Keeping a Computational Lab Notebook & How to Get Programming Help

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- Explanation of why and how you are doing an experiment, as well as the results
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- Lab legacy/institutional memory

Adapted from ‘Keeping a Lab Notebook’, Philip Ryan, Office of Intramural Training and Education (NIH)

Why do we need to keep computational laboratory notebooks?

‘Ten Simple Rules for a Computational Biologist’s Laboratory Notebook.’ S. Schnell, PLOS Computational Biology, 2015.

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"One of the major hurdles I face as the head of a computational biology laboratory is convincing my research team—particularly those pursuing exclusively mathematical and computational modeling—that they need to keep a laboratory notebook. There seems to be a misconception in the computational biology community that a lab notebook is only useful for recording experimental protocols and their results. **A lab notebook is much more than that. It is an organizational tool and memory aid, which serves as the primary record of scientific research and activity for all scientists. It also serves as a legal record of ownership of the ideas and results obtained by a scientist." -S. Schnell**

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- Rule 4: Record all* scientific activities in your lab notebook —it is a chronological log of everything scholarly a scientist does (*more wiggle room on this rule)

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- Rule 9: Make a table of contents for your lab notebook
- Rule 10: Protect your lab notebook—the original belongs to your institution.

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Example Lab Notebook Entry:

180410

Goal: I'm trying to understand how many TCGA KIRC samples have each combination of data types

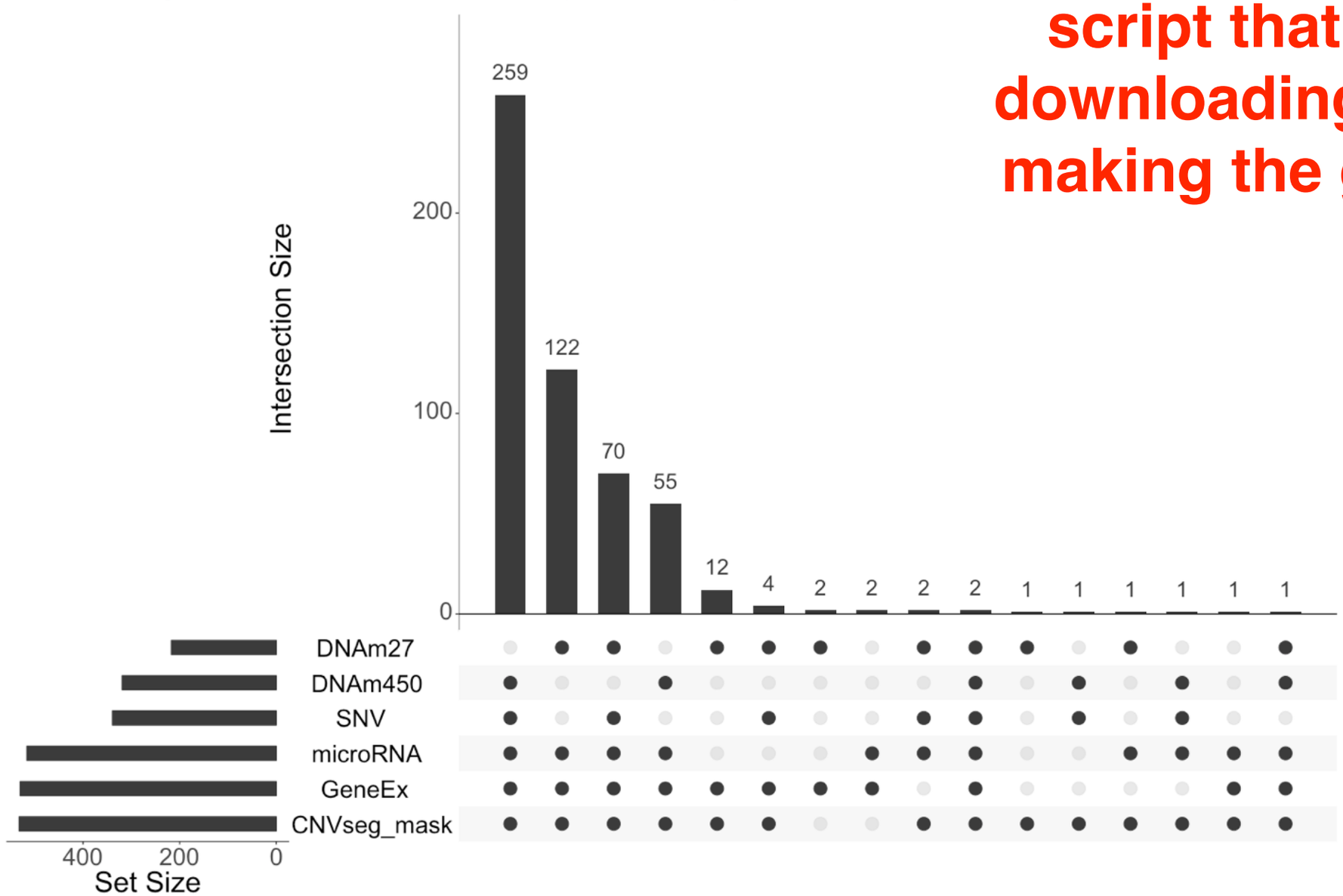
-Working scripts are here: /Data_nonGoogleDrive/TCGAKIRC_TCGAbioinks_180314/getTCGAKIRCdata.R

-I set up tcgabiolinks queries for each dataset (except for clinical) and recorded the number of T/N samples for each

-Analyzed the tumor overlap between datasets, including limiting datasets with Reduce(intersect, list()) notation

-Visually examined the results with UpSetR graph (vignette: https://cran.r-project.org/web/packages/UpSetR/vignettes/basic.usage.html)

/Data_nonGoogleDrive/TCGAKIRC_TCGAbiolinks_180314/KIRC_UpSetRPlot_180410.png



Conclusions: switch from m27 to m450 happened during this dataset so about 25% of tumors have m27k data and rest with m450k data

script that goes from downloading raw data to making the graph below

Example Lab Notebook Entry (continued):

(Partial for Illustrative Purposes) Code to Plot Graph on Previous Slide

```
##visualize intersections
library(UpSetR)
listInput<-list(GeneEx=substr(getResults(query.exp.hg38.KIRC, cols="cases"), 1, 12),
                DNAm450=substr(getResults(query.DNAm450.hg38.KIRC, cols="cases"), 1, 12),
                DNAm27=substr(getResults(query.DNAm27.hg38.KIRC, cols="cases"), 1, 12),
                microRNA=substr(getResults(query.micro.hg38.KIRC, cols="cases"), 1, 12),
                #CNVseg=substr(getResults(query.CNVseg.hg38.KIRC, cols="cases"), 1, 12),
                CNVseg_mask=substr(getResults(query.CNVsegmasked.hg38.KIRC, cols="cases"), 1, 12),
                SNV=substr(getResults(query.SNV.hg38.KIRC, cols="cases"), 1, 12))
#commented out CNVseg because masked has known germline snps removed

str(listInput)

upset(fromList(listInput), order.by=c("freq"), nsets=7, line.size=0, point.size=5, nintersects = NA,
text.scale=3)
#KIRC_UpSetRPlot_180410.png
#nsets shows all 7 data sets
#line.size=0 removes vertical lines in plot
#point.size changes circle sizes
#nintersects says number of intersects to plot
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                microRNA=substr(getResults(query.micro.hg38.KIRC, cols="cases"), 1, 12),
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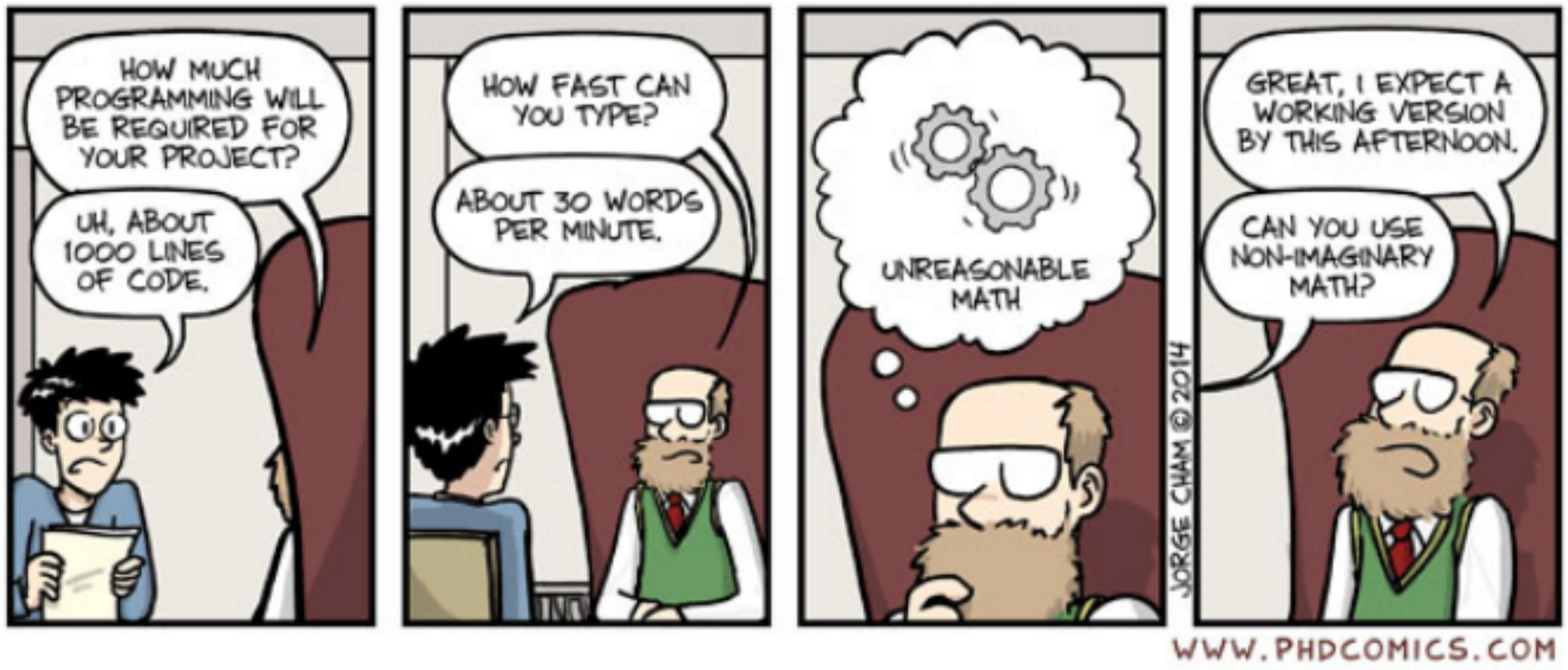
- ✓ consistent naming
- ✓ explain thought process
- ✓ reproducible

How to ask for programming help:



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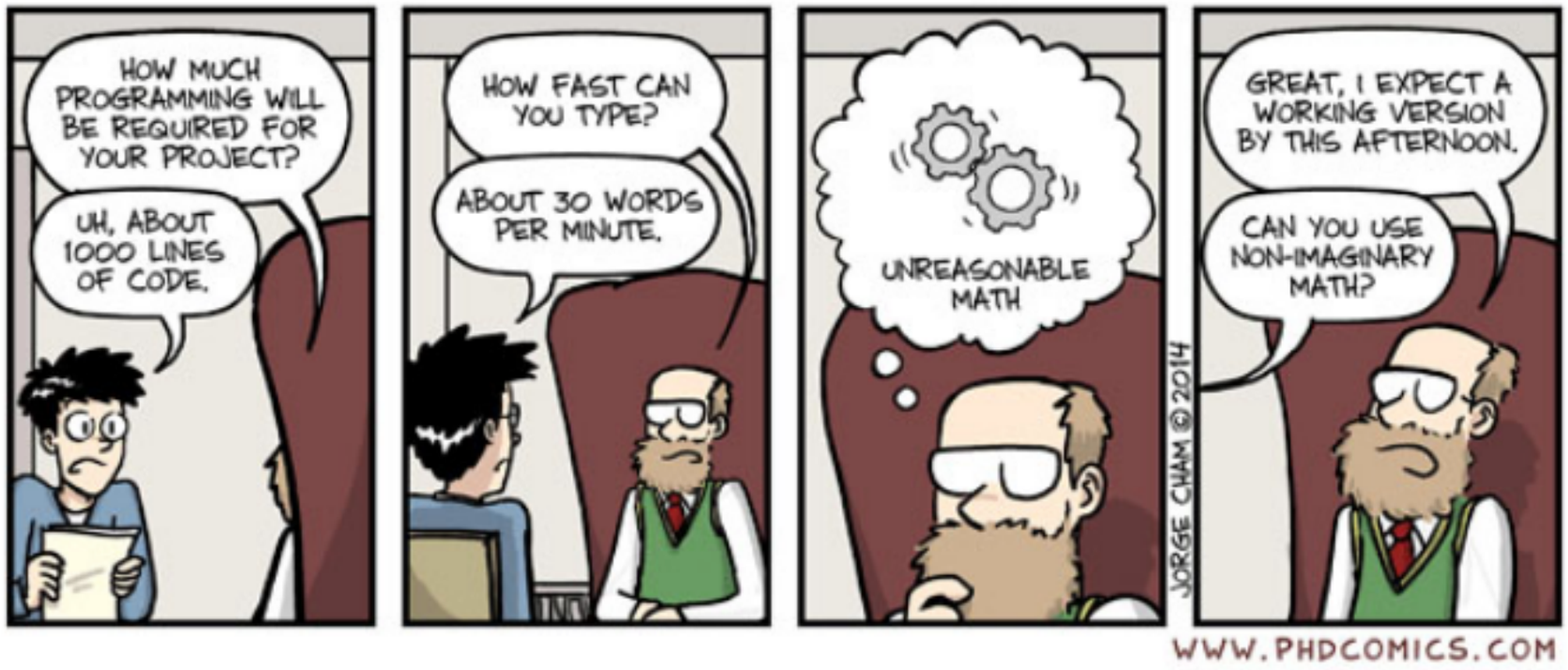

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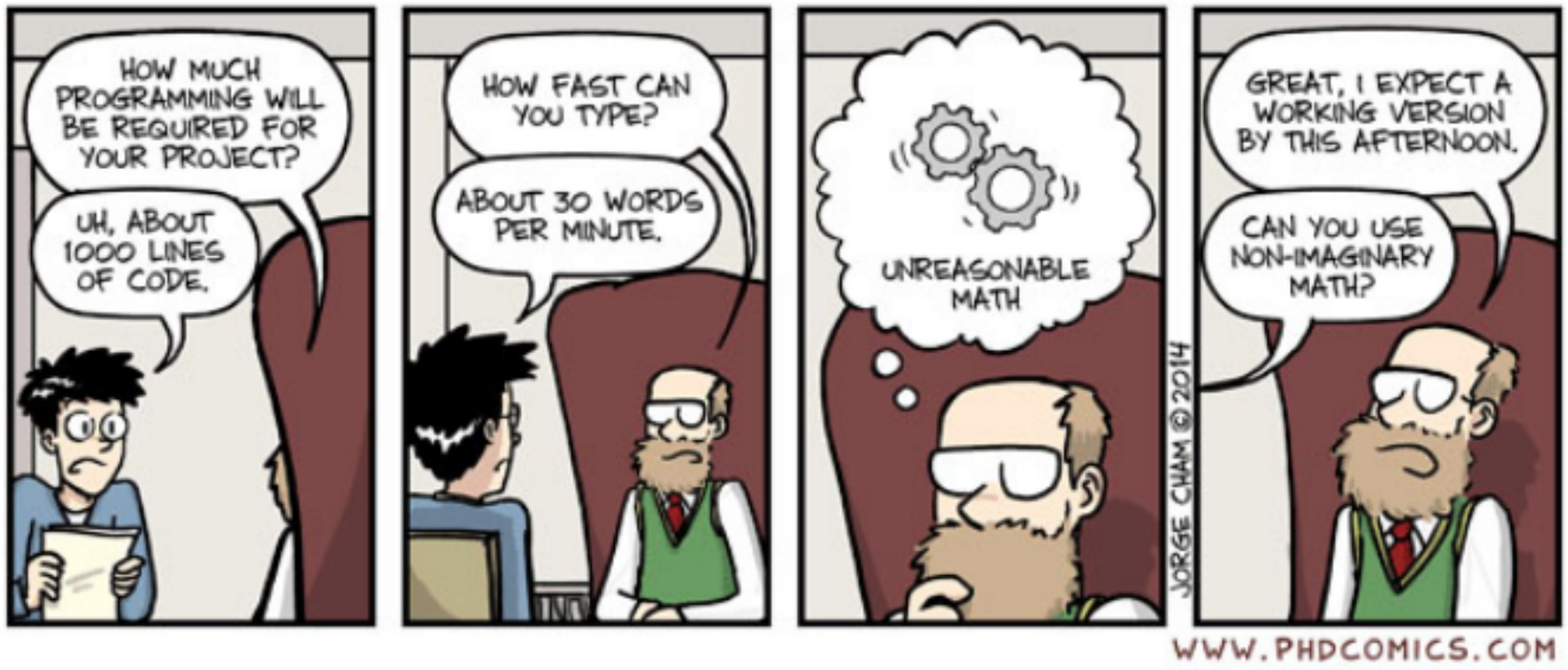

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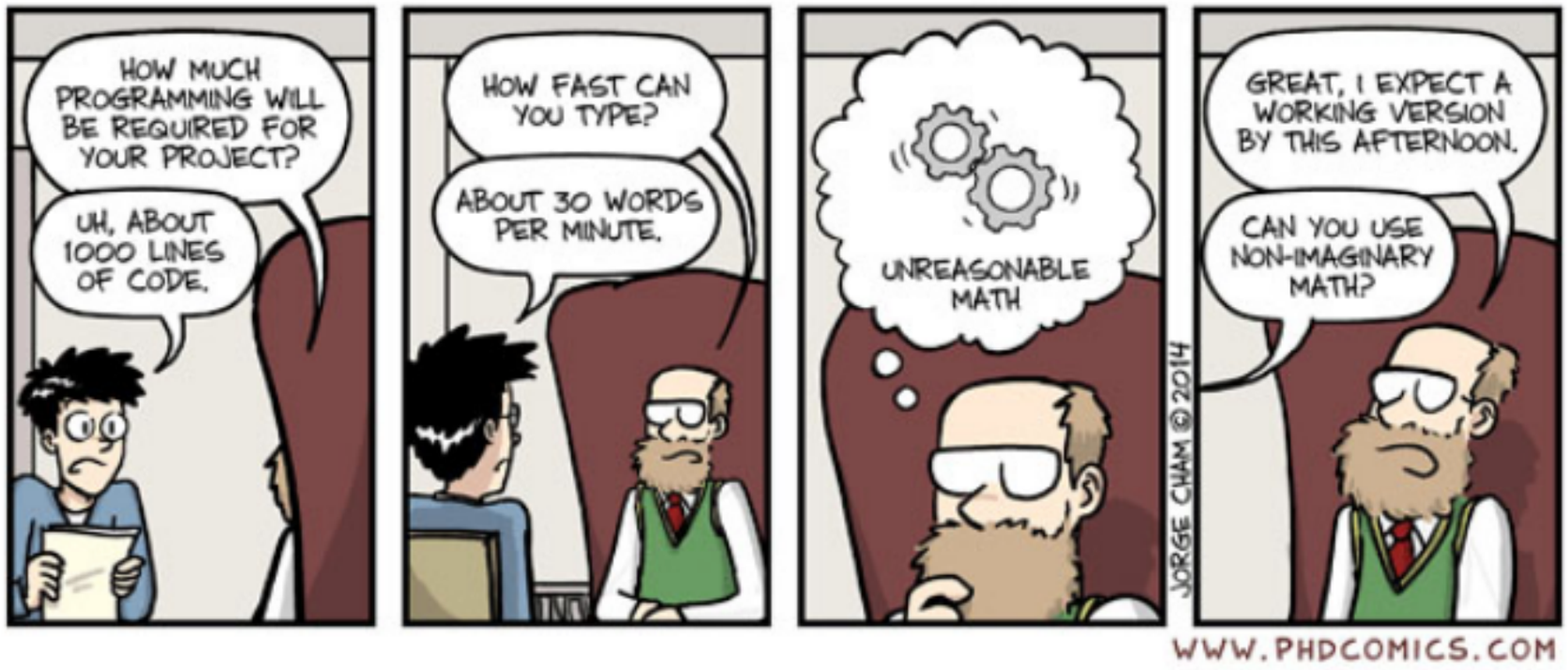

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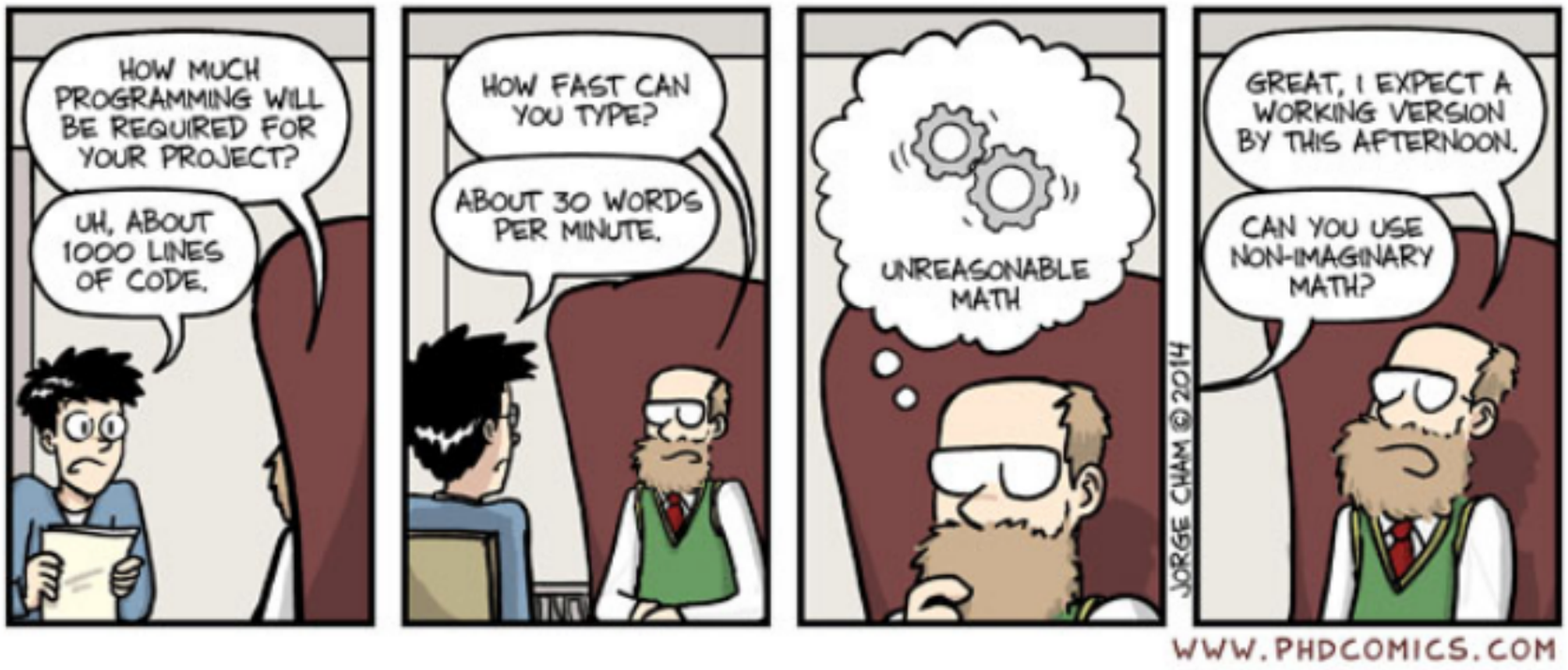

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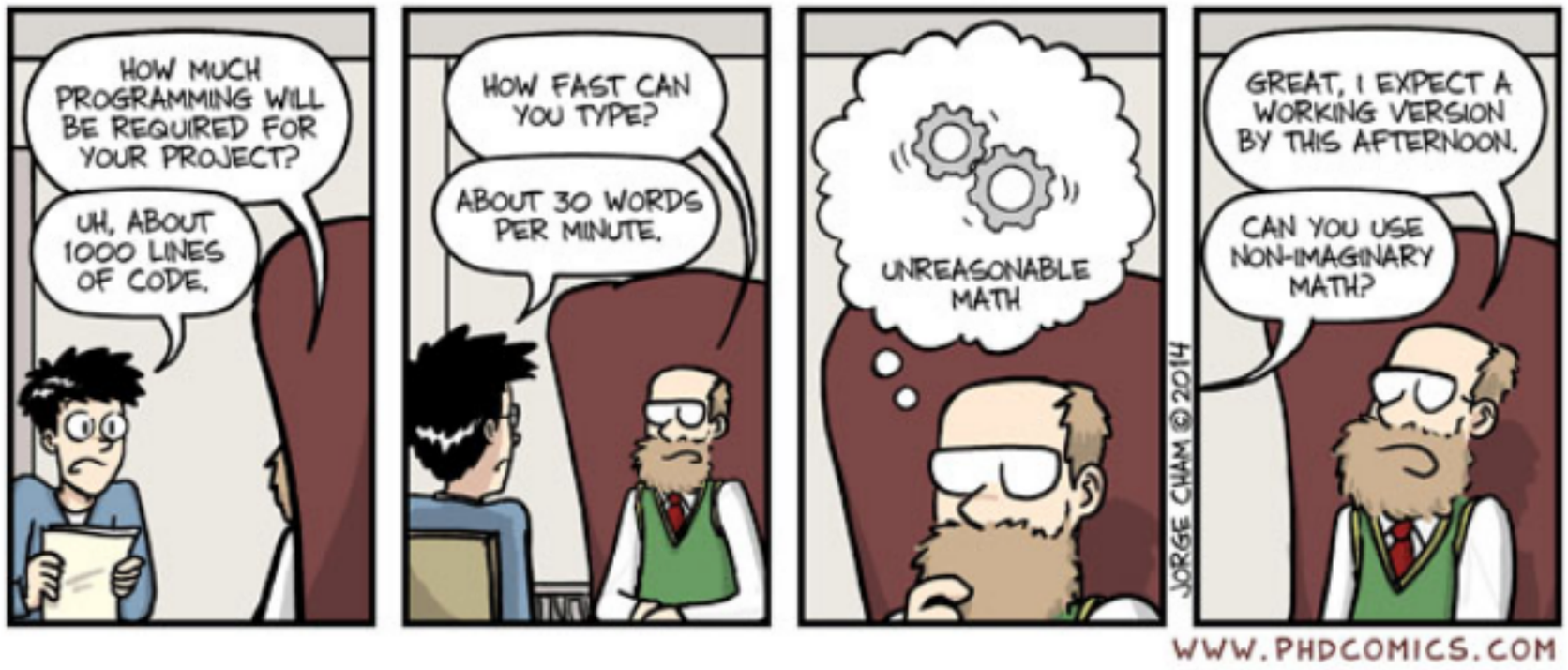

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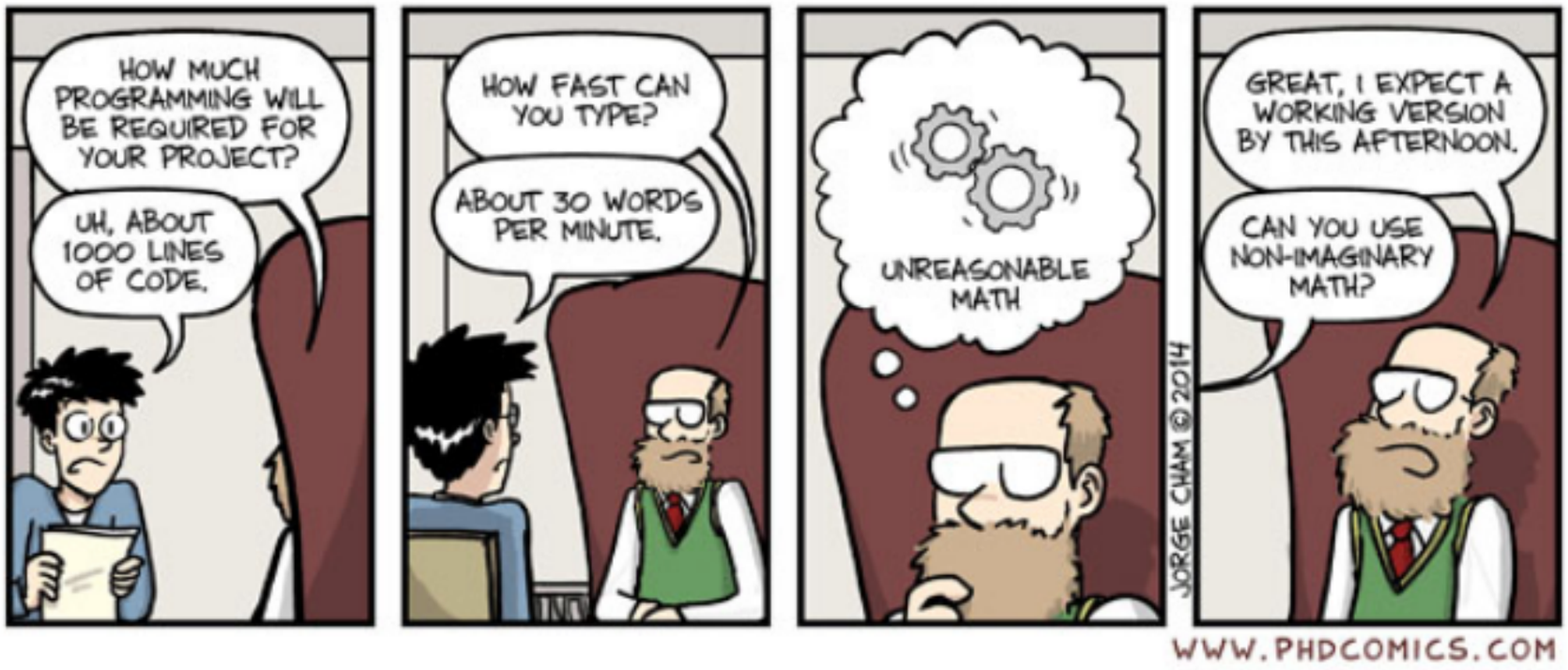

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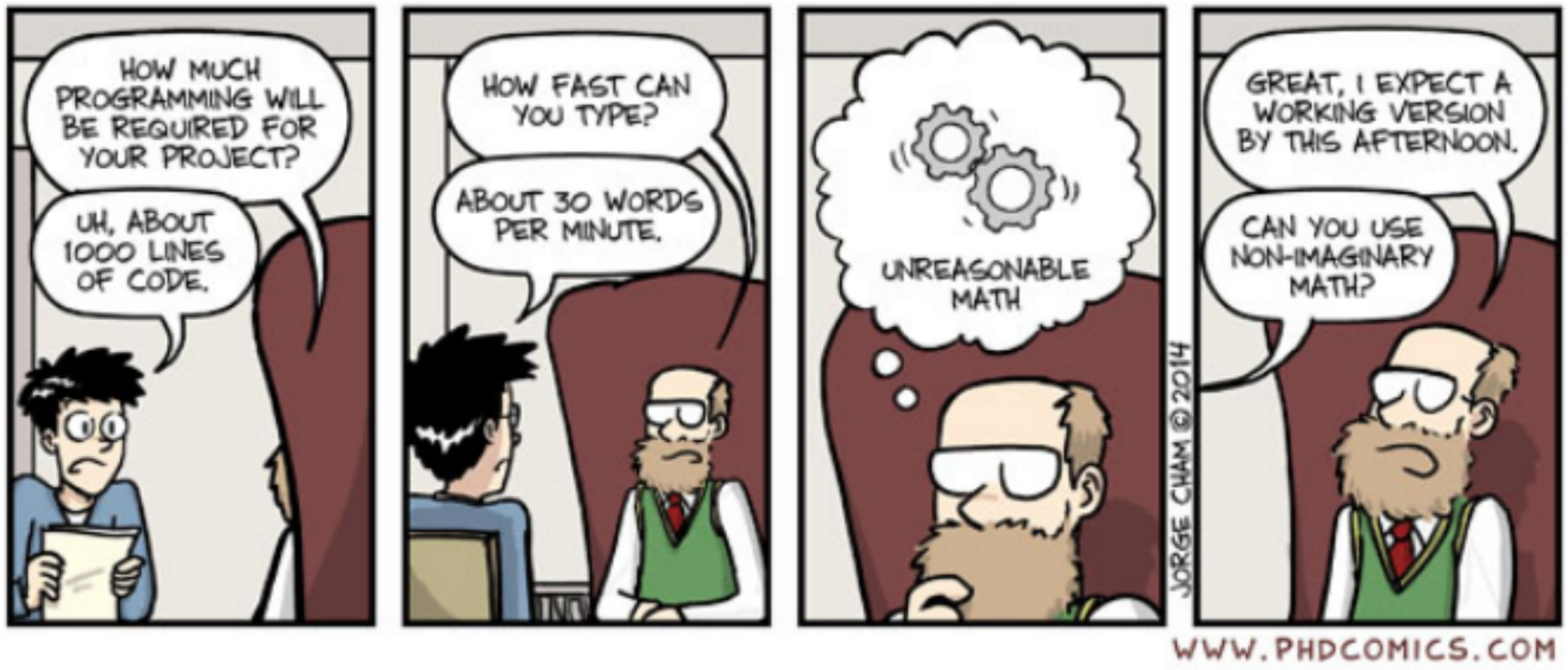

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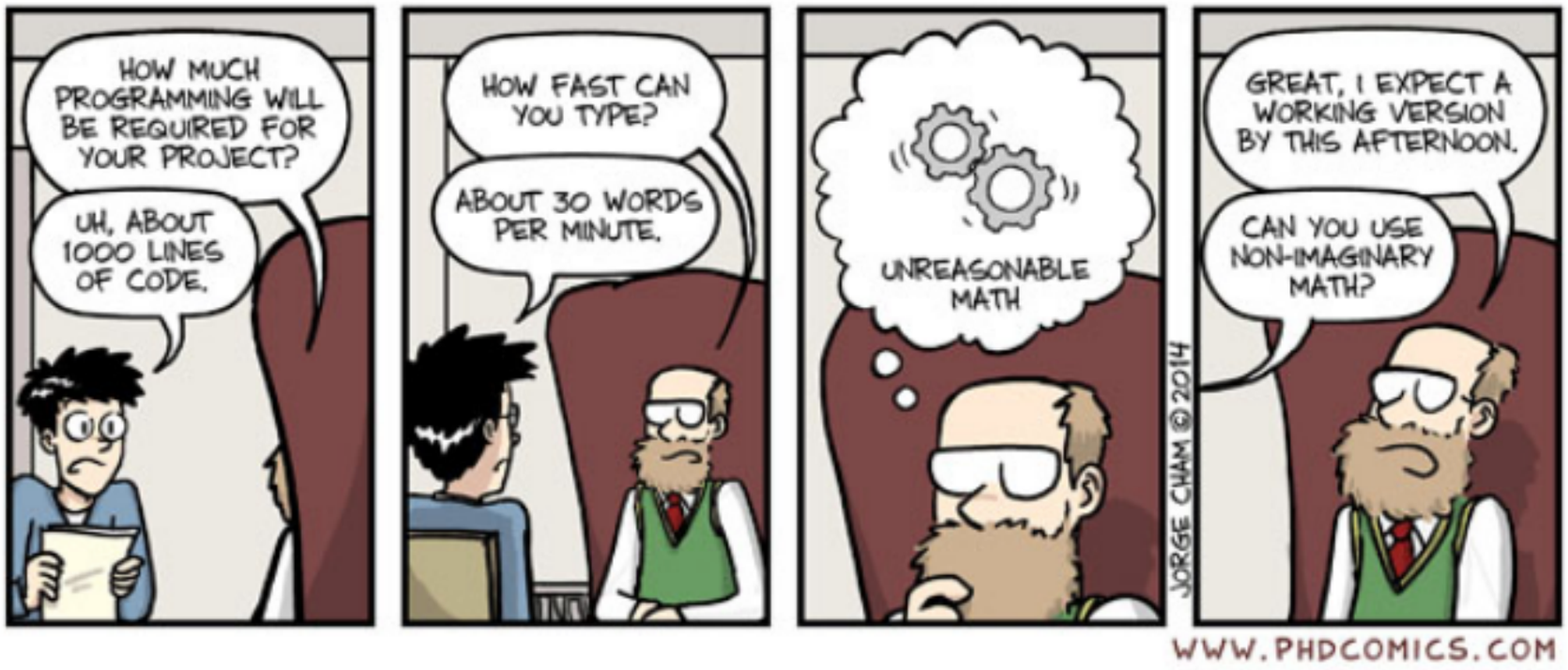
- Be patient and courteous.
- Record your troubleshooting in your lab notebook!

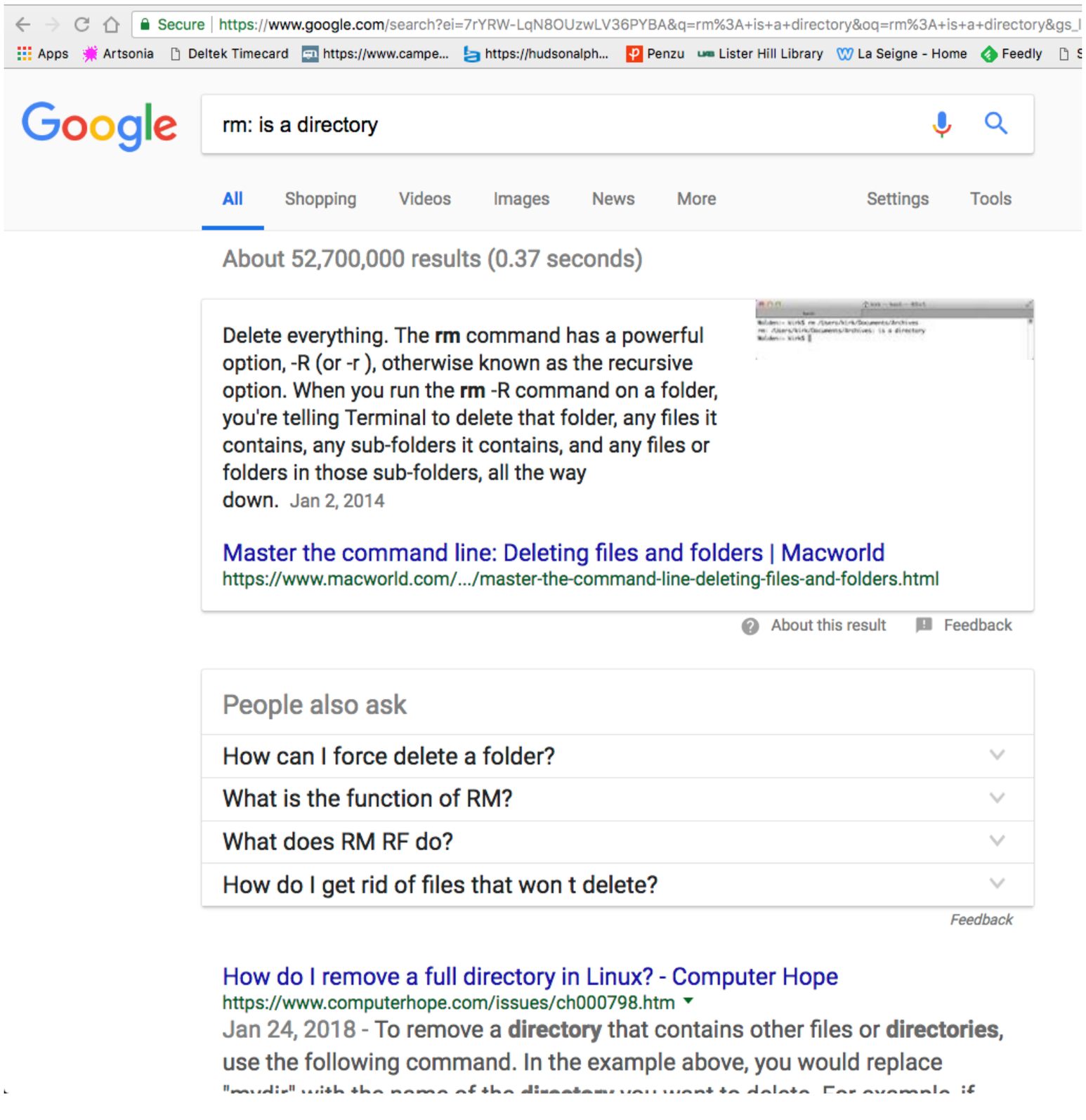


Example 1:
want to delete ‘demo1’ directory

DemoDir — -bash — 80×24

```
Brittany-Lasseigne:DemoDir brittany$ pwd
/Users/brittany/GoogleDrive/Teaching/DemoDir
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$ rm demo1
rm: demo1: is a directory
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$
```

Google the error message:



Check the manual: man rm

DemoDir — less ◂ man rm — 80×29

```
RM(1)                    BSD General Commands Manual                    RM(1)

NAME
     rm, unlink -- remove directory entries

SYNOPSIS
     rm [-dfiPRrvW] file ...
     unlink file

DESCRIPTION
     The rm utility attempts to remove the non-directory type files specified
     on the command line.  If the permissions of the file do not permit writ-
     ing, and the standard input device is a terminal, the user is prompted
     (on the standard error output) for confirmation.

     The options are as follows:

     -R          Attempt to remove the file hierarchy rooted in each file
                 argument.  The -R option implies the -d option.  If the -i
                 option is specified, the user is prompted for confirmation
                 before each directory's contents are processed (as well as
                 before the attempt is made to remove the directory).  If the
                 user does not respond affirmatively, the file hierarchy
                 rooted in that directory is skipped.

     -r          Equivalent to -R.
```

It works!

DemoDir — -bash — 80×24

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/Users/brittany/GoogleDrive/Teaching/DemoDir
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$ rm demo1
rm: demo1: is a directory
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$ rm -R demo1
Brittany-Lasseigne:DemoDir brittany$ ls
Brittany-Lasseigne:DemoDir brittany$
```
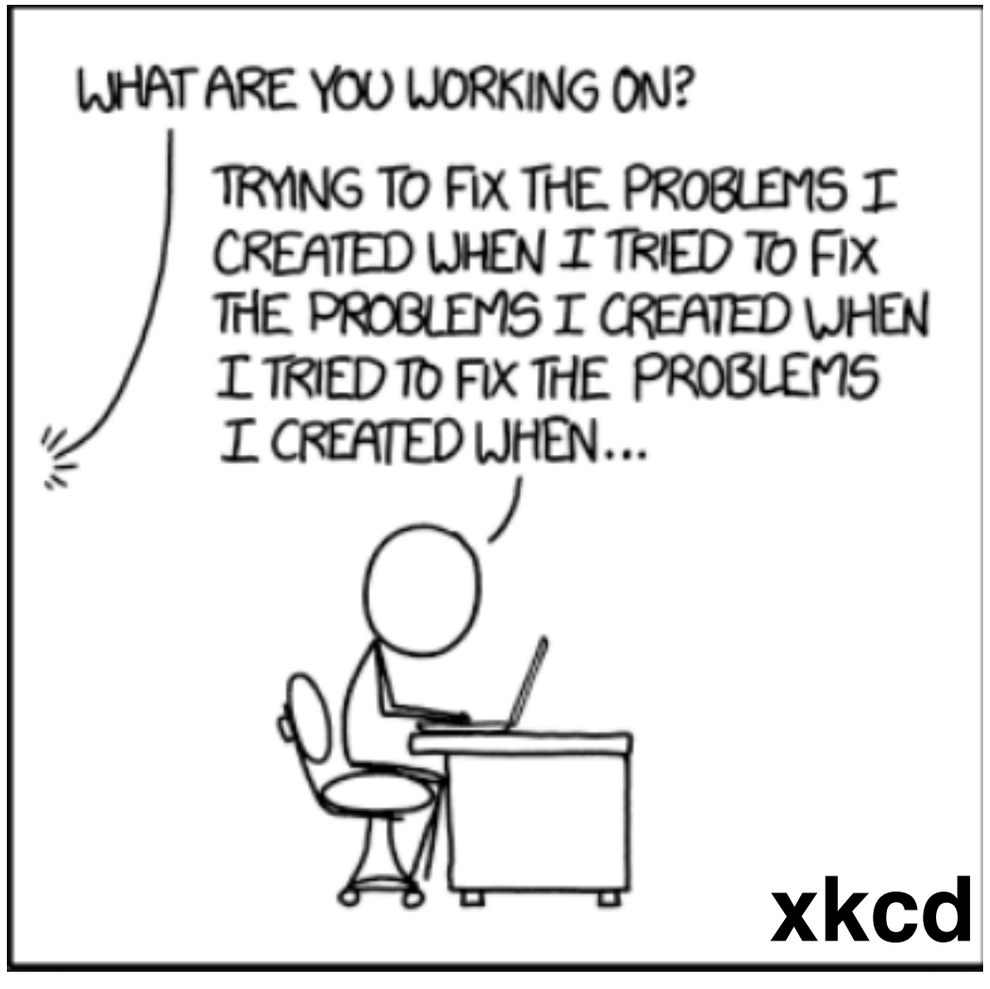

Thanks! Slides available at https://www.lasseigne.org/post/2018-06-04-biotraincompbioworkshop2018/



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