C.E.C.I

Consortium des Equipements
de Calcul Intensif
en Fédération Wallonie-Bruxelles

Introduction to Scripting Languages

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Goal of this session:

“Advocate the use of scripting languages (interpreted languages) and help you choose the most suitable for your needs”

Agenda

1. Interpreters vs compilers
2. Octave, R, Python
3. Graphical User Interfaces & Literate programming
4. Additional Packages/Libraries/Modules
5. What to do when it is too slow
6. Using several of them at the same time

Interpreters vs Compilers

- A **compiler** reads the whole (text) code and produces a separate “binary” file that can be executed by the CPU.

  C/C++, Fortran, Java, Go, Rust, Haskel, ...

- An **interpreter** reads each line of code and executes it by calling the corresponding functionalities in its own code.

  Bash, Python, PHP, Javascript, Ruby, ...

Interpreters vs Compilers

- The ugly truth...
  - Many interpreters will pre-compile the code
  - Some compilers compile not to CPU-specific machine instructions but to bytecode
  - The bytecode interpreters sometimes re-compile the bytecode just before execution (JIT compiling)
  - Interpreters exist for C and C++
  - Compilers exist for Python
  - The interpreter can be compiled or himself interpreted

Interpreters vs Compilers

Compilers

- can apply code-wise powerful optimization
- practically have no run-time overhead

→ Speed

Interpreters

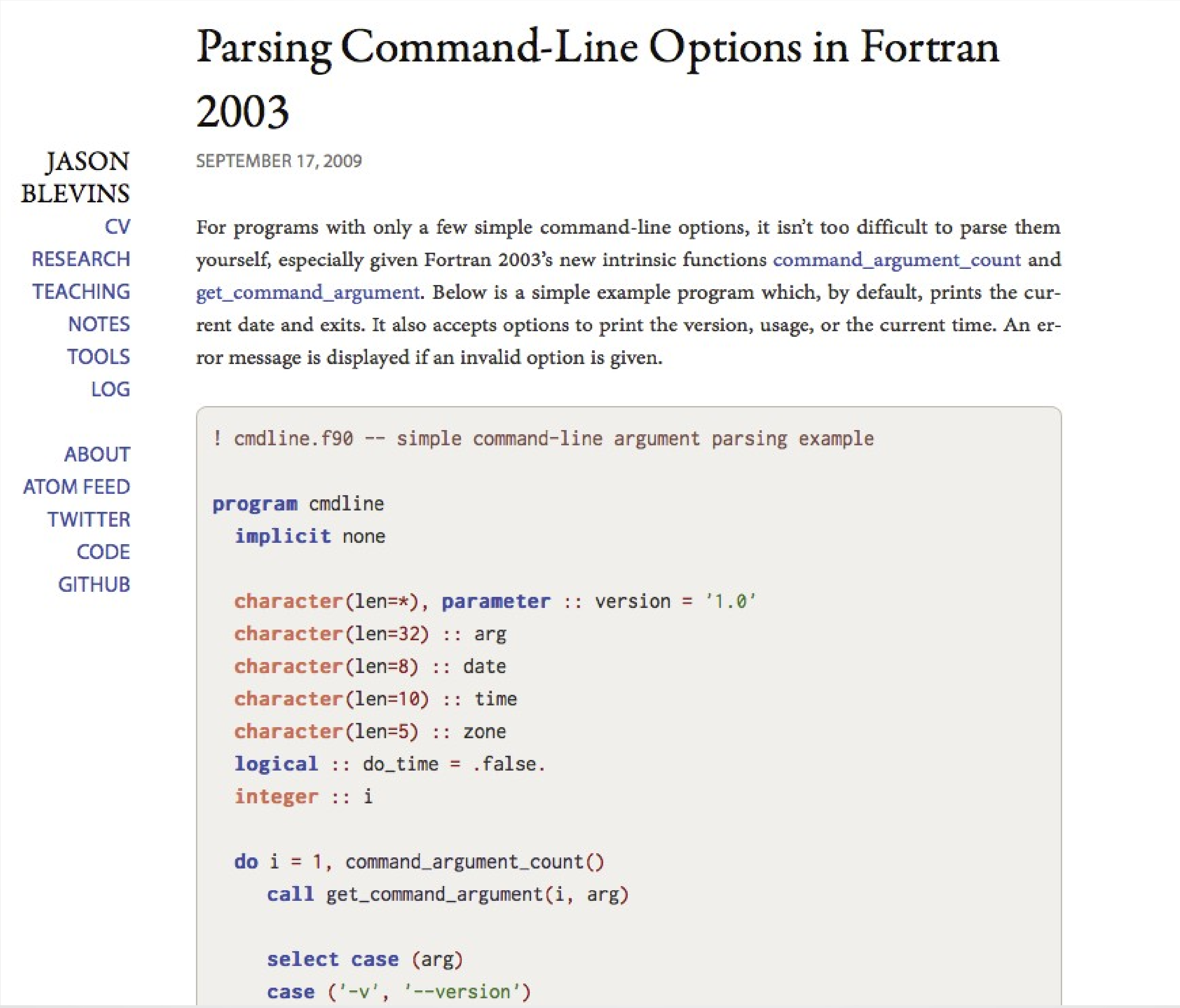
- allow easy code introspection
- offer high-level language constructs and tools

→ Ease of use

Interpreted languages

- Easier to **learn**
  - Many implementation details hidden
  - Can try and test code portions rapidly and easily
- Easier to **exchange**/reuse
  - The scripts are cross-platform by design
  - Often built-in package management
- Faster development
  - More **convenient programming** and shorter programs
    - Offers many simplifications and shortcuts – no need to micromanage memory
    - Built-in support for mundane tasks (handle files, dates, plots, NAs, NANs, ...)
  - **Easier to debug** and profile
    - GUI

Ex.1: argument parsing in Fortran



Parsing Command-Line Options in Fortran 2003

JASON BLEVINS
CV
RESEARCH
TEACHING
NOTES
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LOG

ABOUT
ATOM FEED
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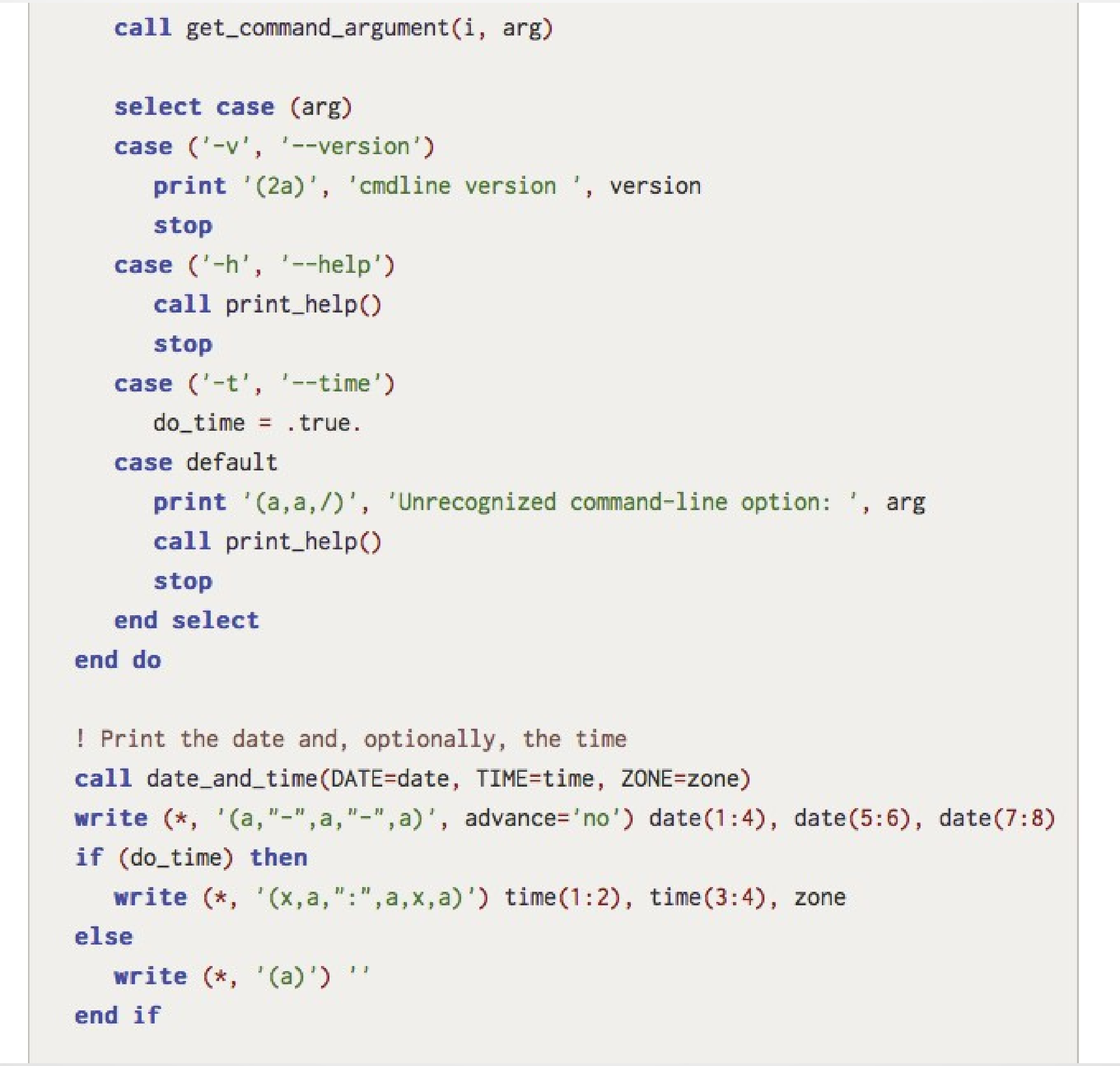
SEPTEMBER 17, 2009

For programs with only a few simple command-line options, it isn't too difficult to parse them yourself, especially given Fortran 2003's new intrinsic functions command_argument_count and get_command_argument. Below is a simple example program which, by default, prints the current date and exits. It also accepts options to print the version, usage, or the current time. An error message is displayed if an invalid option is given.

```
! cmdline.f90 -- simple command-line argument parsing example

program cmdline
  implicit none

  character(len=*), parameter :: version = '1.0'
  character(len=32) :: arg
  character(len=8) :: date
  character(len=10) :: time
  character(len=5) :: zone
  logical :: do_time = .false.
  integer :: i

  do i = 1, command_argument_count()
     call get_command_argument(i, arg)

     select case (arg)
     case ('-v', '--version')
```

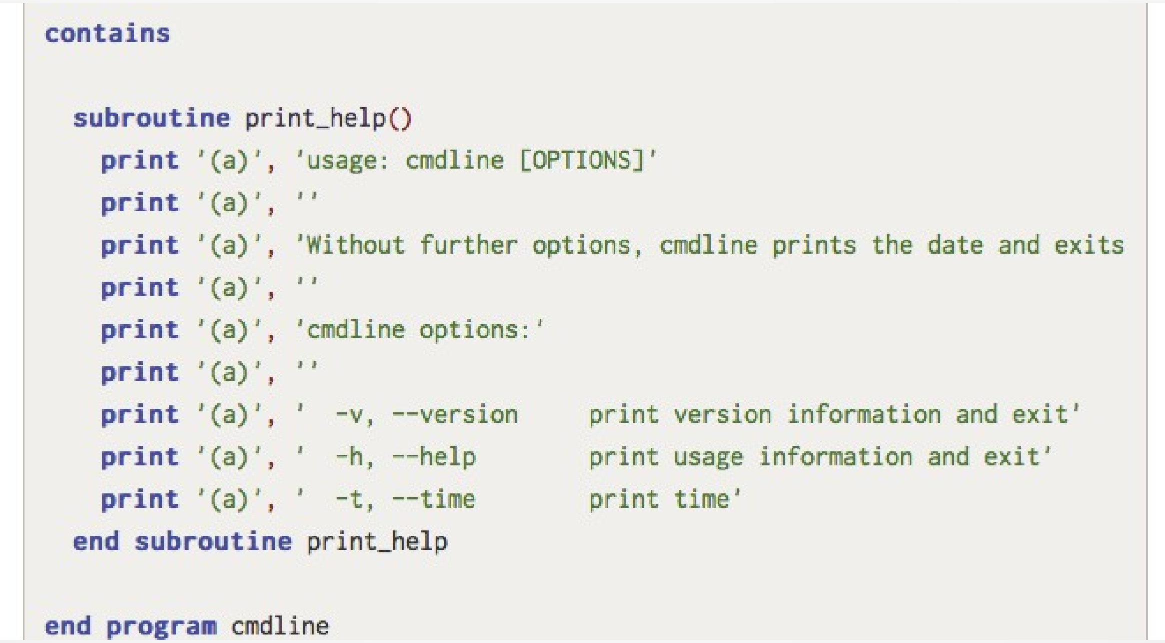
https://docs.python.org/3/library/argparse.html

Ex.1: argument parsing in Fortran



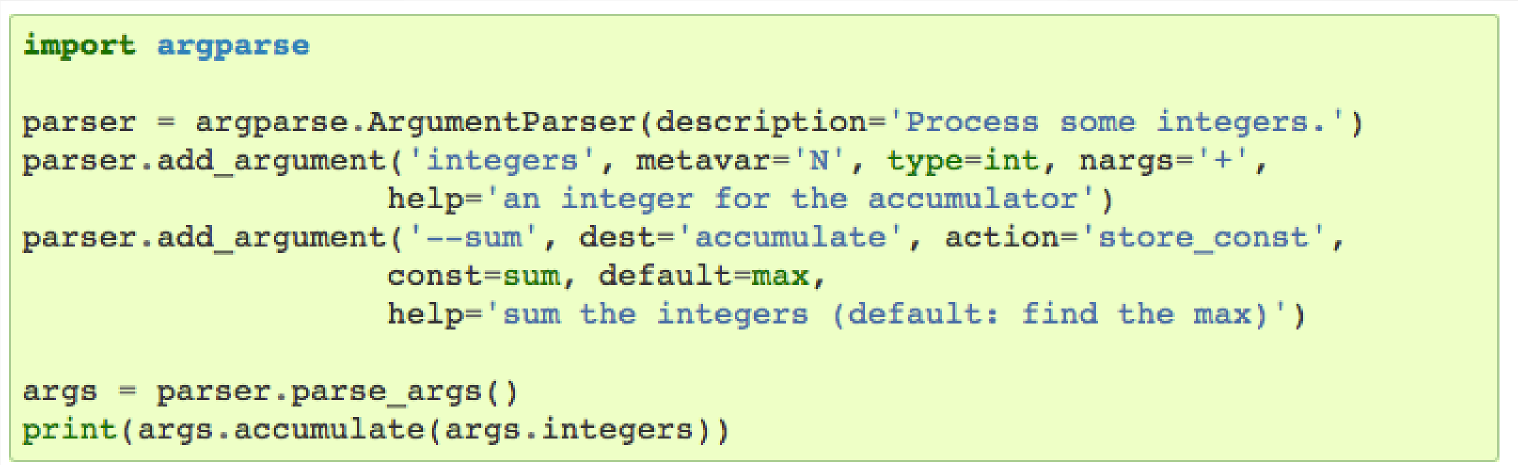
```
   call get_command_argument(i, arg)

   select case (arg)
   case ('-v', '--version')
      print '(2a)', 'cmdline version ', version
      stop
   case ('-h', '--help')
      call print_help()
      stop
   case ('-t', '--time')
      do_time = .true.
   case default
      print '(a,a,/)', 'Unrecognized command-line option: ', arg
      call print_help()
      stop
   end select
end do

! Print the date and, optionally, the time
call date_and_time(DATE=date, TIME=time, ZONE=zone)
write (*, '(a,"-",a,"-",a)', advance='no') date(1:4), date(5:6), date(7:8)
if (do_time) then
   write (*, '(x,a,":",a,x,a)') time(1:2), time(3:4), zone
else
   write (*, '(a)') ''
end if
```

Ex.1: argument parsing in Fortran



```fortran
contains

  subroutine print_help()
    print '(a)', 'usage: cmdline [OPTIONS]'
    print '(a)', ''
    print '(a)', 'Without further options, cmdline prints the date and exits
    print '(a)', ''
    print '(a)', 'cmdline options:'
    print '(a)', ''
    print '(a)', '  -v, --version     print version information and exit'
    print '(a)', '  -h, --help        print usage information and exit'
    print '(a)', '  -t, --time        print time'
  end subroutine print_help

end program cmdline
```

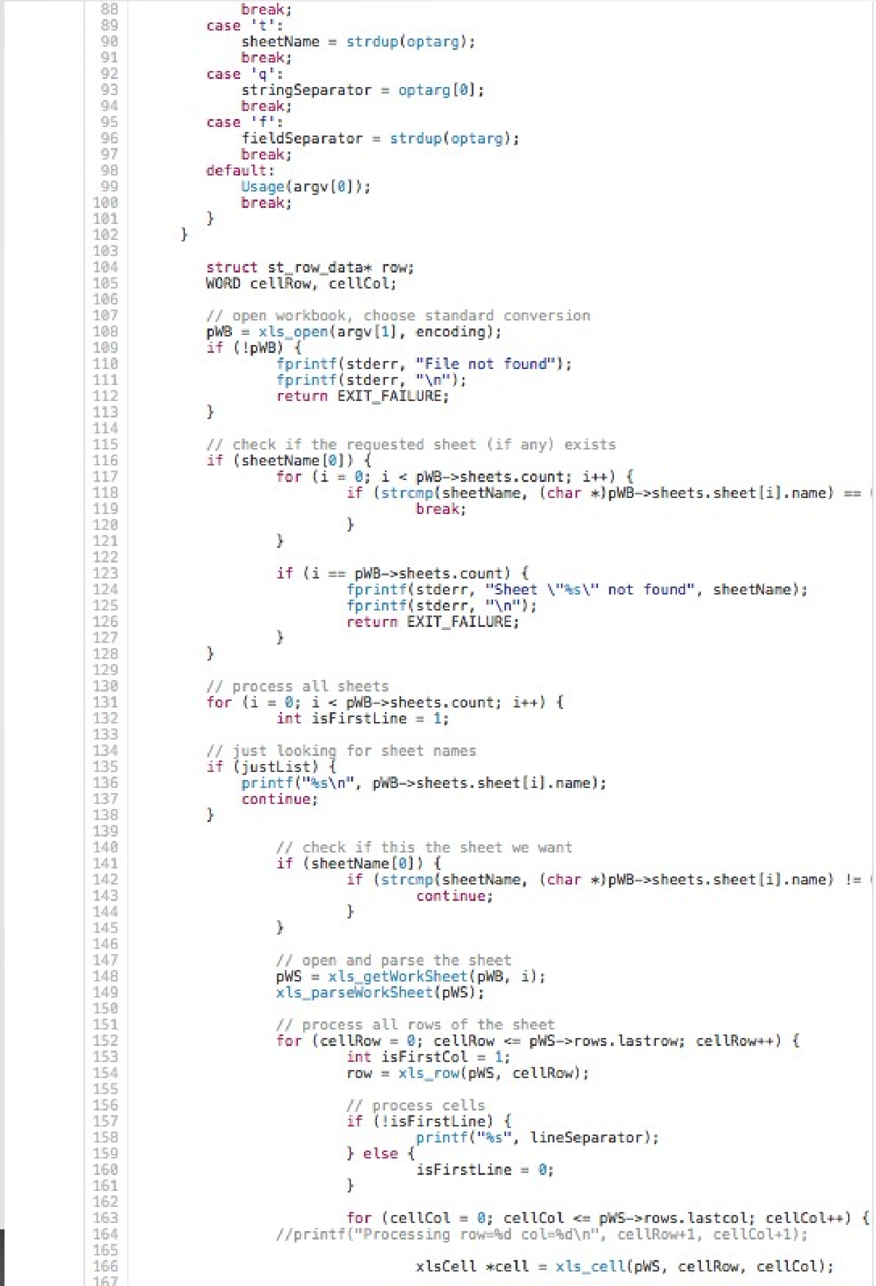
Ex.1: argument parsing in Python



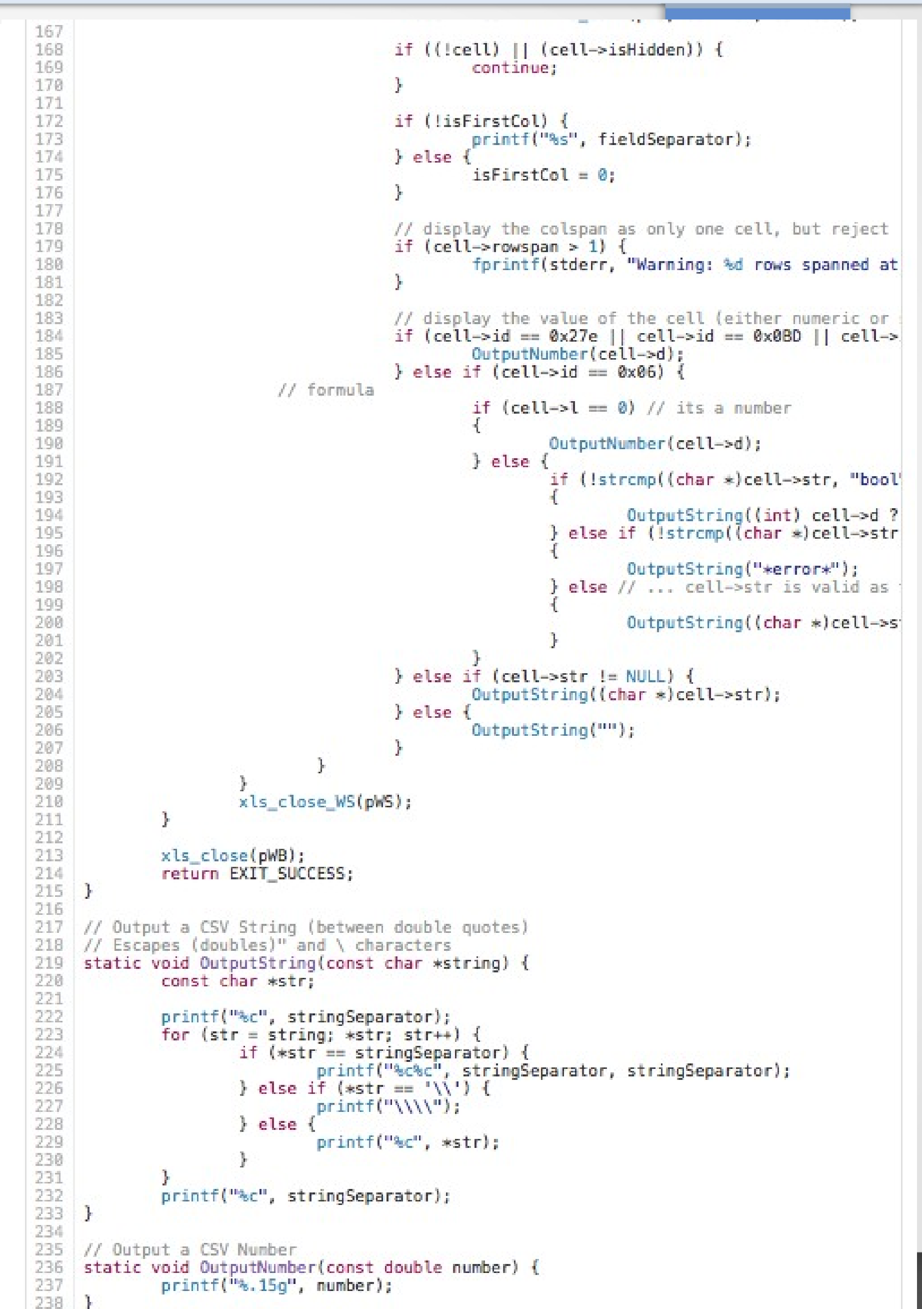
```
import argparse

parser = argparse.ArgumentParser(description='Process some integers.')
parser.add_argument('integers', metavar='N', type=int, nargs='+',
                   help='an integer for the accumulator')
parser.add_argument('--sum', dest='accumulate', action='store_const',
                   const=sum, default=max,
                   help='sum the integers (default: find the max)')

args = parser.parse_args()
print(args.accumulate(args.integers))
```

https://docs.python.org/3/library/argparse.html

Ex.2: Use XLS file in C

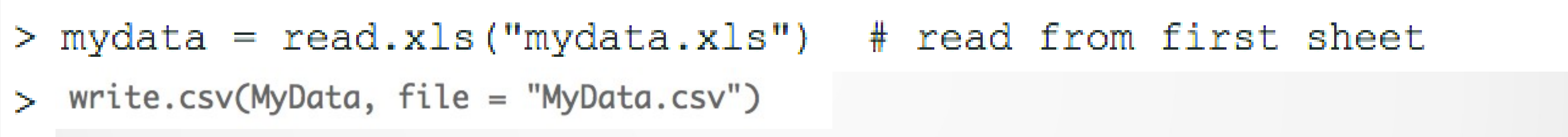


```
            break;
        case 't':
            sheetName = strdup(optarg);
            break;
        case 'q':
            stringSeparator = optarg[0];
            break;
        case 'f':
            fieldSeparator = strdup(optarg);
            break;
        default:
            Usage(argv[0]);
            break;
        }
    }

        struct st_row_data* row;
        WORD cellRow, cellCol;

        // open workbook, choose standard conversion
        pWB = xls_open(argv[1], encoding);
        if (!pWB) {
                fprintf(stderr, "File not found");
                fprintf(stderr, "\n");
                return EXIT_FAILURE;
        }

        // check if the requested sheet (if any) exists
        if (sheetName[0]) {
                for (i = 0; i < pWB->sheets.count; i++) {
                        if (strcmp(sheetName, (char *)pWB->sheets.sheet[i].name) == (
                                break;
                        }
                }

                if (i == pWB->sheets.count) {
                        fprintf(stderr, "Sheet \"%s\" not found", sheetName);
                        fprintf(stderr, "\n");
                        return EXIT_FAILURE;
                }
        }

        // process all sheets
        for (i = 0; i < pWB->sheets.count; i++) {
                int isFirstLine = 1;

        // just looking for sheet names
        if (justList) {
            printf("%s\n", pWB->sheets.sheet[i].name);
            continue;
        }

                // check if this the sheet we want
                if (sheetName[0]) {
                        if (strcmp(sheetName, (char *)pWB->sheets.sheet[i].name) != (
                                continue;
                        }
                }

                // open and parse the sheet
                pWS = xls_getWorkSheet(pWB, i);
                xls_parseWorkSheet(pWS);

                // process all rows of the sheet
                for (cellRow = 0; cellRow <= pWS->rows.lastrow; cellRow++) {
                        int isFirstCol = 1;
                        row = xls_row(pWS, cellRow);

                        // process cells
                        if (!isFirstLine) {
                                printf("%s", lineSeparator);
                        } else {
                                isFirstLine = 0;
                        }

                        for (cellCol = 0; cellCol <= pWS->rows.lastcol; cellCol++) {
                //printf("Processing row=%d col=%d\n", cellRow+1, cellCol+1);

                                xlsCell *cell = xls_cell(pWS, cellRow, cellCol);
```



```
                                        if ((!cell) || (cell->isHidden)) {
                                                continue;
                                        }

                                        if (!isFirstCol) {
                                                printf("%s", fieldSeparator);
                                        } else {
                                                isFirstCol = 0;
                                        }

                                        // display the colspan as only one cell, but reject
                                        if (cell->rowspan > 1) {
                                                fprintf(stderr, "Warning: %d rows spanned at
                                        }

                                        // display the value of the cell (either numeric or
                                        if (cell->id == 0x27e || cell->id == 0x0BD || cell->
                                                OutputNumber(cell->d);
                                        } else if (cell->id == 0x06) {
                       // formula
                                                if (cell->l == 0) // its a number
                                                {
                                                        OutputNumber(cell->d);
                                                } else {
                                                        if (!strcmp((char *)cell->str, "bool'
                                                        {
                                                                OutputString((int) cell->d ?
                                                        } else if (!strcmp((char *)cell->str
                                                        {
                                                                OutputString("*error*");
                                                        } else // ... cell->str is valid as
                                                        {
                                                                OutputString((char *)cell->s
                                                        }
                                                }
                                        } else if (cell->str != NULL) {
                                                OutputString((char *)cell->str);
                                        } else {
                                                OutputString("");
                                        }
                                }
                        }
                        xls_close_WS(pWS);
                }

        xls_close(pWB);
        return EXIT_SUCCESS;
}

// Output a CSV String (between double quotes)
// Escapes (doubles)" and \ characters
static void OutputString(const char *string) {
        const char *str;

        printf("%c", stringSeparator);
        for (str = string; *str; str++) {
                if (*str == stringSeparator) {
                        printf("%c%c", stringSeparator, stringSeparator);
                } else if (*str == '\\') {
                        printf("\\\\");
                } else {
                        printf("%c", *str);
                }
        }
        printf("%c", stringSeparator);
}

// Output a CSV Number
static void OutputNumber(const double number) {
        printf("%.15g", number);
}
```

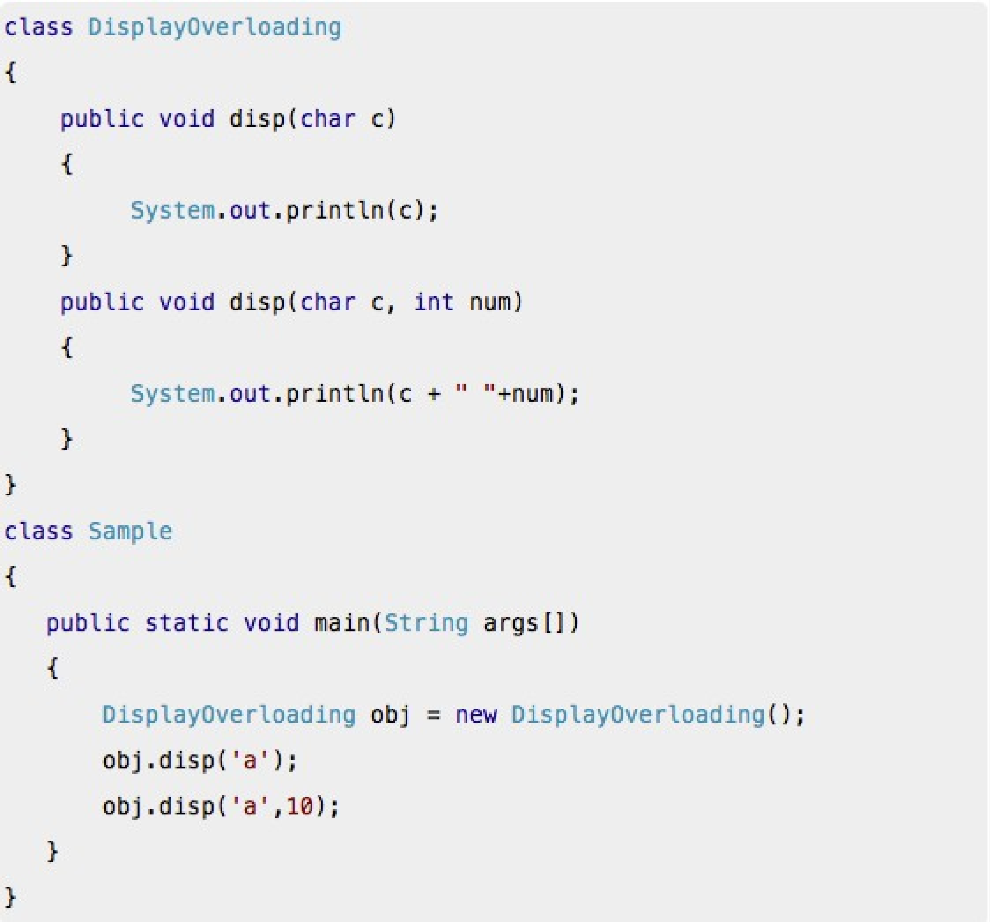
Ex.2: Use XLS file in R



```
> mydata = read.xls("mydata.xls")  # read from first sheet
> write.csv(MyData, file = "MyData.csv")
```

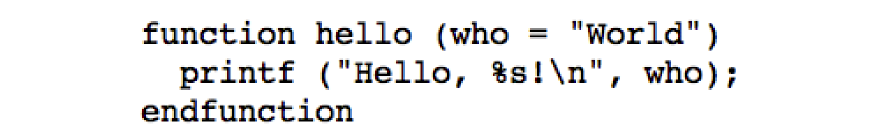
https://cran.r-project.org/web/packages/gdata/

Ex.3: default args in Java



```
class DisplayOverloading
{
    public void disp(char c)
    {
         System.out.println(c);
    }
    public void disp(char c, int num)
    {
         System.out.println(c + " "+num);
    }
}
class Sample
{
   public static void main(String args[])
   {
       DisplayOverloading obj = new DisplayOverloading();
       obj.disp('a');
       obj.disp('a',10);
   }
}
```

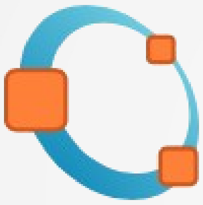
Ex.3: default args in Octave



```
function hello (who = "World")
  printf ("Hello, %s!\n", who);
endfunction
```

https://www.gnu.org/software/octave/doc/interpreter/Default-Arguments.html

1.



Why those three?

Why those three?

- All very much used in scientific applications

  R (S/SPlus): strong for statistics

  Octave (Matlab): strong for engineering

  Python Scipy/Numpy (Canopy,Anaconda): strong for data science
- All free and free.
- Fun fact: All started as wrappers for Fortran code!

Why those three?

By contrast,

- Ruby, Perl: smaller bioinformatics-only community
- Javascript, PHP, Bash, TCL, Lua: totally different goal
- Matlab, IDL, Mathematica: not free
- Julia: very young – good luck to get help when needed

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Not true anymore.
Worth considering !

(but not yet in this session...)

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Some Julia in here...

2.

TripleQuickstart

Operators and assignment

a=1; b=2;	a=1; b=1	a<-1; b<-2
a + b	a + b or add(a,b)	a + b
a - b	a - b or subtract(a,b)	a - b
a * b	a * b or multiply(a,b)	a * b
a / b	a / b or divide(a,b)	a / b

a .^ b	a ** b
	power(a,b)
	pow(a,b)
		a ^ b

rem(a,b)	a % b
	remainder(a,b)
	fmod(a,b)
		a %% b

http://sebastianraschka.com/Articles/2014_matrix_cheatsheet_table.html

Building arrays/matrices

from numpy import *

1:10	arange(1,11, dtype=Float)	seq(10) or 1:10
	range(1,11)	
0:9	arange(10.)	seq(0,length=10)
1:3:10	arange(1,11,3)	seq(1,10,by=3)
10:-1:1	arange(10,0,-1)	seq(10,1) or 10:1
10:-3:1	arange(10,0,-3)	seq(from=10,to=1,by=-3)
linspace(1,10,7)	linspace(1,10,7)	seq(1,10,length=7)
reverse(a)	a[::-1] or	rev(a)
a(:) = 3	a.fill(3), a[:] = 3	

a=reshape(1:9, 3, 3)	a = reshape(arange(1,10),[3,3])
	a = arange(1,10).reshape(3,3)
		a=array(1:9, dim=c(3,3))

http://sebastianraschka.com/Articles/2014_matrix_cheatsheet_table.html

Indexing/slicing

a(2,3)	a[1,2]	a[2,3]
a(1,:)	a[0,]	a[1,]
a(:,1)	a[:,0]	a[,1]
a([1 3],[1 4]);	a.take([0,2]).take([0,3], axis=1)	
a(2:end,:)	a[1:,]	a[-1,]
a(end-1:end,:)	a[-2:,]	
a(1:2:end,:)	a[::2,:]	
	a[...,2]	
		a[-2,-3]
a(:,[1 3 4])	a.take([0,2,3],axis=1)	a[,-2]
	a.diagonal(offset=0)	

http://sebastianraschka.com/Articles/2014_matrix_cheatsheet_table.html

Searching arrays/matrices

C.E.C.I

find(a)	a.ravel().nonzero()	which(a != 0)
[i j] = find(a)	(i,j) = a.nonzero() (i,j) = where(a!=0)	which(a != 0, arr.ind=T)

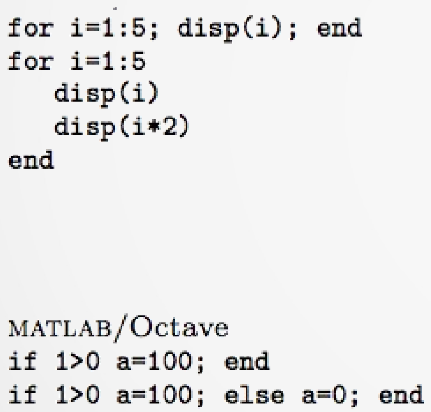
[i j v] = find(a)	v = a.compress((a!=0).flat)
	v = extract(a!=0,a)
		ij <- which(a != 0, arr.ind=T); v <- a[ij]

find(a>5.5)	(a>5.5).nonzero()	which(a>5.5)
	a.compress((a>5.5).flat)	ij <- which(a>5.5, arr.ind=T); v <- a[ij]

a .* (a>5.5)	where(a>5.5,0,a) or a * (a>5.5)
	a.put(2,indices)	

http://mathesaurus.sourceforge.net/matlab-python-xref.pdf

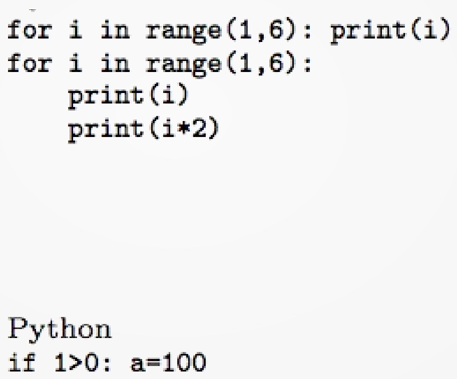
Control structures



```
for i=1:5; disp(i); end
for i=1:5
   disp(i)
   disp(i*2)
end
```

MATLAB/Octave

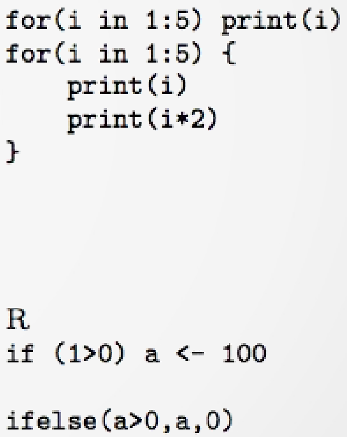
```
if 1>0 a=100; end
if 1>0 a=100; else a=0; end
```



```
for i in range(1,6): print(i)
for i in range(1,6):
    print(i)
    print(i*2)
```

Python

```
if 1>0: a=100
```



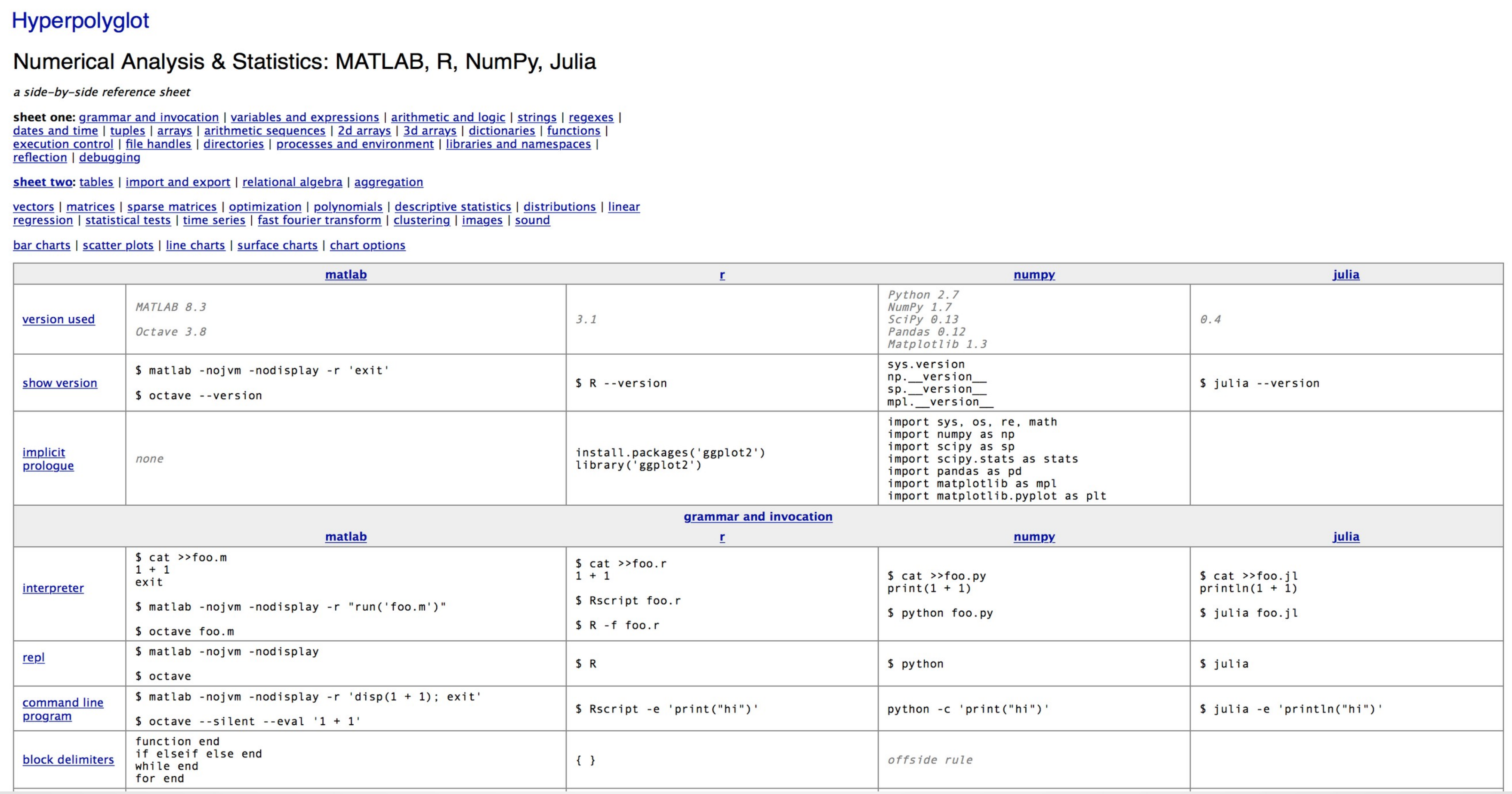
```
for(i in 1:5) print(i)
for(i in 1:5) {
    print(i)
    print(i*2)
}
```

R

```
if (1>0) a <- 100

ifelse(a>0,a,0)
```

http://mathesaurus.sourceforge.net/matlab-python-xref.pdf

More complete list



Hyperpolyglot

Numerical Analysis & Statistics: MATLAB, R, NumPy, Julia

a side-by-side reference sheet

sheet one: grammar and invocation | variables and expressions | arithmetic and logic | strings | regexes | dates and time | tuples | arrays | arithmetic sequences | 2d arrays | 3d arrays | dictionaries | functions | execution control | file handles | directories | processes and environment | libraries and namespaces | reflection | debugging

sheet two: tables | import and export | relational algebra | aggregation

vectors | matrices | sparse matrices | optimization | polynomials | descriptive statistics | distributions | linear regression | statistical tests | time series | fast fourier transform | clustering | images | sound

bar charts | scatter plots | line charts | surface charts | chart options

	matlab	r	numpy	julia
version used	*MATLAB 8.3* *Octave 3.8*	*3.1*	*Python 2.7* *NumPy 1.7* *SciPy 0.13* *Pandas 0.12* *Matplotlib 1.3*	*0.4*

show version	`$ matlab -nojvm -nodisplay -r 'exit'`
	`$ octave --version`
		`$ R --version`	`sys.version`
			`np.__version__`
			`sp.__version__`
			`mpl.__version__`
				`$ julia --version`

implicit prologue	*none*	`install.packages('ggplot2')`
		`library('ggplot2')`
			`import sys, os, re, math`
			`import numpy as np`
			`import scipy as sp`
			`import scipy.stats as stats`
			`import pandas as pd`
			`import matplotlib as mpl`
			`import matplotlib.pyplot as plt`	

grammar and invocation				
	matlab	r	numpy	julia

interpreter	`$ cat >>foo.m`
	`1 + 1`
	`exit`
	`$ matlab -nojvm -nodisplay -r "run('foo.m')"`
	`$ octave foo.m`
		`$ cat >>foo.r`
		`1 + 1`
		`$ Rscript foo.r`
		`$ R -f foo.r`
			`$ cat >>foo.py`
			`print(1 + 1)`
			`$ python foo.py`
				`$ cat >>foo.jl`
				`println(1 + 1)`
				`$ julia foo.jl`

repl	`$ matlab -nojvm -nodisplay`
	`$ octave`
		`$ R`	`$ python`	`$ julia`

command line program	`$ matlab -nojvm -nodisplay -r 'disp(1 + 1); exit'`
	`$ octave --silent --eval '1 + 1'`
		`$ Rscript -e 'print("hi")'`	`python -c 'print("hi")'`	`$ julia -e 'println("hi")'`

block delimiters	`function end`
	`if elseif else end`
	`while end`
	`for end`
		`{ }`	*offside rule*	

http://hyperpolyglot.org/numerical-analysis

3.

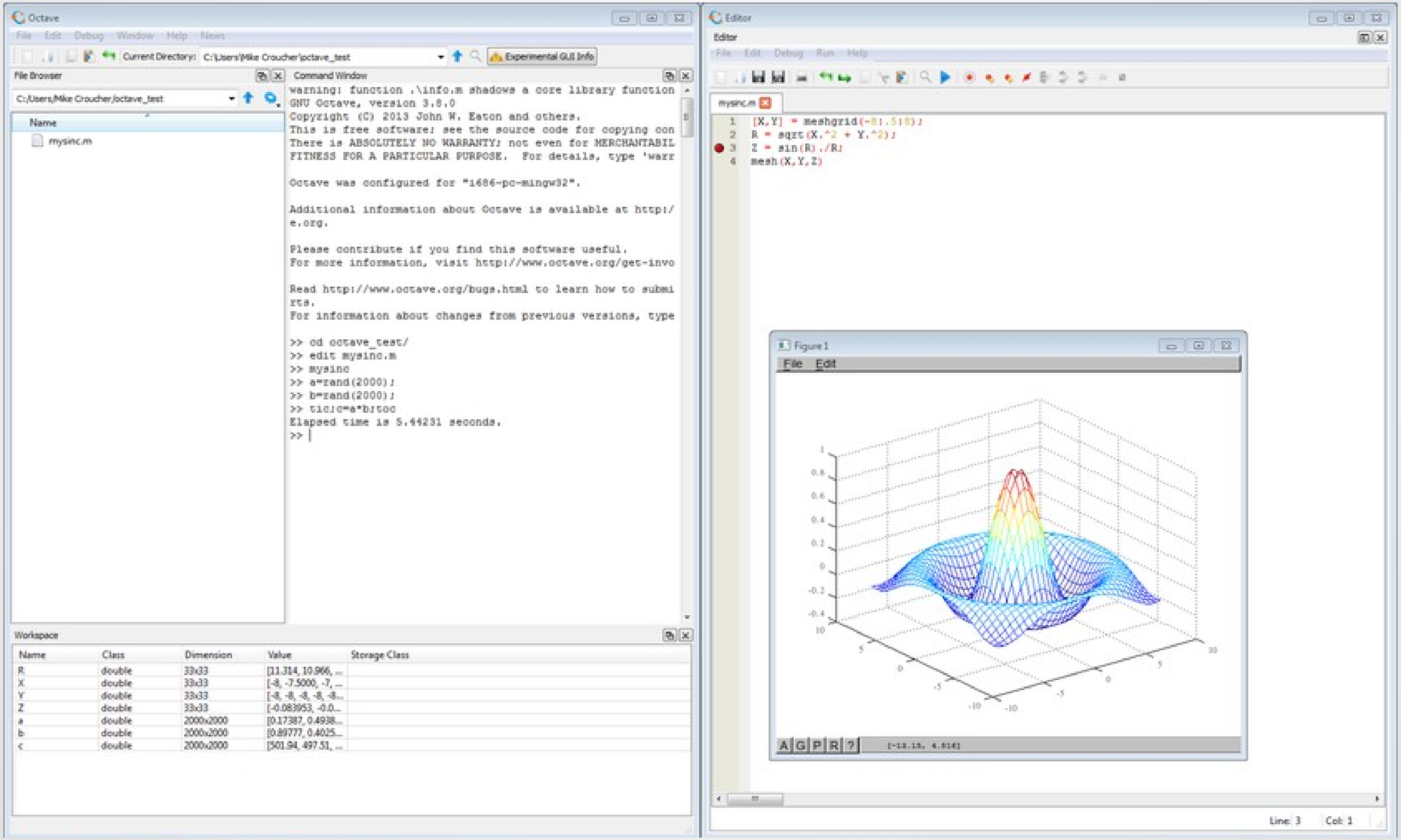
Graphical User Interfaces

Editing, debugging, accessing the doc, made easy

Literate programming

Authoring dynamic documents with code in them

Octave



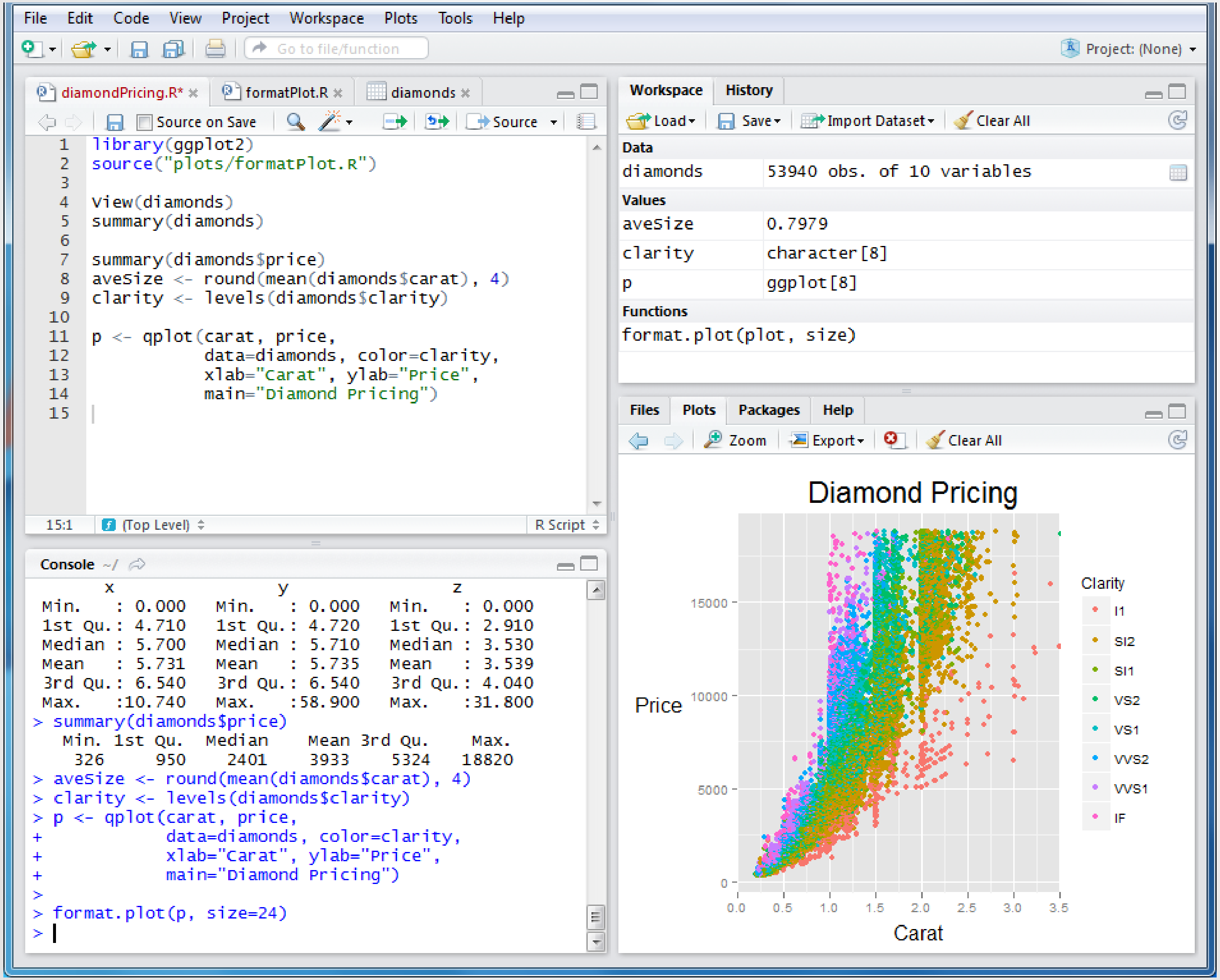
```
warning: function .\info.m shadows a core library function
GNU Octave, version 3.8.0
Copyright (C) 2013 John W. Eaton and others.
This is free software; see the source code for copying con
There is ABSOLUTELY NO WARRANTY; not even for MERCHANTABIL
FITNESS FOR A PARTICULAR PURPOSE.  For details, type 'warr

Octave was configured for "i686-pc-mingw32".

Additional information about Octave is available at http:/
e.org.

Please contribute if you find this software useful.
For more information, visit http://www.octave.org/get-invo

Read http://www.octave.org/bugs.html to learn how to submi
rts.
For information about changes from previous versions, type

>> cd octave_test/
>> edit mysinc.m
>> mysinc
>> a=rand(2000);
>> b=rand(2000);
>> tic;c=a*b;toc
Elapsed time is 5.44231 seconds.
>> 
```

Workspace

Name	Class	Dimension	Value	Storage Class
R	double	33x33	[11.314, 10.966, ...	
X	double	33x33	[-8, -7.5000, -7, ...	
Y	double	33x33	[-8, -8, -8, -8, -8...	
Z	double	33x33	[-0.083953, -0.0...	
a	double	2000x2000	[0.17387, 0.4938...	
b	double	2000x2000	[0.89777, 0.4025...	
c	double	2000x2000	[501.94, 497.51, ...	

```
[X,Y] = meshgrid(-8:.5:8);
R = sqrt(X.^2 + Y.^2);
Z = sin(R)./R;
mesh(X,Y,Z)
```

Rstudio

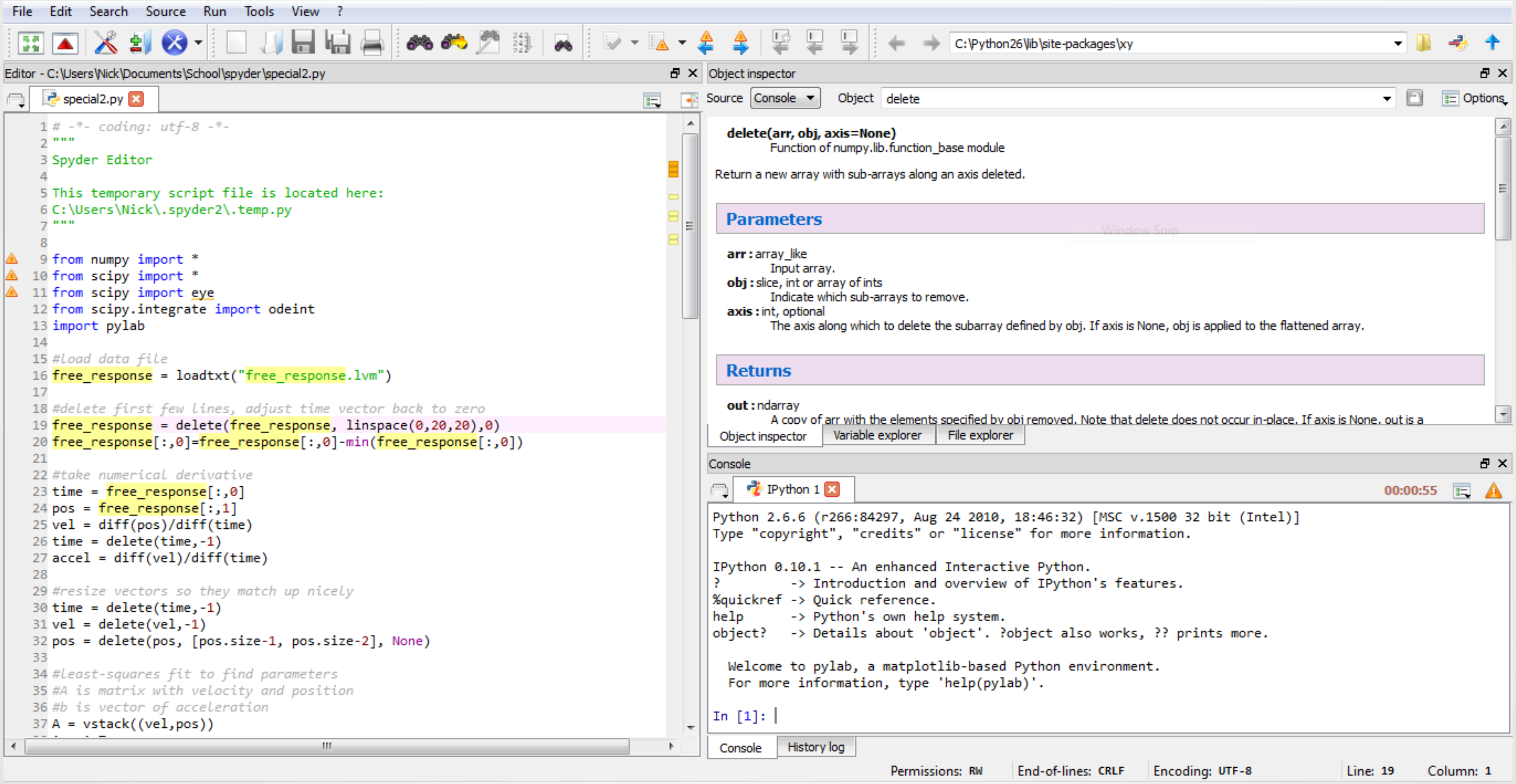


```
library(ggplot2)
source("plots/formatPlot.R")

View(diamonds)
summary(diamonds)

summary(diamonds$price)
aveSize <- round(mean(diamonds$carat), 4)
clarity <- levels(diamonds$clarity)

p <- qplot(carat, price,
           data=diamonds, color=clarity,
           xlab="Carat", ylab="Price",
           main="Diamond Pricing")
```

Data	
diamonds	53940 obs. of 10 variables
Values	
aveSize	0.7979
clarity	character[8]
p	ggplot[8]
Functions	
format.plot(plot, size)	

```
        x                y                z        
 Min.   : 0.000   Min.   : 0.000   Min.   : 0.000  
 1st Qu.: 4.710   1st Qu.: 4.720   1st Qu.: 2.910  
 Median : 5.700   Median : 5.710   Median : 3.530  
 Mean   : 5.731   Mean   : 5.735   Mean   : 3.539  
 3rd Qu.: 6.540   3rd Qu.: 6.540   3rd Qu.: 4.040  
 Max.   :10.740   Max.   :58.900   Max.   :31.800  
> summary(diamonds$price)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max. 
    326     950    2401    3933    5324   18820 
> aveSize <- round(mean(diamonds$carat), 4)
> clarity <- levels(diamonds$clarity)
> p <- qplot(carat, price,
+            data=diamonds, color=clarity,
+            xlab="Carat", ylab="Price",
+            main="Diamond Pricing")
>
> format.plot(p, size=24)
> 
```

Spyder



```python
# -*- coding: utf-8 -*-
"""
Spyder Editor

This temporary script file is located here:
C:\Users\Nick\.spyder2\.temp.py
"""

from numpy import *
from scipy import *
from scipy import eye
from scipy.integrate import odeint
import pylab

#load data file
free_response = loadtxt("free_response.lvm")

#delete first few lines, adjust time vector back to zero
free_response = delete(free_response, linspace(0,20,20),0)
free_response[:,0]=free_response[:,0]-min(free_response[:,0])

#take numerical derivative
time = free_response[:,0]
pos = free_response[:,1]
vel = diff(pos)/diff(time)
time = delete(time,-1)
accel = diff(vel)/diff(time)

#resize vectors so they match up nicely
time = delete(time,-1)
vel = delete(vel,-1)
pos = delete(pos, [pos.size-1, pos.size-2], None)

#least-squares fit to find parameters
#A is matrix with velocity and position
#b is vector of acceleration
A = vstack((vel,pos))
```

delete(arr, obj, axis=None)
Function of numpy.lib.function_base module

Return a new array with sub-arrays along an axis deleted.

Parameters

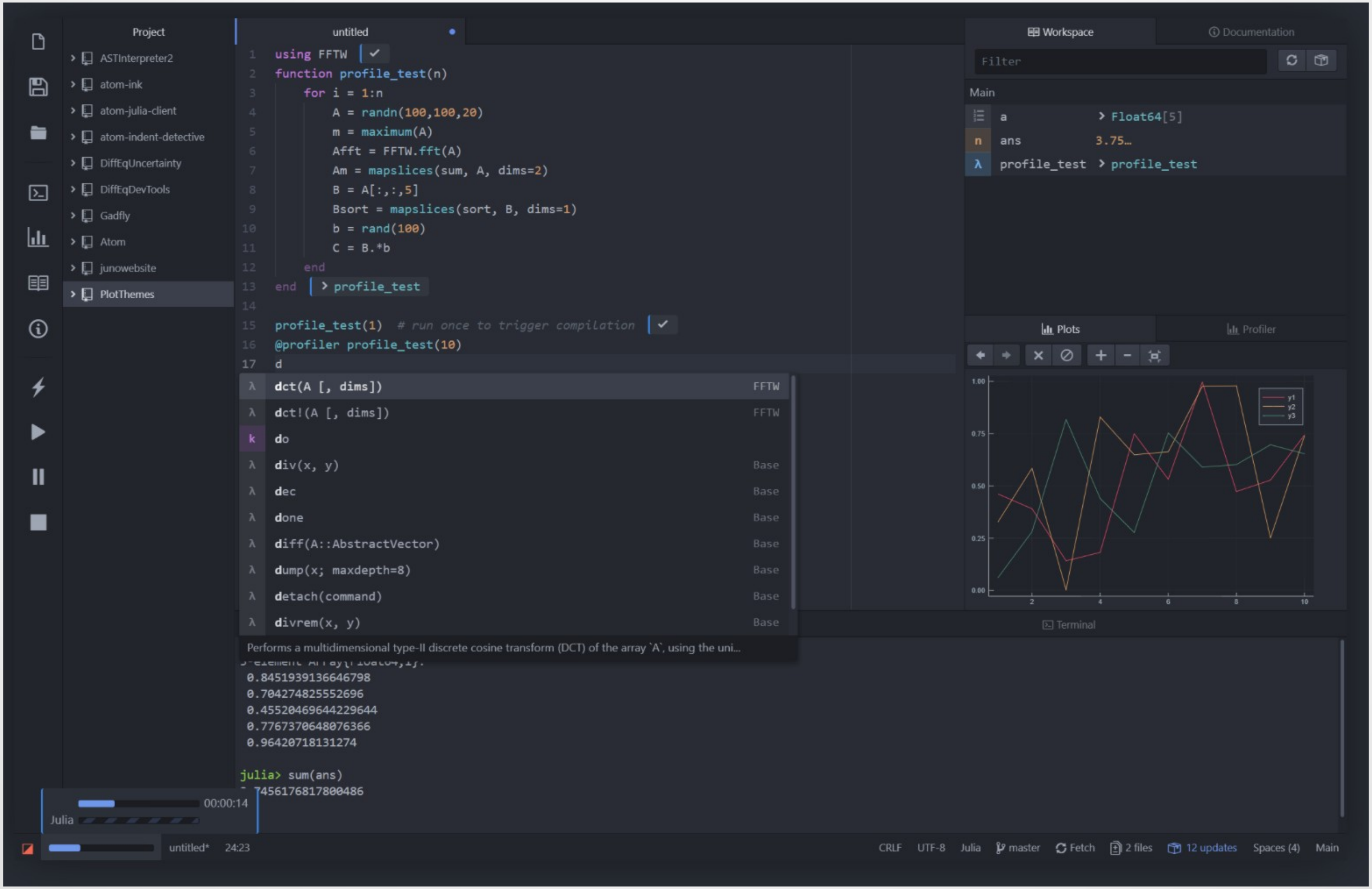
arr : array_like
Input array.
obj : slice, int or array of ints
Indicate which sub-arrays to remove.
axis : int, optional
The axis along which to delete the subarray defined by obj. If axis is None, obj is applied to the flattened array.

Returns

out : ndarray
A copy of arr with the elements specified by obj removed. Note that delete does not occur in-place. If axis is None, out is a

```
Python 2.6.6 (r266:84297, Aug 24 2010, 18:46:32) [MSC v.1500 32 bit (Intel)]
Type "copyright", "credits" or "license" for more information.

IPython 0.10.1 -- An enhanced Interactive Python.
?         -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help      -> Python's own help system.
object?   -> Details about 'object'. ?object also works, ?? prints more.

  Welcome to pylab, a matplotlib-based Python environment.
  For more information, type 'help(pylab)'.

In [1]: |
```

Juno



```
using FFTW ✓
function profile_test(n)
    for i = 1:n
        A = randn(100,100,20)
        m = maximum(A)
        Afft = FFTW.fft(A)
        Am = mapslices(sum, A, dims=2)
        B = A[:,:,5]
        Bsort = mapslices(sort, B, dims=1)
        b = rand(100)
        C = B.*b
    end
end  > profile_test

profile_test(1)  # run once to trigger compilation  ✓
@profiler profile_test(10)
d
```

```
λ  dct(A [, dims])              FFTW
λ  dct!(A [, dims])             FFTW
k  do
λ  div(x, y)                    Base
λ  dec                          Base
λ  done                         Base
λ  diff(A::AbstractVector)      Base
λ  dump(x; maxdepth=8)          Base
λ  detach(command)              Base
λ  divrem(x, y)                 Base
```

Performs a multidimensional type-II discrete cosine transform (DCT) of the array `A`, using the uni...

```
a             > Float64[5]
ans           3.75…
profile_test  > profile_test
```

```
5-element Array{Float64,1}:
 0.8451939136646798
 0.704274825552696
 0.45520469644229644
 0.7767370648076366
 0.96420718131274

julia> sum(ans)
 745617681780486
```

3.

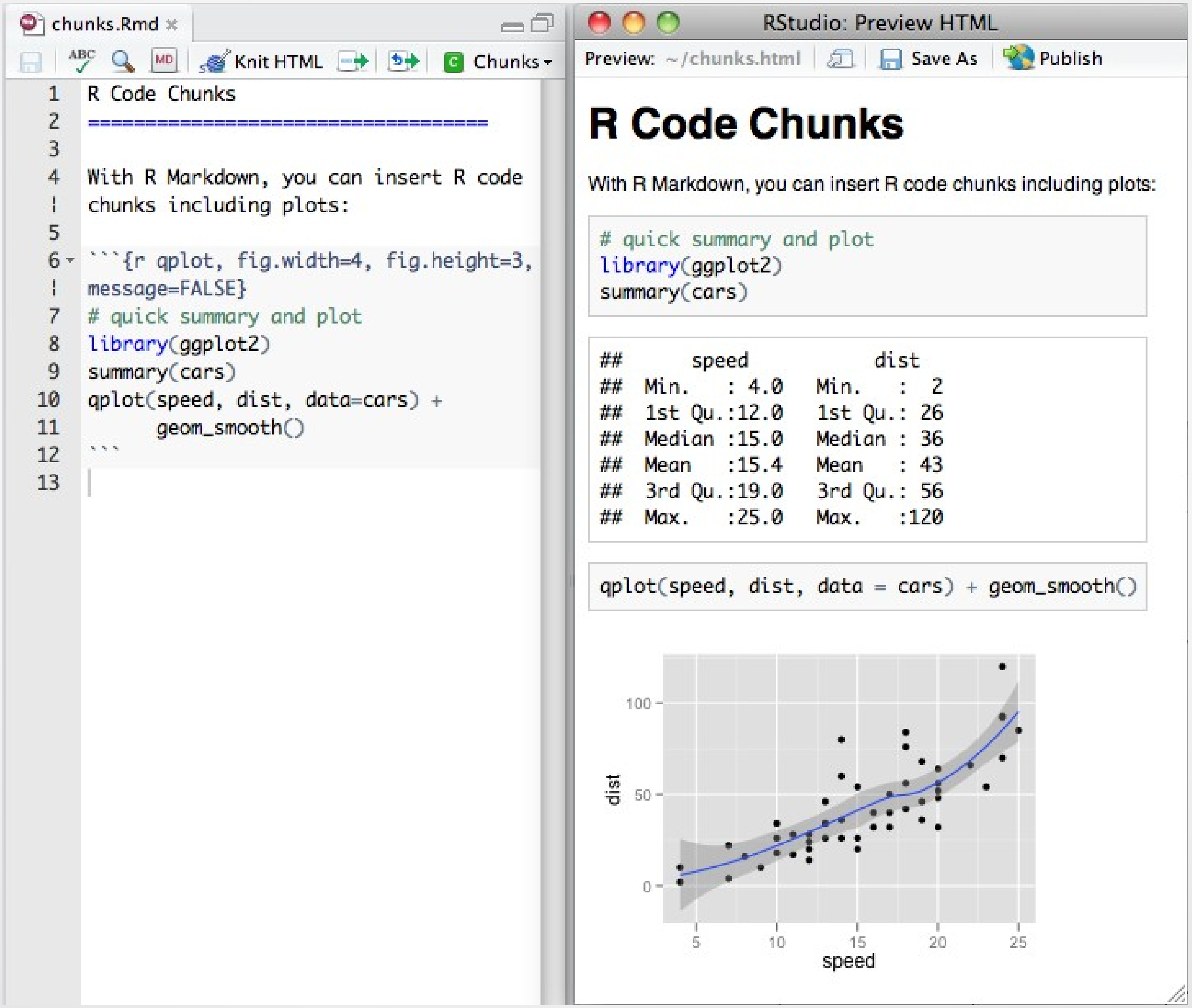
Graphical User Interfaces

Editing, debugging, accessing the doc, made easy

Literate programming

Authoring HTML or LaTeX documents
with code and results in them

RMarkdown and KnitR



~~~
R Code Chunks
====================================

With R Markdown, you can insert R code
chunks including plots:

```{r qplot, fig.width=4, fig.height=3,
message=FALSE}
# quick summary and plot
library(ggplot2)
summary(cars)
qplot(speed, dist, data=cars) +
      geom_smooth()
```

~~~

R Code Chunks

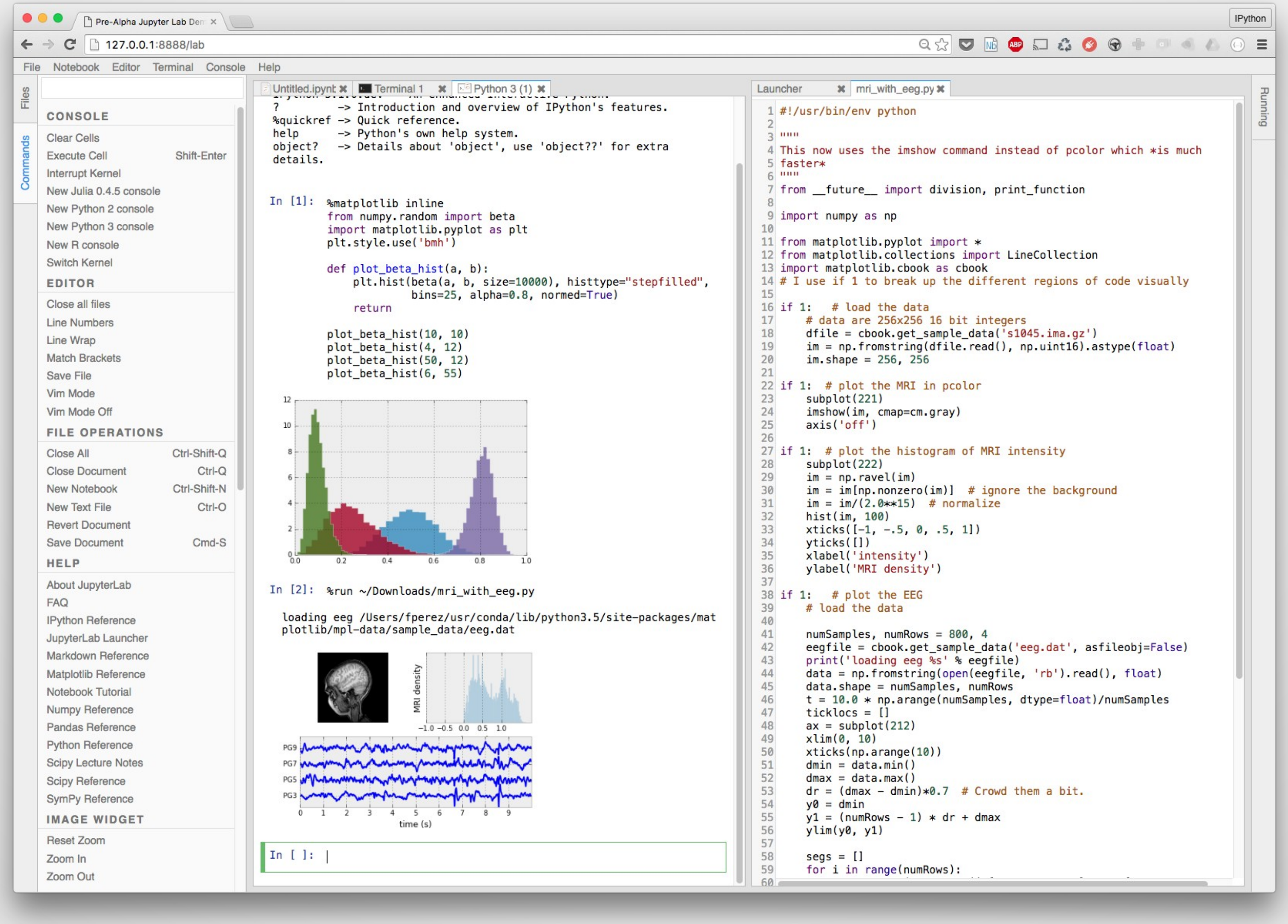
With R Markdown, you can insert R code chunks including plots:

```
# quick summary and plot
library(ggplot2)
summary(cars)
```

```
##      speed           dist    
##  Min.   : 4.0   Min.   :  2  
##  1st Qu.:12.0   1st Qu.: 26  
##  Median :15.0   Median : 36  
##  Mean   :15.4   Mean   : 43  
##  3rd Qu.:19.0   3rd Qu.: 56  
##  Max.   :25.0   Max.   :120  
```

```
qplot(speed, dist, data = cars) + geom_smooth()
```

Jupyter notebooks



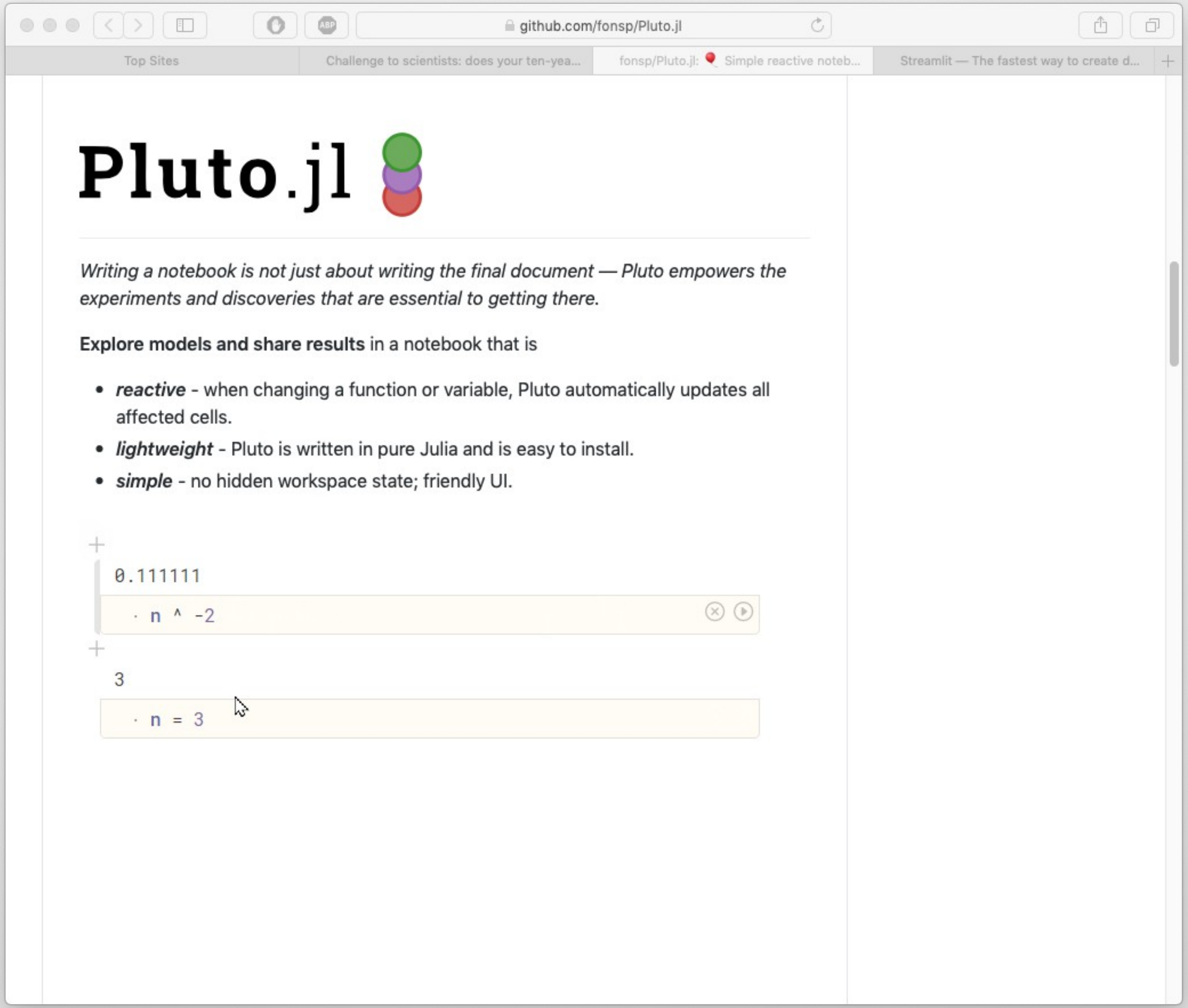
```
?         -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help      -> Python's own help system.
object?   -> Details about 'object', use 'object??' for extra
details.


In [1]:  %matplotlib inline
         from numpy.random import beta
         import matplotlib.pyplot as plt
         plt.style.use('bmh')

         def plot_beta_hist(a, b):
             plt.hist(beta(a, b, size=10000), histtype="stepfilled",
                      bins=25, alpha=0.8, normed=True)
             return

         plot_beta_hist(10, 10)
         plot_beta_hist(4, 12)
         plot_beta_hist(50, 12)
         plot_beta_hist(6, 55)
```

```
In [2]:  %run ~/Downloads/mri_with_eeg.py

 loading eeg /Users/fperez/usr/conda/lib/python3.5/site-packages/mat
 plotlib/mpl-data/sample_data/eeg.dat
```

```
In [ ]:
```

```
#!/usr/bin/env python

"""
This now uses the imshow command instead of pcolor which *is much
faster*
"""
from __future__ import division, print_function

import numpy as np

from matplotlib.pyplot import *
from matplotlib.collections import LineCollection
import matplotlib.cbook as cbook
# I use if 1 to break up the different regions of code visually

if 1:   # load the data
    # data are 256x256 16 bit integers
    dfile = cbook.get_sample_data('s1045.ima.gz')
    im = np.fromstring(dfile.read(), np.uint16).astype(float)
    im.shape = 256, 256

if 1:  # plot the MRI in pcolor
    subplot(221)
    imshow(im, cmap=cm.gray)
    axis('off')

if 1:  # plot the histogram of MRI intensity
    subplot(222)
    im = np.ravel(im)
    im = im[np.nonzero(im)]  # ignore the background
    im = im/(2.0**15)  # normalize
    hist(im, 100)
    xticks([-1, -.5, 0, .5, 1])
    yticks([])
    xlabel('intensity')
    ylabel('MRI density')

if 1:   # plot the EEG
    # load the data

    numSamples, numRows = 800, 4
    eegfile = cbook.get_sample_data('eeg.dat', asfileobj=False)
    print('loading eeg %s' % eegfile)
    data = np.fromstring(open(eegfile, 'rb').read(), float)
    data.shape = numSamples, numRows
    t = 10.0 * np.arange(numSamples, dtype=float)/numSamples
    ticklocs = []
    ax = subplot(212)
    xlim(0, 10)
    xticks(np.arange(10))
    dmin = data.min()
    dmax = data.max()
    dr = (dmax - dmin)*0.7  # Crowd them a bit.
    y0 = dmin
    y1 = (numRows - 1) * dr + dmax
    ylim(y0, y1)

    segs = []
    for i in range(numRows):
```

Julia notebooks



github.com/fonsp/Pluto.jl
Top Sites
Challenge to scientists: does your ten-yea...
fonsp/Pluto.jl: 🎈 Simple reactive noteb...
Streamlit — The fastest way to create d...

Pluto.jl

Writing a notebook is not just about writing the final document — Pluto empowers the experiments and discoveries that are essential to getting there.

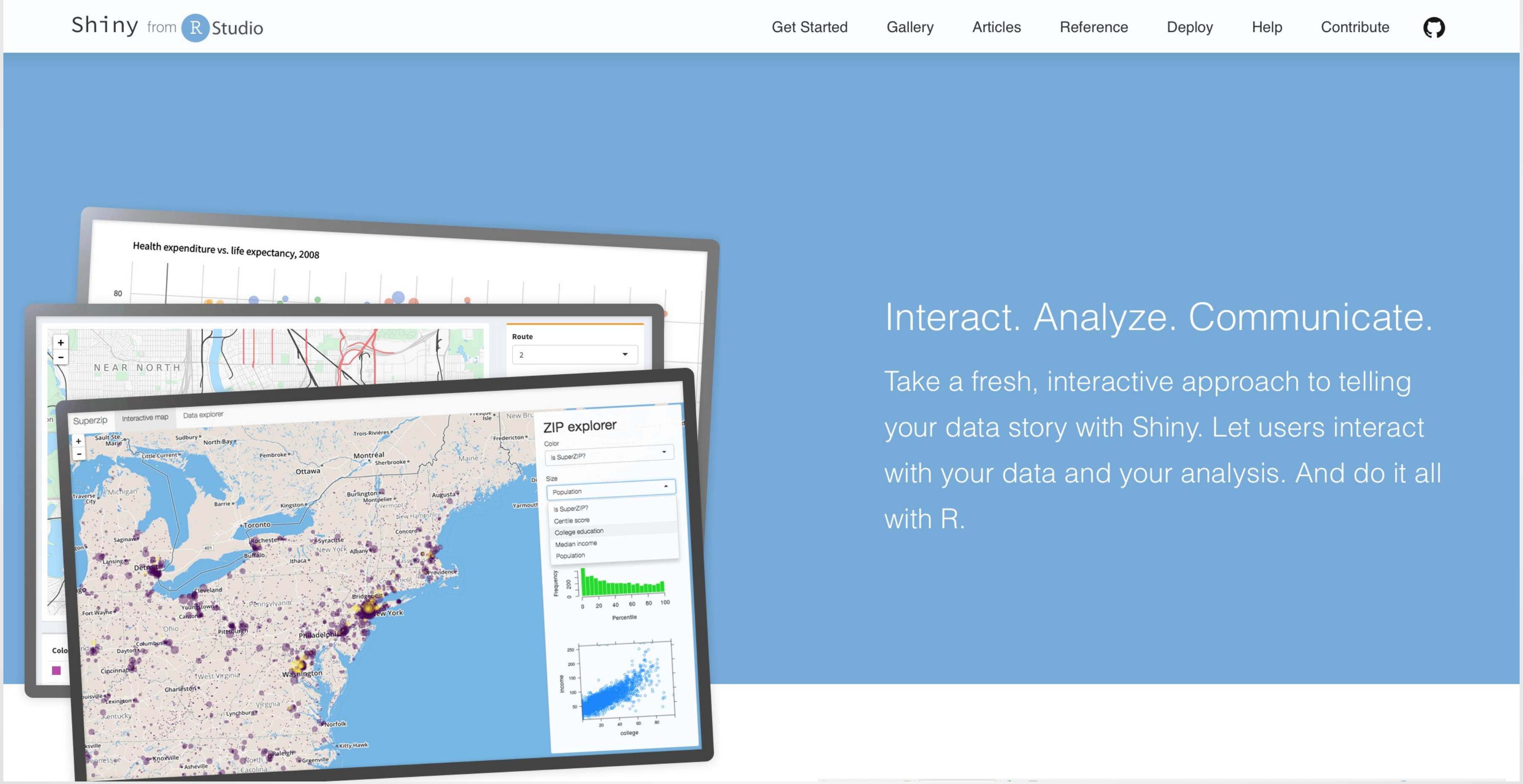
Explore models and share results in a notebook that is

- ***reactive*** - when changing a function or variable, Pluto automatically updates all affected cells.
- ***lightweight*** - Pluto is written in pure Julia and is easy to install.
- ***simple*** - no hidden workspace state; friendly UI.

```
0.111111
n ^ -2
```

```
3
n = 3
```

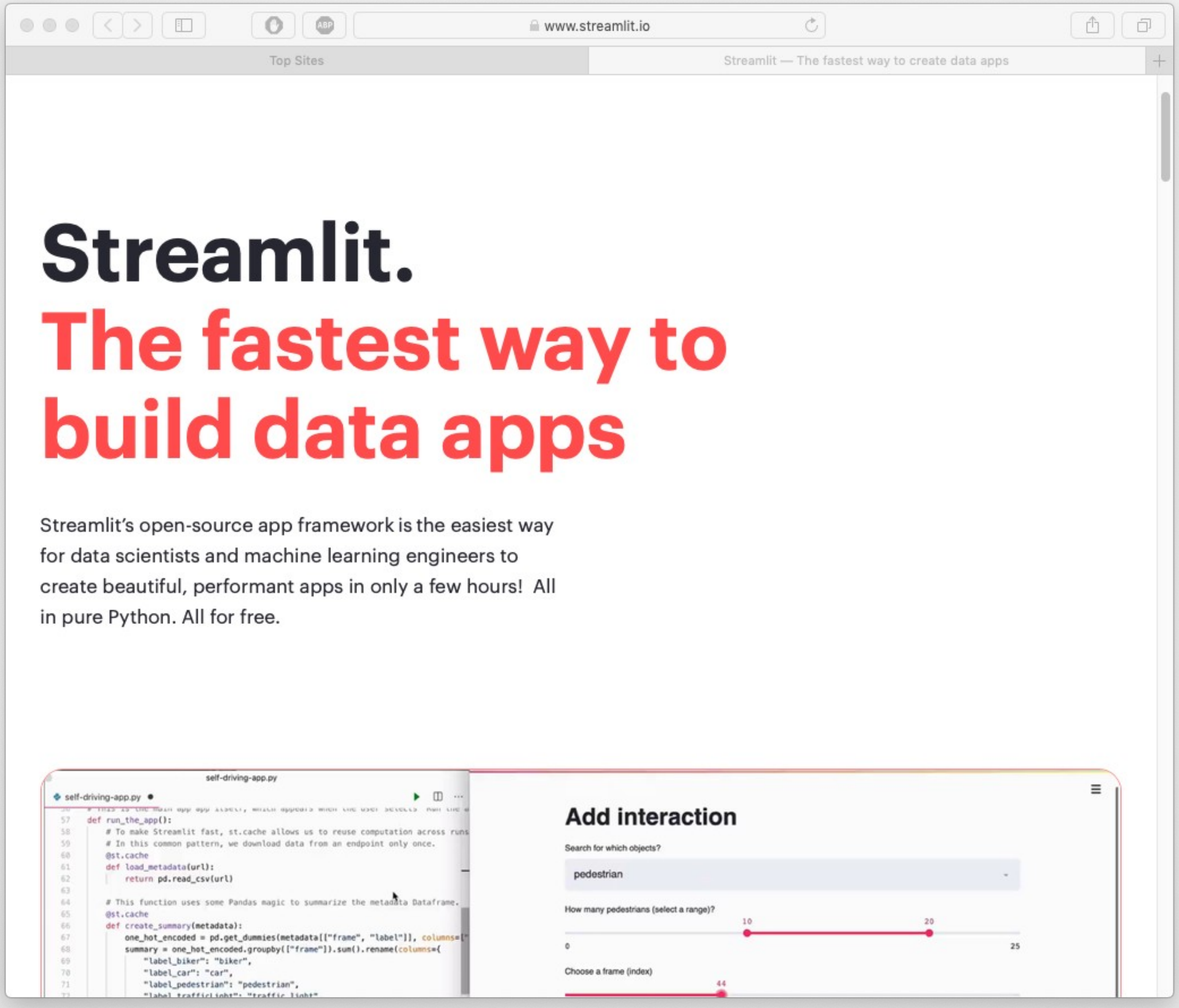
Shiny



Interact. Analyze. Communicate.

Take a fresh, interactive approach to telling your data story with Shiny. Let users interact with your data and your analysis. And do it all with R.

Streamlit



Streamlit.

The fastest way to build data apps

Streamlit's open-source app framework is the easiest way for data scientists and machine learning engineers to create beautiful, performant apps in only a few hours! All in pure Python. All for free.

```
def run_the_app():
    # To make Streamlit fast, st.cache allows us to reuse computation across runs
    # In this common pattern, we download data from an endpoint only once.
    @st.cache
    def load_metadata(url):
        return pd.read_csv(url)

    # This function uses some Pandas magic to summarize the metadata Dataframe.
    @st.cache
    def create_summary(metadata):
        one_hot_encoded = pd.get_dummies(metadata[["frame", "label"]], columns=["
        summary = one_hot_encoded.groupby(["frame"]).sum().rename(columns={
            "label_biker": "biker",
            "label_car": "car",
            "label_pedestrian": "pedestrian",
```

Add interaction

Search for which objects?

pedestrian

How many pedestrians (select a range)?

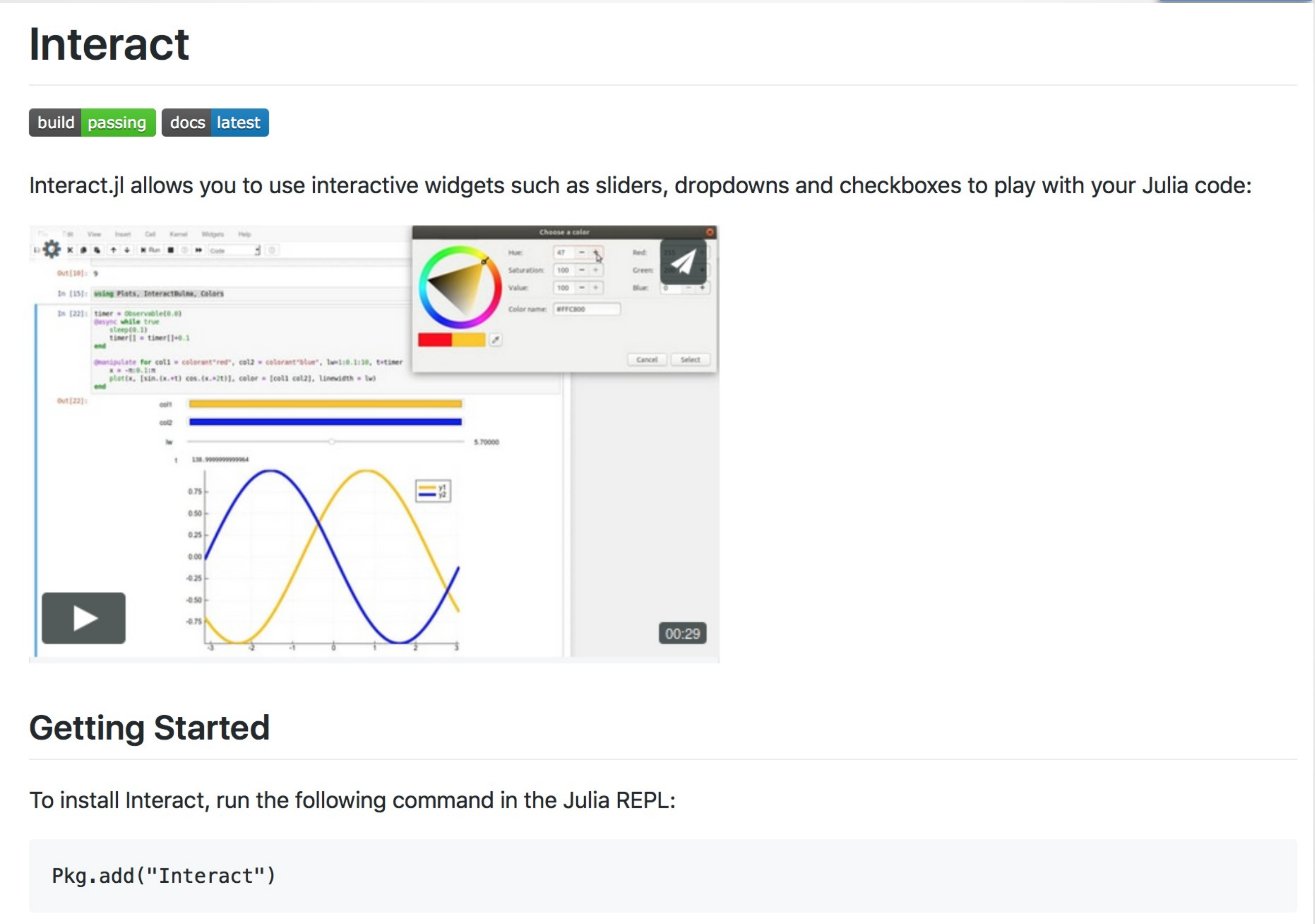
10 20

0 25

Choose a frame (index)

44

Interact.jl



Interact

Interact.jl allows you to use interactive widgets such as sliders, dropdowns and checkboxes to play with your Julia code:

```
Out[10]: 9

In [15]: using Plots, InteractBulma, Colors

In [22]: timer = Observable(0.0)
         @async while true
             sleep(0.1)
             timer[] = timer[]+0.1
         end

         @manipulate for col1 = colorant"red", col2 = colorant"blue", lw=1:0.1:10, t=timer
             x = -π:0.1:π
             plot(x, [sin.(x.+t) cos.(x.+2t)], color = [col1 col2], linewidth = lw)
         end

Out[22]:
```

Hue: 47
Saturation: 100
Value: 100
Color name: #FFC800

Getting Started

To install Interact, run the following command in the Julia REPL:

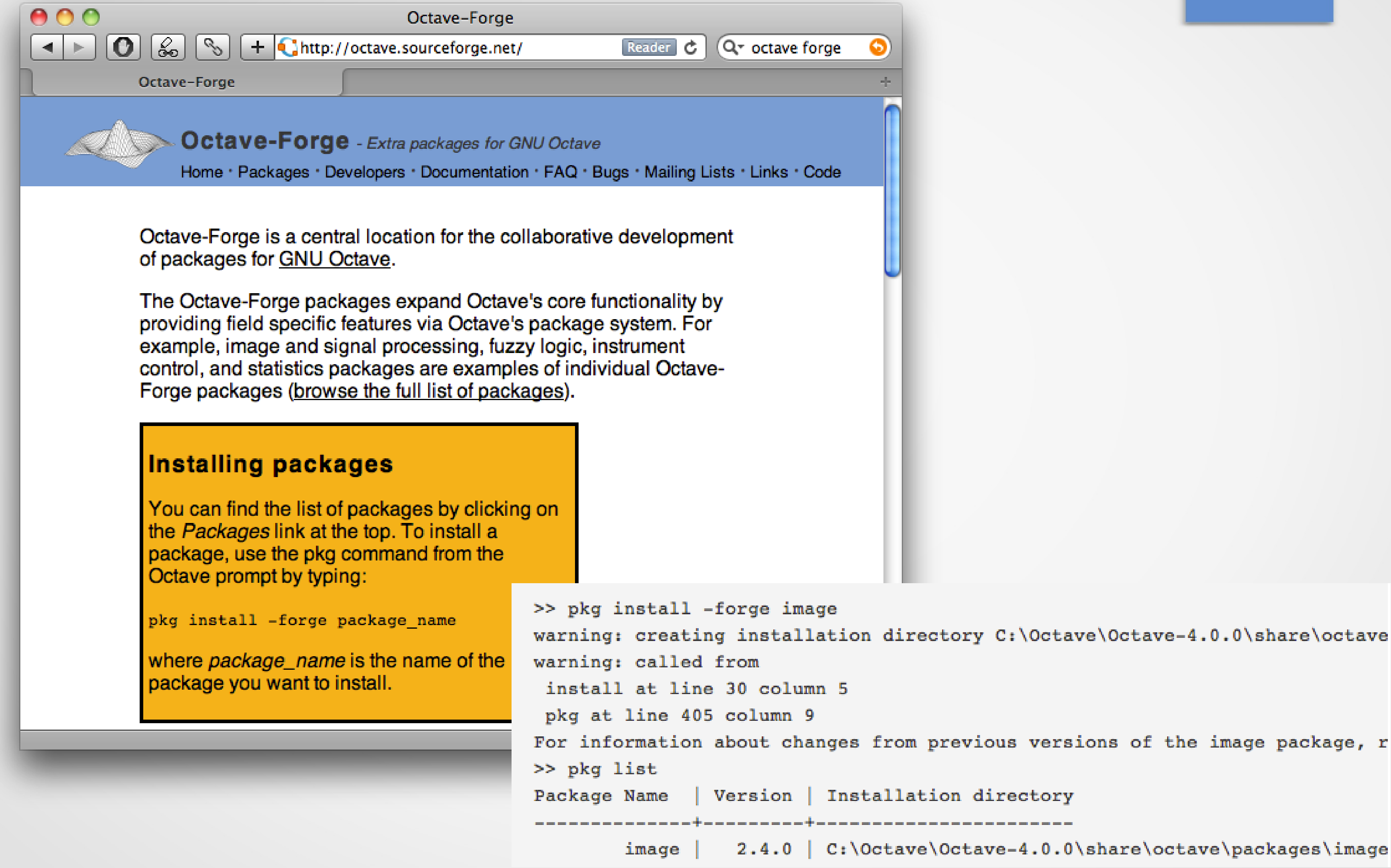
```
Pkg.add("Interact")
```

4.

Extensions

Packages – Libraries – Modules

Octave Forge



Octave-Forge - *Extra packages for GNU Octave*

Home · Packages · Developers · Documentation · FAQ · Bugs · Mailing Lists · Links · Code

Octave-Forge is a central location for the collaborative development of packages for GNU Octave.

The Octave-Forge packages expand Octave's core functionality by providing field specific features via Octave's package system. For example, image and signal processing, fuzzy logic, instrument control, and statistics packages are examples of individual Octave-Forge packages (browse the full list of packages).

Installing packages

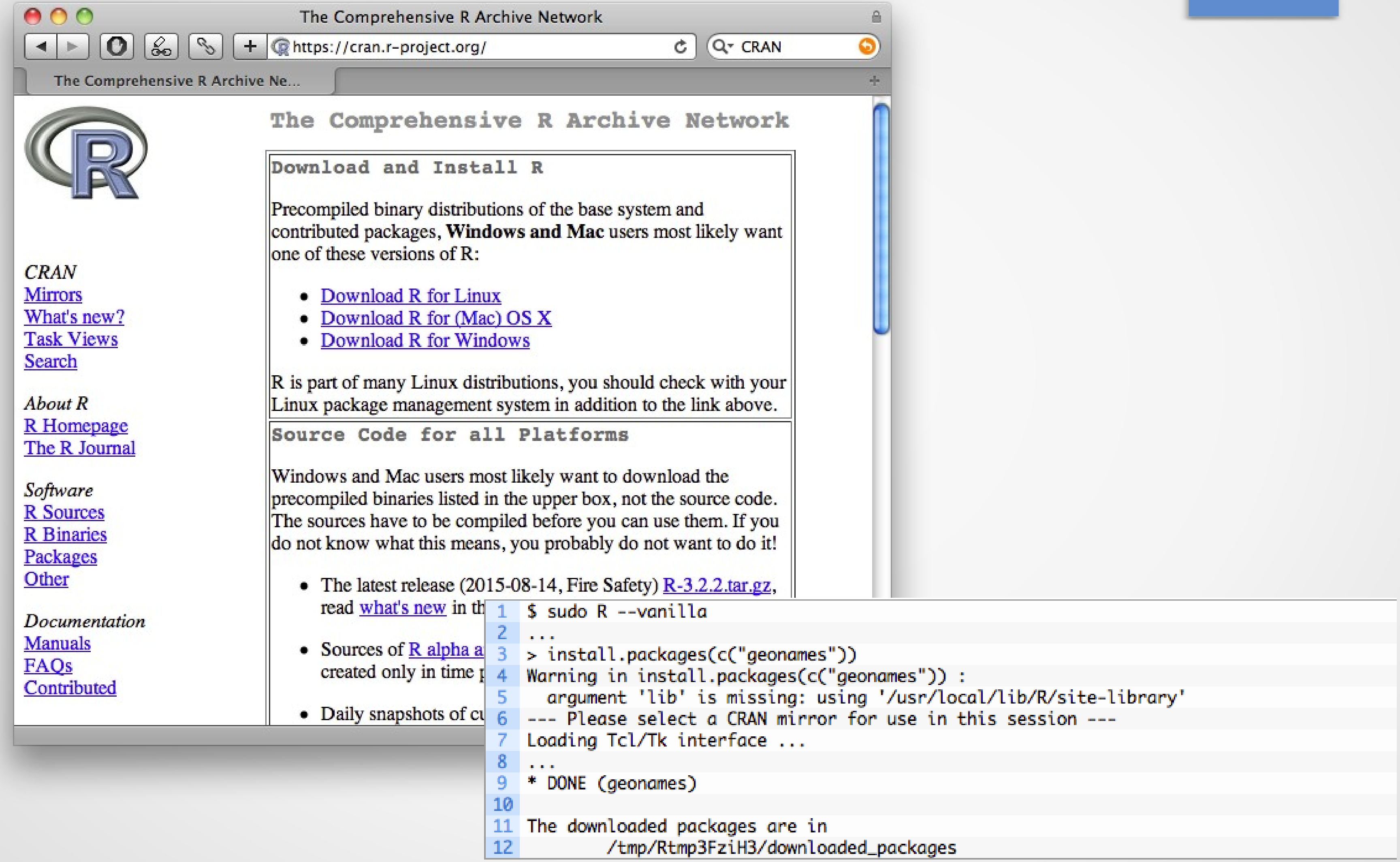
You can find the list of packages by clicking on the *Packages* link at the top. To install a package, use the pkg command from the Octave prompt by typing:

```
pkg install -forge package_name
```

where *package_name* is the name of the package you want to install.

```
>> pkg install -forge image
warning: creating installation directory C:\Octave\Octave-4.0.0\share\octave
warning: called from
 install at line 30 column 5
 pkg at line 405 column 9
For information about changes from previous versions of the image package, r
>> pkg list
Package Name  | Version | Installation directory
--------------+---------+-----------------------
        image |   2.4.0 | C:\Octave\Octave-4.0.0\share\octave\packages\image
```

CRAN



The Comprehensive R Archive Network

https://cran.r-project.org/

The Comprehensive R Archive Network

CRAN
Mirrors
What's new?
Task Views
Search

About R
R Homepage
The R Journal

Software
R Sources
R Binaries
Packages
Other

Documentation
Manuals
FAQs
Contributed

Download and Install R

Precompiled binary distributions of the base system and contributed packages, **Windows and Mac** users most likely want one of these versions of R:

- Download R for Linux
- Download R for (Mac) OS X
- Download R for Windows

R is part of many Linux distributions, you should check with your Linux package management system in addition to the link above.

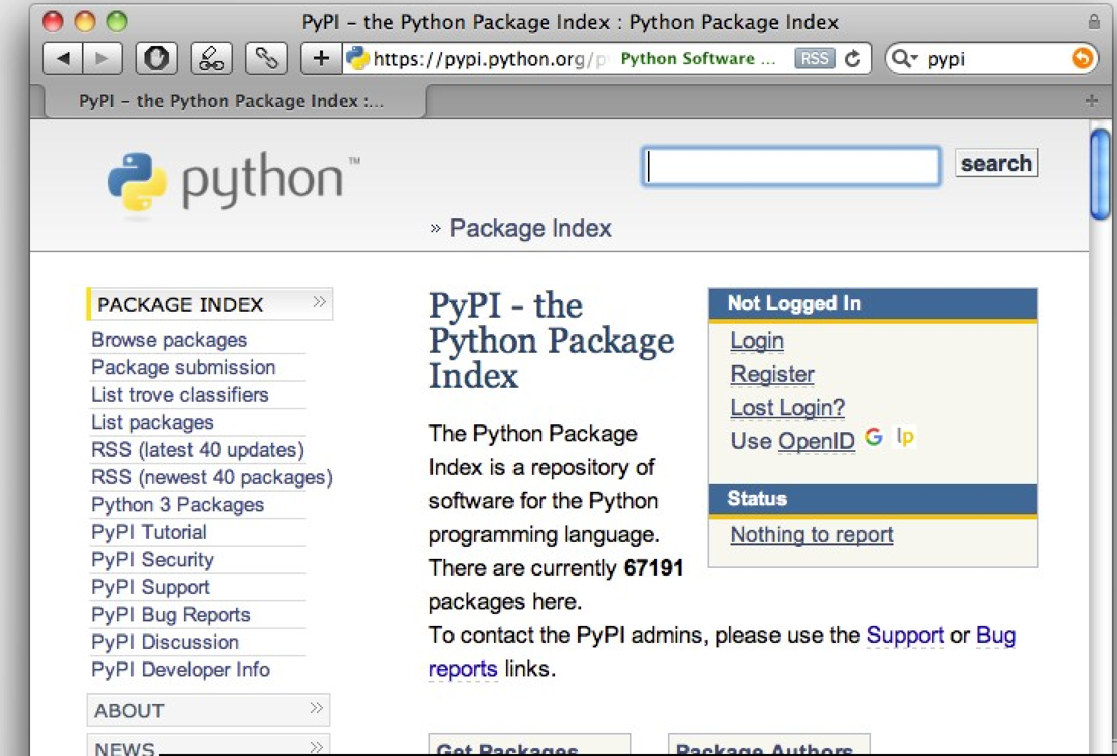
Source Code for all Platforms

Windows and Mac users most likely want to download the precompiled binaries listed in the upper box, not the source code. The sources have to be compiled before you can use them. If you do not know what this means, you probably do not want to do it!

- The latest release (2015-08-14, Fire Safety) R-3.2.2.tar.gz, read what's new in th
- Sources of R alpha a created only in time f
- Daily snapshots of cu

```
$ sudo R --vanilla
...
> install.packages(c("geonames"))
Warning in install.packages(c("geonames")) :
  argument 'lib' is missing: using '/usr/local/lib/R/site-library'
--- Please select a CRAN mirror for use in this session ---
Loading Tcl/Tk interface ...
...
* DONE (geonames)

The downloaded packages are in
        /tmp/Rtmp3FziH3/downloaded_packages
```

PyPI



PyPI - the Python Package Index : Python Package Index

https://pypi.python.org/p

» Package Index

PACKAGE INDEX
- Browse packages
- Package submission
- List trove classifiers
- List packages
- RSS (latest 40 updates)
- RSS (newest 40 packages)
- Python 3 Packages
- PyPI Tutorial
- PyPI Security
- PyPI Support
- PyPI Bug Reports
- PyPI Discussion
- PyPI Developer Info

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COMM

PyPI - the Python Package Index

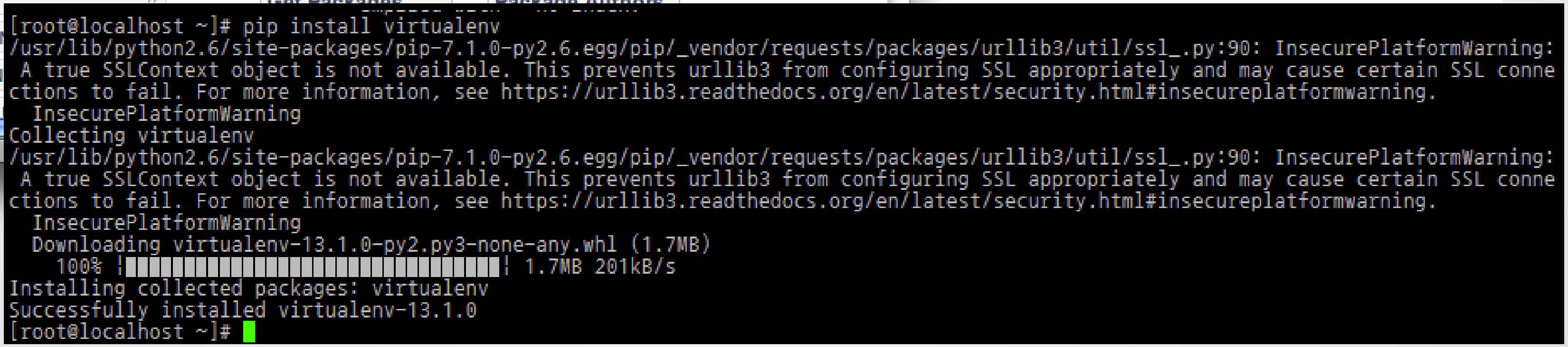
The Python Package Index is a repository of software for the Python programming language. There are currently **67191** packages here.

To contact the PyPI admins, please use the Support or Bug reports links.

Not Logged In
- Login
- Register
- Lost Login?
- Use OpenID

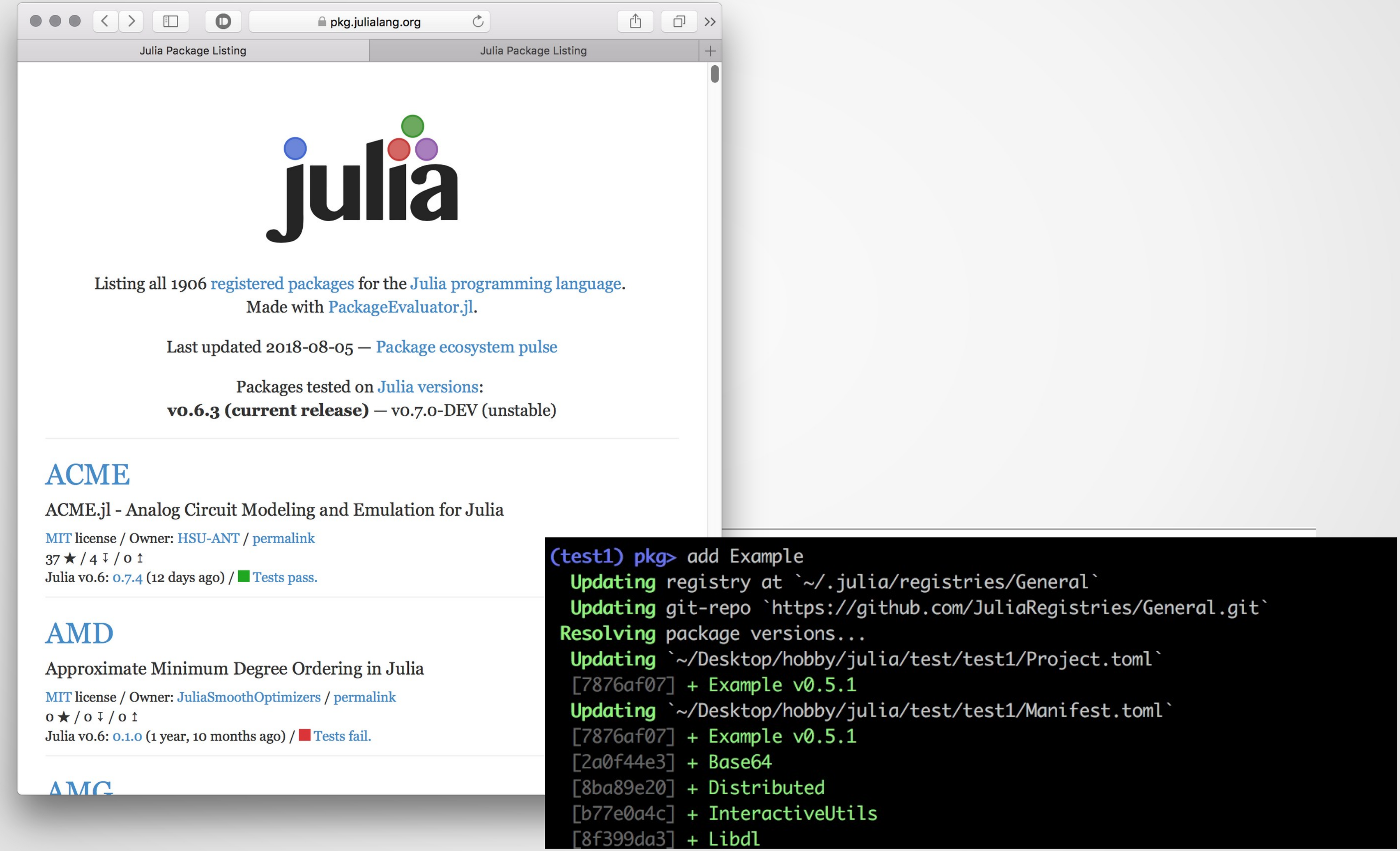
Status
- Nothing to report

Get Packages   Package Authors



```
[root@localhost ~]# pip install virtualenv
/usr/lib/python2.6/site-packages/pip-7.1.0-py2.6.egg/pip/_vendor/requests/packages/urllib3/util/ssl_.py:90: InsecurePlatformWarning:
 A true SSLContext object is not available. This prevents urllib3 from configuring SSL appropriately and may cause certain SSL conne
ctions to fail. For more information, see https://urllib3.readthedocs.org/en/latest/security.html#insecureplatformwarning.
  InsecurePlatformWarning
Collecting virtualenv
/usr/lib/python2.6/site-packages/pip-7.1.0-py2.6.egg/pip/_vendor/requests/packages/urllib3/util/ssl_.py:90: InsecurePlatformWarning:
 A true SSLContext object is not available. This prevents urllib3 from configuring SSL appropriately and may cause certain SSL conne
ctions to fail. For more information, see https://urllib3.readthedocs.org/en/latest/security.html#insecureplatformwarning.
  InsecurePlatformWarning
  Downloading virtualenv-13.1.0-py2.py3-none-any.whl (1.7MB)
    100% |████████████████████████████████| 1.7MB 201kB/s
Installing collected packages: virtualenv
Successfully installed virtualenv-13.1.0
[root@localhost ~]#
```

Julia package ecosystem



Listing all 1906 registered packages for the Julia programming language.
Made with PackageEvaluator.jl.

Last updated 2018-08-05 — Package ecosystem pulse

Packages tested on Julia versions:
v0.6.3 (current release) — v0.7.0-DEV (unstable)

ACME

ACME.jl - Analog Circuit Modeling and Emulation for Julia

MIT license / Owner: HSU-ANT / permalink
37 ★ / 4 ↧ / 0 ↥
Julia v0.6: 0.7.4 (12 days ago) / 🟩 Tests pass.

AMD

Approximate Minimum Degree Ordering in Julia

MIT license / Owner: JuliaSmoothOptimizers / permalink
0 ★ / 0 ↧ / 0 ↥
Julia v0.6: 0.1.0 (1 year, 10 months ago) / 🟥 Tests fail.

AMG

```
(test1) pkg> add Example
  Updating registry at `~/.julia/registries/General`
  Updating git-repo `https://github.com/JuliaRegistries/General.git`
 Resolving package versions...
  Updating `~/Desktop/hobby/julia/test/test1/Project.toml`
  [7876af07] + Example v0.5.1
  Updating `~/Desktop/hobby/julia/test/test1/Manifest.toml`
  [7876af07] + Example v0.5.1
  [2a0f44e3] + Base64
  [8ba89e20] + Distributed
  [b77e0a4c] + InteractiveUtils
  [8f399da3] + Libdl
```

5. General tips when it is slow

- Program thoughtfully:
  - Use vectorized functions
  - Avoid loops
  - Preallocate
  - Force type
  - Avoid copy-on-write
- Link to fast libraries (C/C++, Fortran, Java)
- Write low-level parts in C or Fortran
- Compile – jit
- Go parallel

6. Bridges

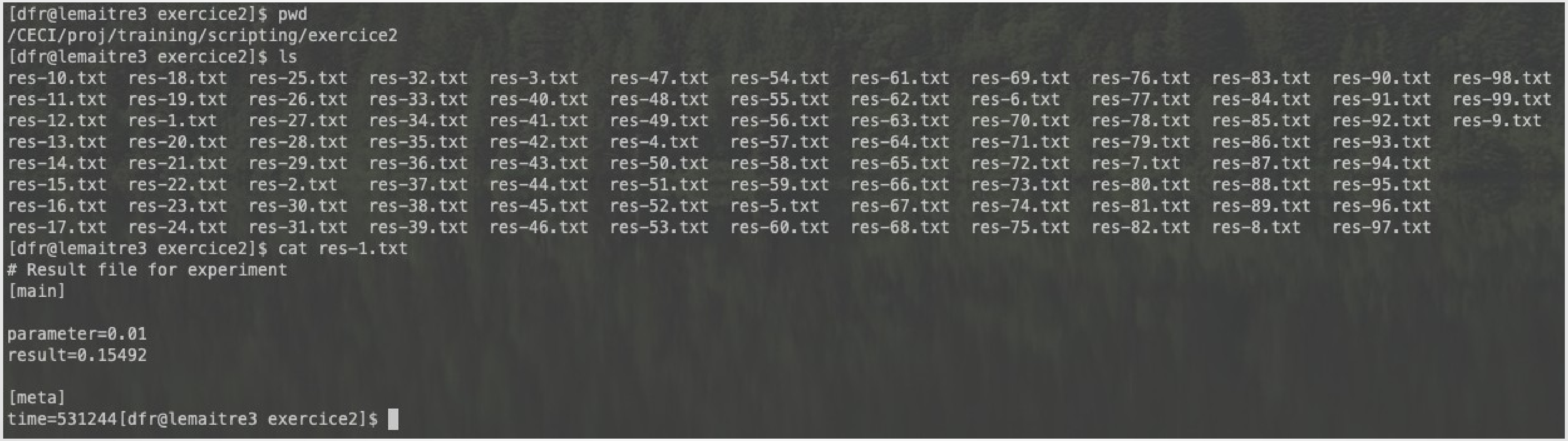
Python	→	R	http://rpython.r-forge.r-project.org/
Octave	→	Python	https://pypi.python.org/pypi/oct2py
R	→	Python	http://rpy.sourceforge.net/
Octave	→	R	https://cran.r-project.org/web/packages/RcppOctave
Python	→	Octave	https://github.com/daniel-e/pyoctave
R	→	Octave	http://www.omegahat.org/ROctave/
R	→	Julia	https://github.com/Non-Contradiction/JuliaCall
Julia	→	R	https://github.com/JuliaInterop/RCall.jl
Python	→	Julia	https://github.com/JuliaPy/pyjulia
Julia	→	Python	https://github.com/JuliaPy/PyCall.jl

So..

Fast to learn
Fast to code

Challenge

- Look at the files in /CECI/proj/training/scripting/exercice2 on any CÉCI cluster



```
[dfr@lemaitre3 exercice2]$ pwd
/CECI/proj/training/scripting/exercice2
[dfr@lemaitre3 exercice2]$ ls
res-10.txt  res-18.txt  res-25.txt  res-32.txt  res-3.txt   res-47.txt  res-54.txt  res-61.txt  res-69.txt  res-76.txt  res-83.txt  res-90.txt  res-98.txt
res-11.txt  res-19.txt  res-26.txt  res-33.txt  res-40.txt  res-48.txt  res-55.txt  res-62.txt  res-6.txt   res-77.txt  res-84.txt  res-91.txt  res-99.txt
res-12.txt  res-1.txt   res-27.txt  res-34.txt  res-41.txt  res-49.txt  res-56.txt  res-63.txt  res-70.txt  res-78.txt  res-85.txt  res-92.txt  res-9.txt
res-13.txt  res-20.txt  res-28.txt  res-35.txt  res-42.txt  res-4.txt   res-57.txt  res-64.txt  res-71.txt  res-79.txt  res-86.txt  res-93.txt
res-14.txt  res-21.txt  res-29.txt  res-36.txt  res-43.txt  res-50.txt  res-58.txt  res-65.txt  res-72.txt  res-7.txt   res-87.txt  res-94.txt
res-15.txt  res-22.txt  res-2.txt   res-37.txt  res-44.txt  res-51.txt  res-59.txt  res-66.txt  res-73.txt  res-80.txt  res-88.txt  res-95.txt
res-16.txt  res-23.txt  res-30.txt  res-38.txt  res-45.txt  res-52.txt  res-5.txt   res-67.txt  res-74.txt  res-81.txt  res-89.txt  res-96.txt
res-17.txt  res-24.txt  res-31.txt  res-39.txt  res-46.txt  res-53.txt  res-60.txt  res-68.txt  res-75.txt  res-82.txt  res-8.txt   res-97.txt
[dfr@lemaitre3 exercice2]$ cat res-1.txt
# Result file for experiment
[main]

parameter=0.01
result=0.15492

[meta]
time=531244[dfr@lemaitre3 exercice2]$ █
```

- We will pretend they are the result of running 100 jobs that take an input parameter and output a result (.INI file)

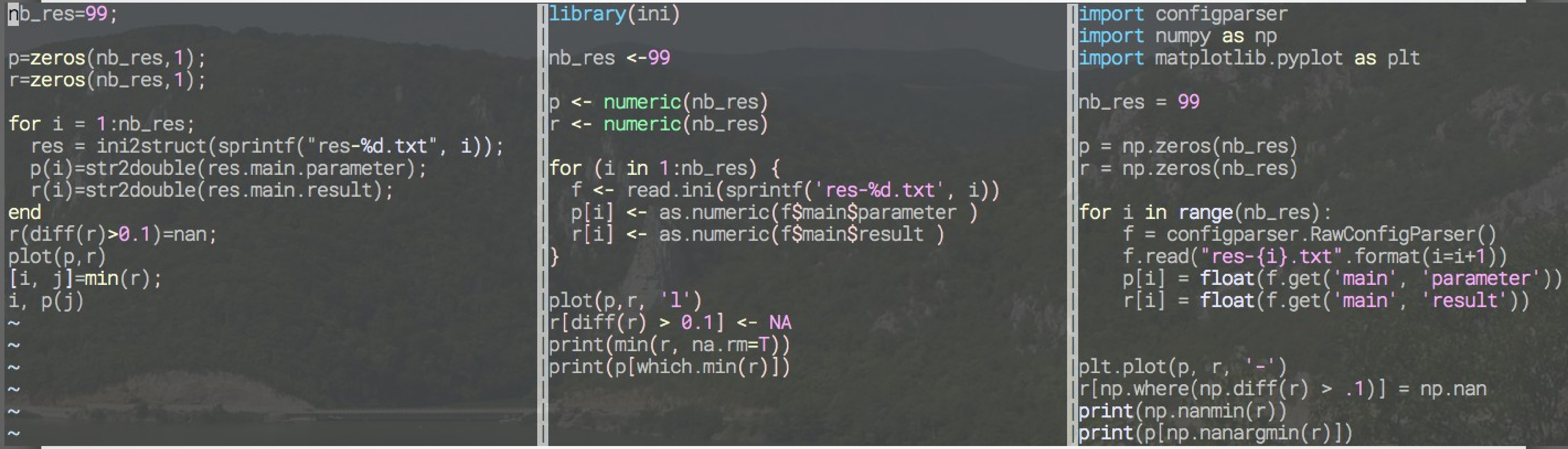
Challenge

- Find for which value of 'parameter' is 'result' the lowest.
- Course of action:
  - Read all files and parse them (you might need to install additional packages/libraries/modules)
  - Build two arrays one of parameter values and the other one for result values
  - Remove problematic values (plotting might help here)
  - Find minimum

Challenge

- Pseudo code:
  - “Activate” extension for .ini files
  - Initialize two arrays to hold the values
  - For-loop 1-99 :
    - Read file (using a ready-made extension)
    - Store values in corresponding arrays
  - Remove from array values that show too large a difference between consecutive values (slicing)
  - Find index of minimum value in one array and the corresponding value in the other array

Possible solution



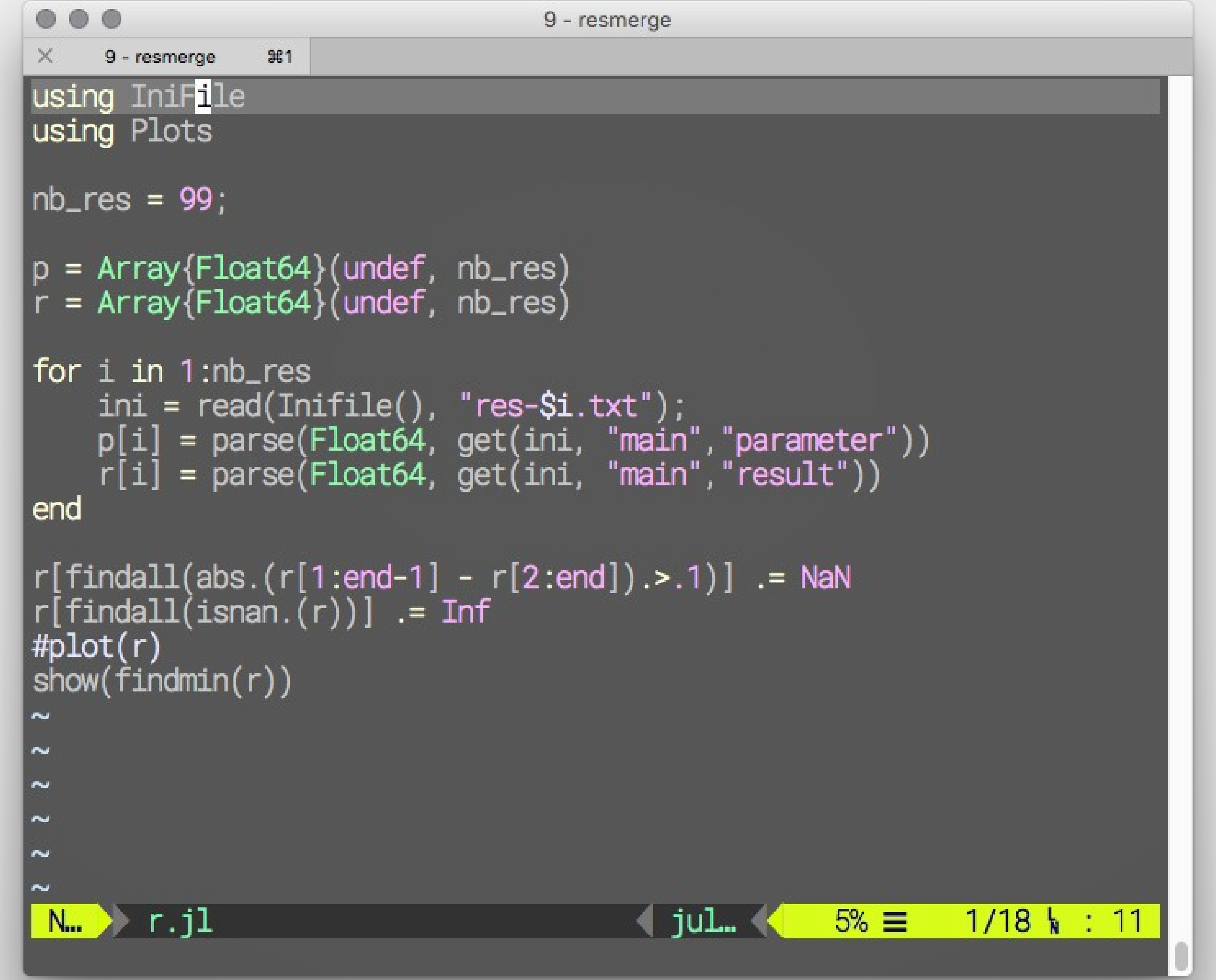
```
nb_res=99;

p=zeros(nb_res,1);
r=zeros(nb_res,1);

for i = 1:nb_res;
  res = ini2struct(sprintf("res-%d.txt", i));
  p(i)=str2double(res.main.parameter);
  r(i)=str2double(res.main.result);
end
r(diff(r)>0.1)=nan;
plot(p,r)
[i, j]=min(r);
i, p(j)
~
~
~
~
~
~
```

```
library(ini)

nb_res <-99

p <- numeric(nb_res)
r <- numeric(nb_res)

for (i in 1:nb_res) {
  f <- read.ini(sprintf('res-%d.txt', i))
  p[i] <- as.numeric(f$main$parameter )
  r[i] <- as.numeric(f$main$result )
}

plot(p,r, 'l')
r[diff(r) > 0.1] <- NA
print(min(r, na.rm=T))
print(p[which.min(r)])
```

```
import configparser
import numpy as np
import matplotlib.pyplot as plt

nb_res = 99

p = np.zeros(nb_res)
r = np.zeros(nb_res)

for i in range(nb_res):
    f = configparser.RawConfigParser()
    f.read("res-{i}.txt".format(i=i+1))
    p[i] = float(f.get('main', 'parameter'))
    r[i] = float(f.get('main', 'result'))


plt.plot(p, r, '-')
r[np.where(np.diff(r) > .1)] = np.nan
print(np.nanmin(r))
print(p[np.nanargmin(r)])
```

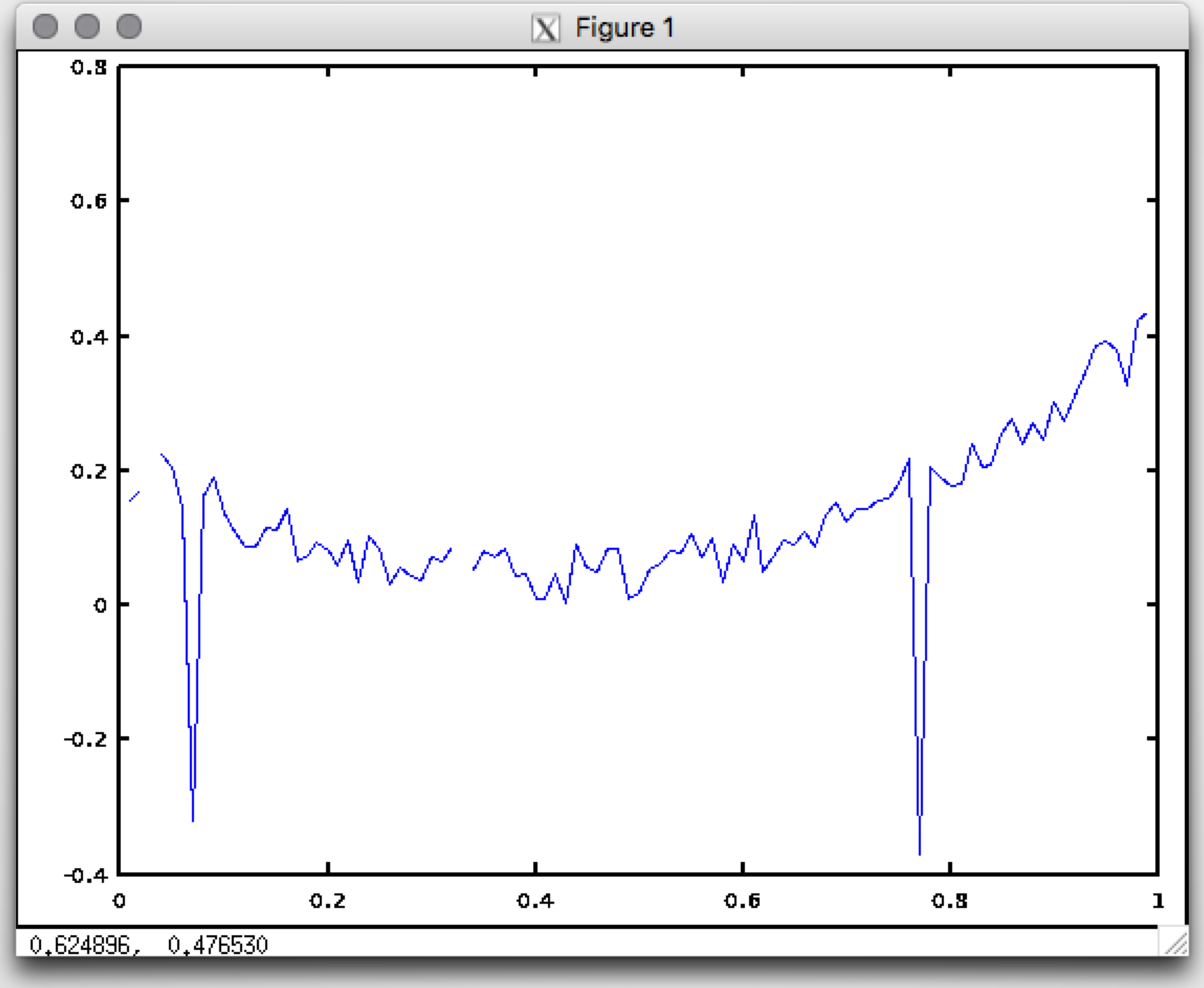
- https://nl.mathworks.com/matlabcentral/fileexchange/17177-ini2struct
- https://cran.r-project.org/web/packages/ini/index.html
- https://docs.python.org/3/library/configparser.html

Possible solution



```
using IniFile
using Plots

nb_res = 99;

p = Array{Float64}(undef, nb_res)
r = Array{Float64}(undef, nb_res)

for i in 1:nb_res
    ini = read(Inifile(), "res-$i.txt");
    p[i] = parse(Float64, get(ini, "main","parameter"))
    r[i] = parse(Float64, get(ini, "main","result"))
end

r[findall(abs.(r[1:end-1] - r[2:end]).>.1)] .= NaN
r[findall(isnan.(r))] .= Inf
#plot(r)
show(findmin(r))
~
~
~
~
~
~
```

Challenge



0.624896, 0.476530

Summary

Octave, R, Python (and Julia)

Much more programmer-friendly than C/C++/Fortran

Still able to use fast compiled code

Focus on the unsolved problems

Try all and choose one

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Introduction to Scripting Languages

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