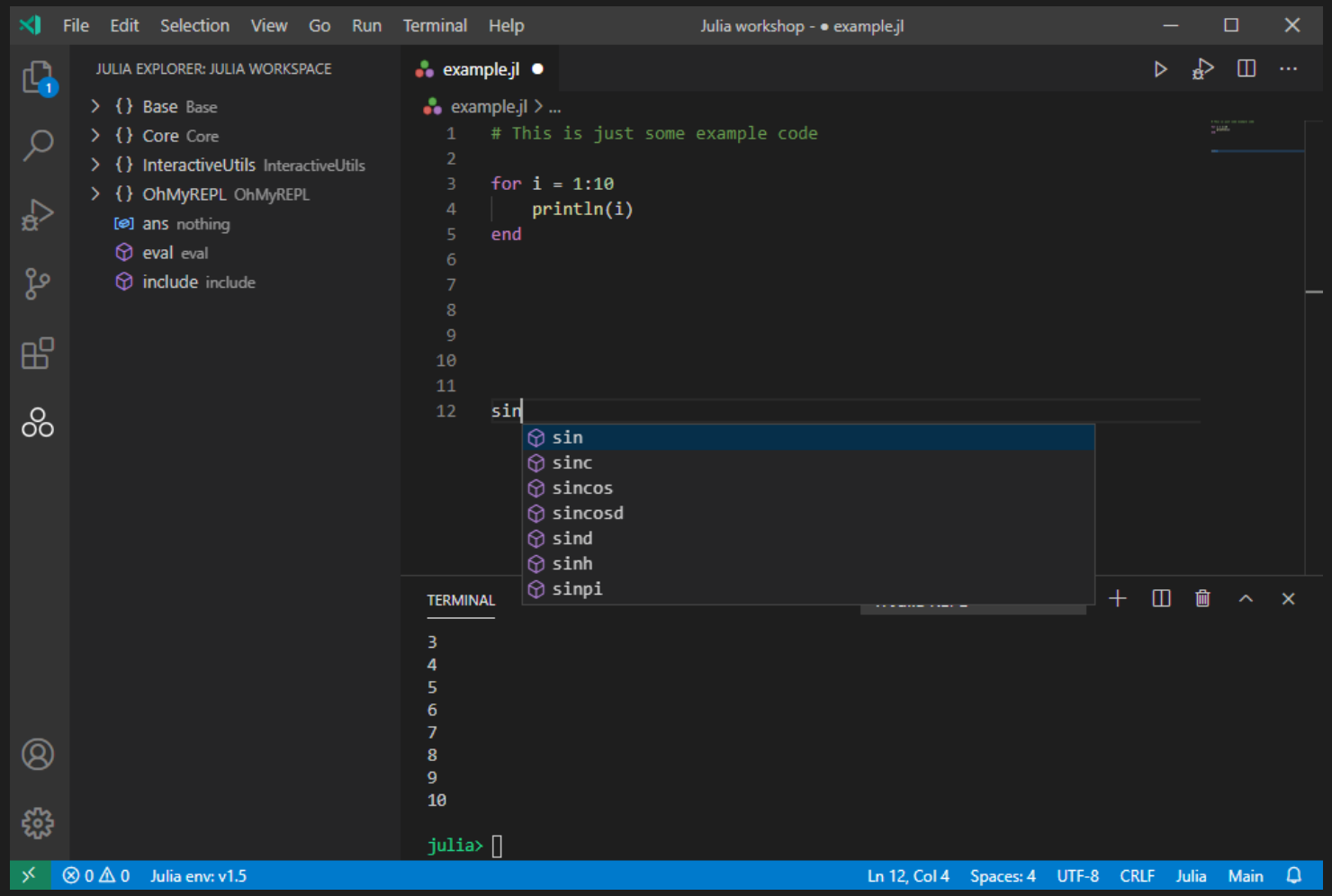
- Install Julia (https://julialang.org/)
- Install VS Code (https://code.visualstudio.com/)
- Install Julia extension in VS Code:





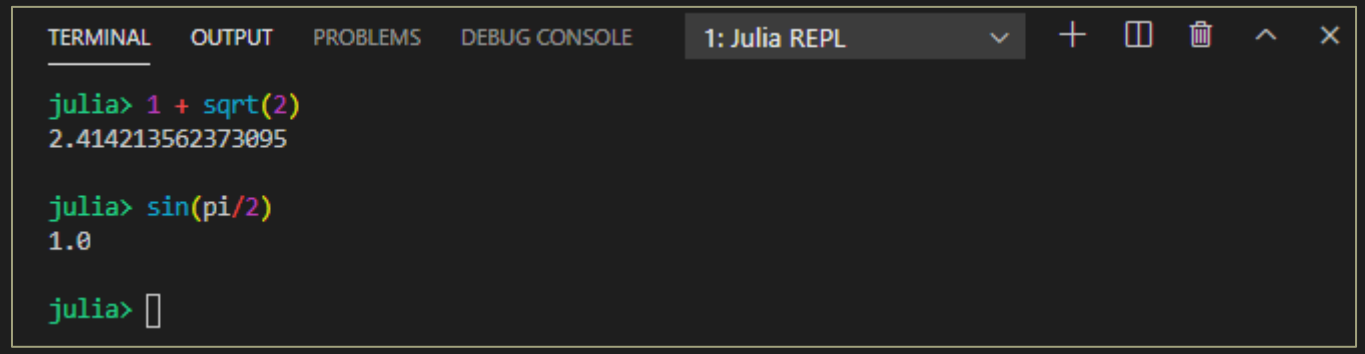
VS code

- Arguably, the best code editor currently available
- Fast and versatile
- Integrated terminal, code runner, debugger, git
- Powerful extension system
- Hit CTRL+SHIFT+P to access all commands
- Use TAB to autocomplete
- Learn basic keyboard shortcuts
- Let's explore it!



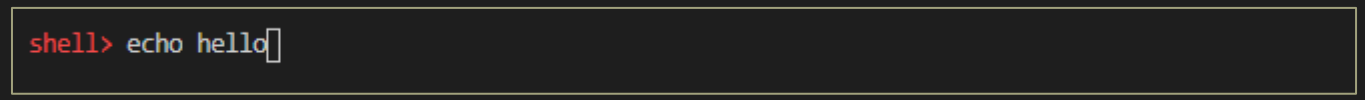
The julia REPL

- The most well-designed terminal we have ever seen!



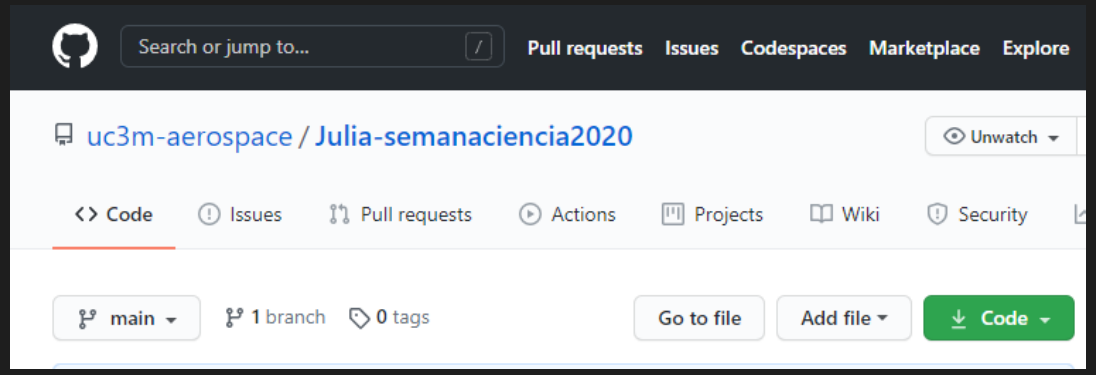
- Get inline help on any function by hitting “?” Try it!

- Shell escape (to run OS commands): hit “;”



Code templates

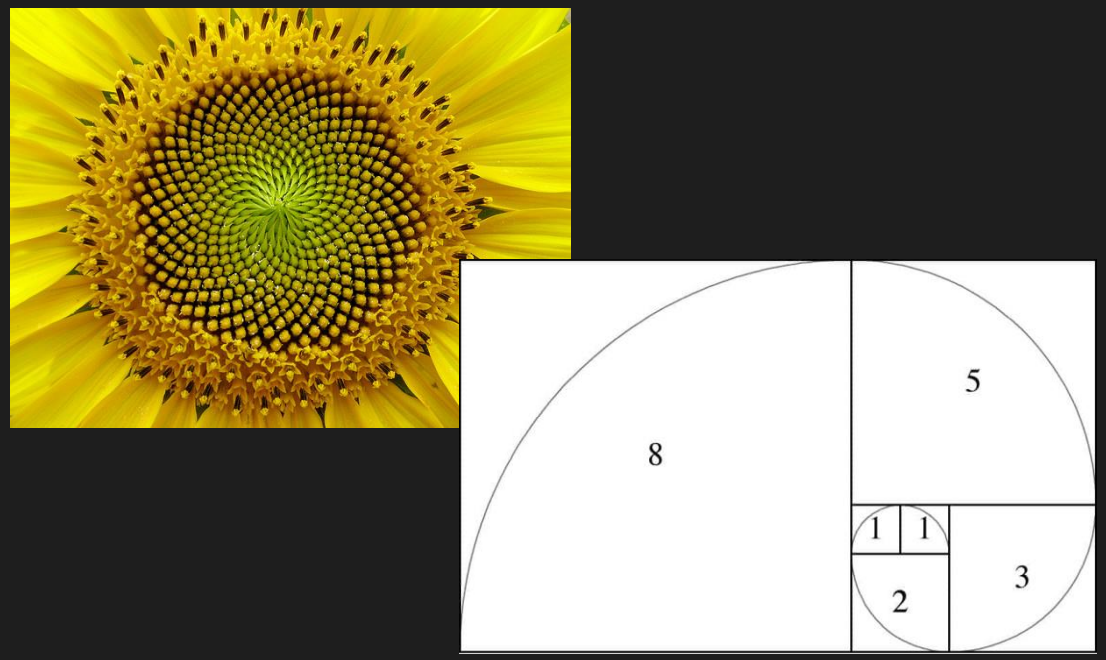
- The templates and the reference solutions for the activities of this workshop can be found at https://github.com/uc3m-aerospace/Julia-semanaciencia2020



- Git is a versioning system. When coding, you will want to save your code and all the development history. Git is the tool!
- GitHub is an online service to store git repositories. It has tons of functionality. You can get a full account for free with your student/staff email

Fibonacci's numbers

- The Fibonacci sequence appears in a surprising number of very different fields. From the structure of spiral galaxies, to the way seeds are arranged in a sunflower, to economics and even art.
- Create a function to compute and print the first n Fibonacci numbers
- Use this function from the REPL to show that F_{n+1}/F_n approaches φ when n is large



$$F_0 = 0,$$
$$F_1 = 1,$$
$$F_n = F_{n-1} + F_{n-2}$$

0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, …

$$\lim_{n\to\infty} \frac{F_{n+1}}{F_n} = \varphi = \frac{\sqrt{5}+1}{2}$$

Fibonacci's numbers

- Functions are used to encapsulate code that can be called from the REPL or other code. Here is a very simple example:

```
function add1(input)
    output = input + 1
    return output
end
```

- Create a function that takes as input the number `N` of Fibonacci numbers to compute
- Initialize the vector `F` where you will store your computed numbers with `F = zeros(N)`
- You can access any entry of the vector using brackets. `F[1]` is the first element and `F[end]` the last one.
- You probably want to set `F[1] = 0, F[2] = 1`
- Create a loop to compute the rest of the Fibonacci numbers:

```
for i = i1:iend
    # Do stuff
end
```

$$F_0 = 0,$$
$$F_1 = 1,$$
$$F_n = F_{n-1} + F_{n-2}$$

Fibonacci's numbers (Hints cont.)

- Now iterate through the rest of the terms of the series
- How to use a loop? The simplest way is to use a semicolon range operator. Initially i = i1 and increases 1 each iteration, the last iteration is i = iend
- Print each term of the series using println(). Finally try to retrieve the approximate value of φ using the values stored in F

Is it a multiple of 7?

- I never know if a number like 841288 is a multiple of 7 or not!
- Create a function that takes an input number and returns "`It is a multiple of 7`" or "`It is not a multiple of 7`" accordingly
- Run the function from REPL to check if 841288 and/or 122145 are multiples of 7

- How to run conditional code?

```
if condition
    # What to do if true
else
    # What to do if false
end
```

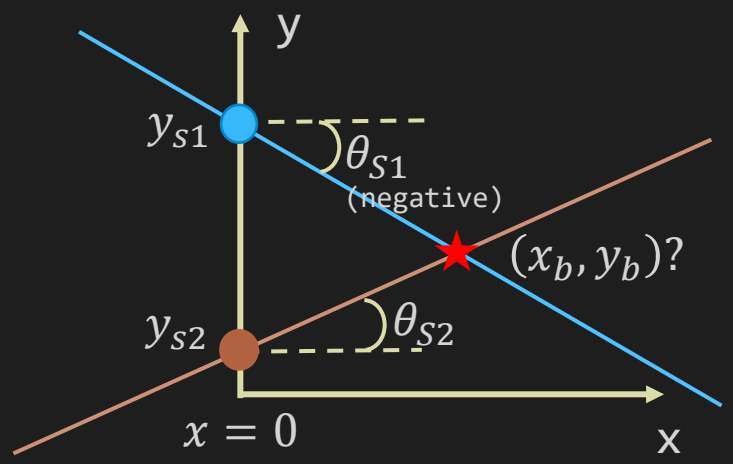
- Equality condition: `a == b` is true if a is equal to b
- To compute the remainder of `x/y`, use `x % y`
- Print to console with `println()`

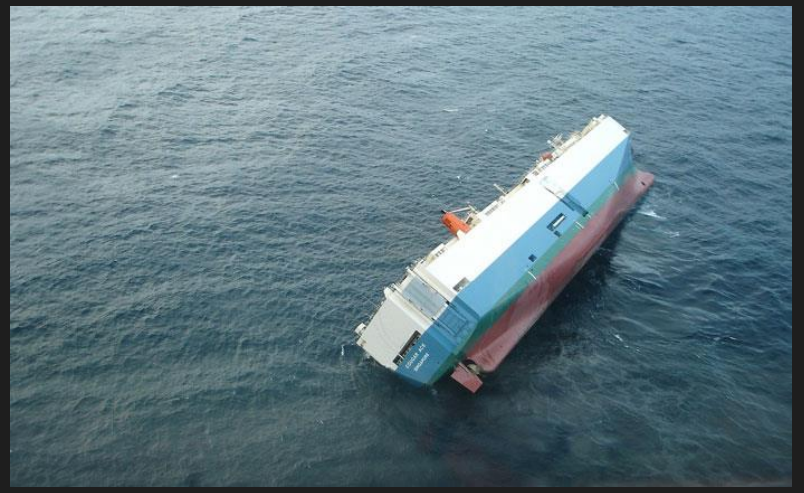
Locate that ship!

- Imagine a ship in distress sends a signal to two stations on the coast, of which we know their position. The stations only know the *angle* at which the signal arrives, nothing more. Can we locate the ship?
- Write the equations for the two straight lines and find the intersection by solving the resulting linear system
- Write the system of equations in matrix form $\boldsymbol{Ax} = \boldsymbol{c}$

$$\begin{bmatrix} \tan(\theta_{S1}) & -1 \\ \tan(\theta_{S2}) & -1 \end{bmatrix} \cdot \begin{pmatrix} x_b \\ y_b \end{pmatrix} = \begin{pmatrix} -y_{s1} \\ -y_{s2} \end{pmatrix}$$

$$y = n + mx,$$
$$m = \tan(\theta),$$
$$n = y(x = 0)$$





- The ship location belongs to both lines:

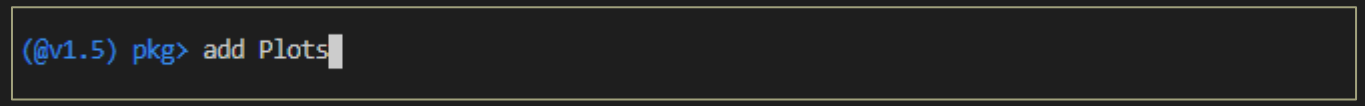
$$y_b = n_1 + m_1 x_b$$
$$y_b = n_2 + m_2 x_b$$

- We have a linear system of 2 equations with 2 unknowns

$$\begin{bmatrix} \tan(\theta_{S1}) & -1 \\ \tan(\theta_{S2}) & -1 \end{bmatrix} \cdot \begin{pmatrix} x_b \\ y_b \end{pmatrix} = \begin{pmatrix} -y_{s1} \\ -y_{s2} \end{pmatrix}$$

julia packages

- Remember the REPL? Enter Pkg mode by hitting “]”



- The Pkg mode allows installing, removing, and maintaining packages
- Install the Plots package for the next activity
- The first time you use a package, it will be compiled. This will take some time (just for the first time or if the package is updated)

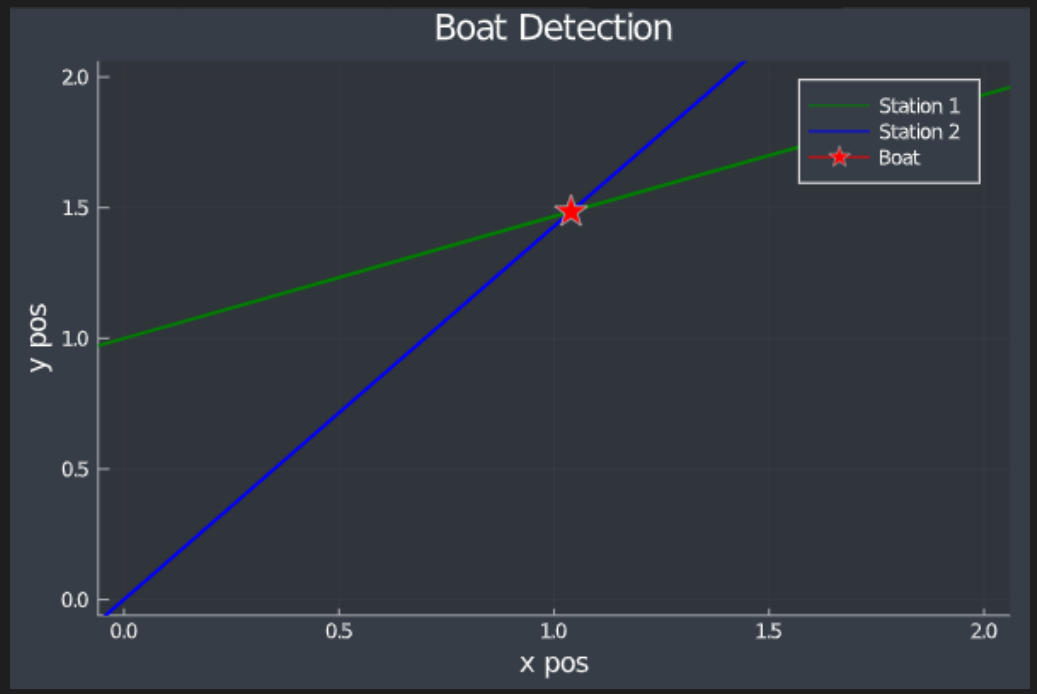
Now, show me the ship!

- It would be great if we could see the result of our previous work!
- Plot the two lines of the previous example and add a marker at the intersection.

- You must first load the Plots package with

```
using Plots
```

- Have a look at the Plots.jl documentation for style and attributes: http://docs.juliaplots.org/



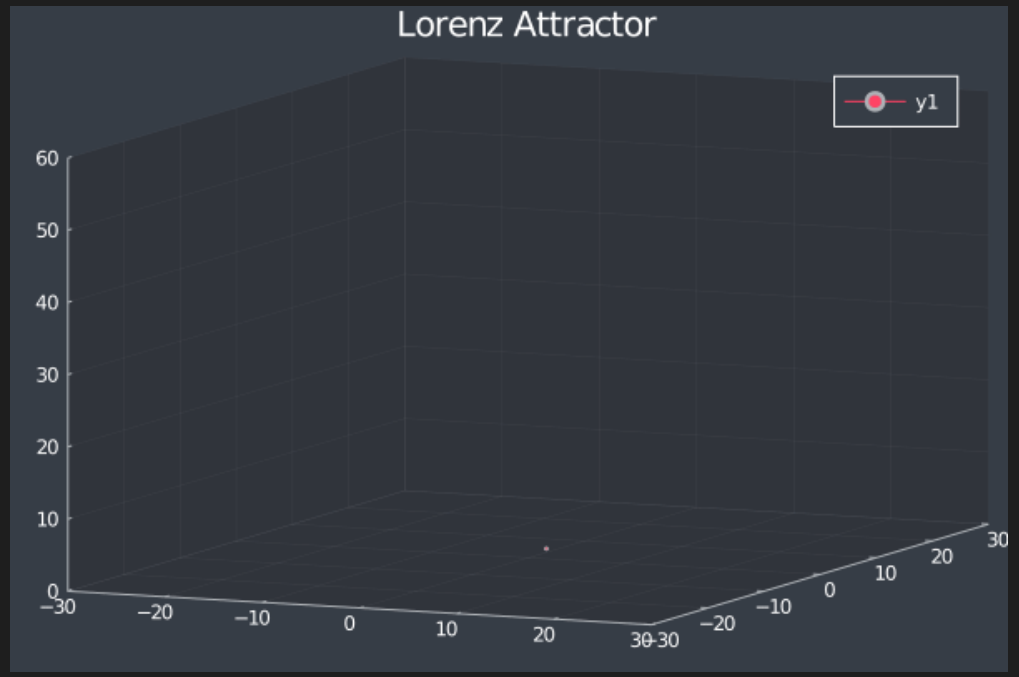
The Lorenz attractor

- Chaos is everywhere and unpredictable. A simple model of atmospheric convection proposed in 1963 by Edward Lorenz already shows this. Similar equations appear in many other applications: Lasers, electrical systems, chemical reactions...
- System of ordinary Differential Equations:

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = x(\rho - z) - y$$
$$\frac{dz}{dt} = xy - \beta z$$

- The Forward Euler Method can integrate this system numerically:

$$x(t + \Delta t) = x(t) + \frac{dx}{dt}\Delta t$$



$\sigma = 10,\ \rho = 28,\ \beta = 8/3$

The Lorenz attractor

- Create a function that advances x, y, z one small timestep $\mathrm{d}t$ using Euler's forward method. Use the parameters on the right.
- Use this function to advance the solution, starting with:

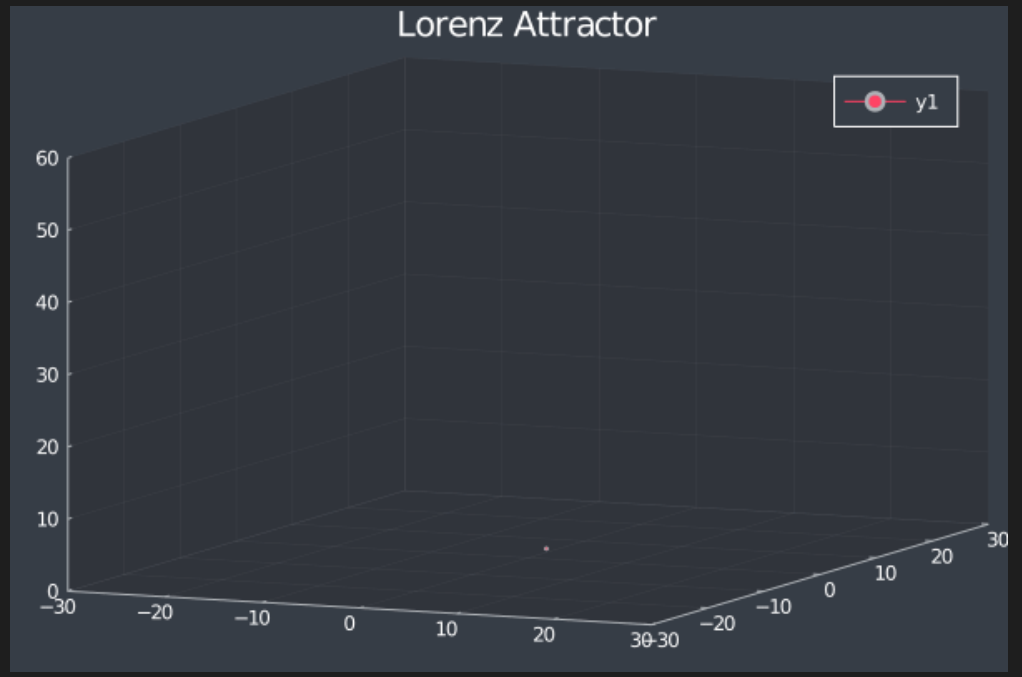
```
dt = 0.02
σ  = 10
ρ  = 28
β  = 8/3
```

```
x0 = 1
y0 = 1
z0 = 1
```

- Plot the resulting trajectory

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = x(\rho - z) - y$$
$$\frac{dz}{dt} = xy - \beta z$$

$$x(t + \Delta t) = x(t) + \frac{dx}{dt}\Delta t$$



Other capabilities of julia

- We have barely scratched the surface!
- Julia's main strength is the multiple dispatch system based on types

```
mutable struct Point
    x::Float64
    y::Float64
end

A = Point(1.23, 5.55)
A.x
```

```
function compute_average(numbers::Float64)

function compute_average(numbers::Int32)
```

- Common types are Float64, Int32…
  But you can create your own types!
- Macros are functions with a convenient syntax (@ syntax)

```
@time myfunction(a,b,c)
```

- Unit testing is included out of the box

```
using Test
@test myfunction(a,b,c)
```

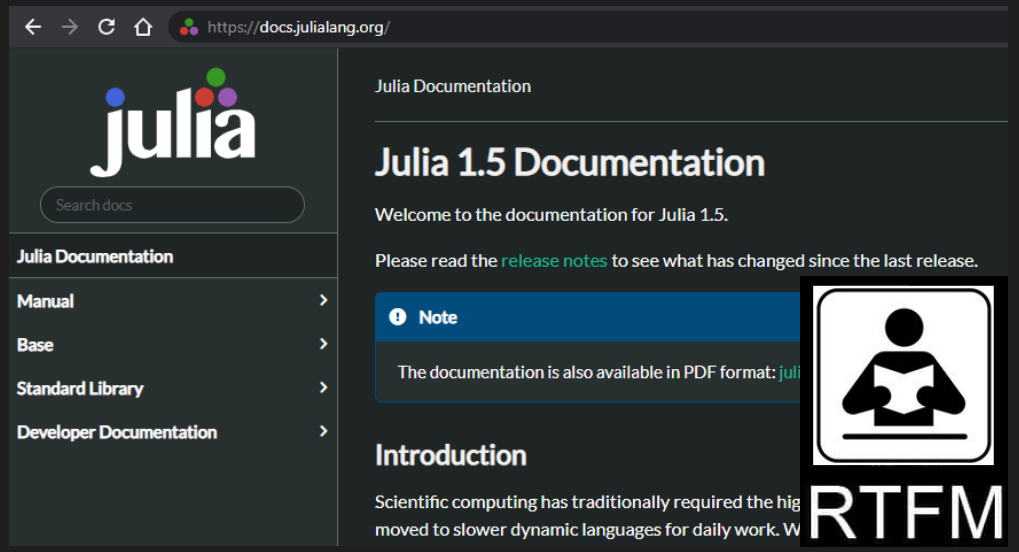
- Julia can run in multithreaded and distributed mode out of the box

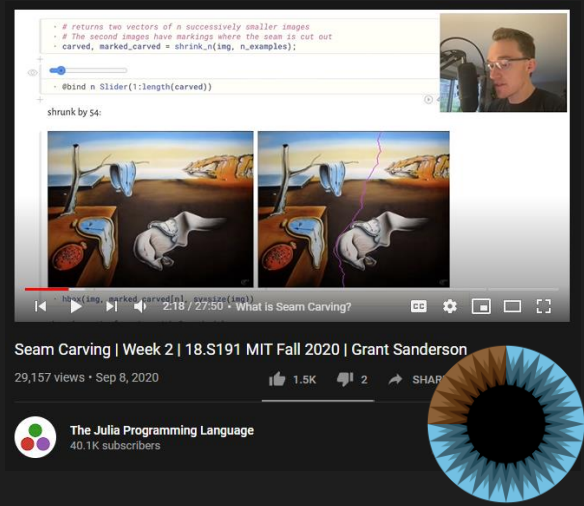
Interesting packages

- There are tons of packages with extra functionality!
  - DifferentialEquations: amazing library to solve ODEs, PDEs
  - JuliaFEM: finite element method library
  - Pluto: reactive notebooks (see also IJulia in Jupyter)
  - Flux: machine learning
  - JuMP: optimization
  - PyCall: call python functions from julia
  - Revise: update function definitions atomatically as you work
  - OhMyREPL: adds some oomph to the REPL
  - MPI: parallel computing with MPI
  - CUDA: use your GPU for parallel computing
  - HDF5: read/write to this format of data files
  - PackageCompiler: compile julia code
- Check out juliahub.com, juliaobserver.com, juliapackages.com for more

Where to learn more and get help?

- Remember the "?" help function of the REPL
- Documentation! docs.julialang.org
- Tutorials, books and videos
- https://exercism.io/tracks/julia
- Great online course by MIT on YouTube with the participation of 3blue1brown
- Read the performance tips: docs.julialang.org/en/v1/manual/performance-tips/#man-performance-tips
- How do I...? Just google it!



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