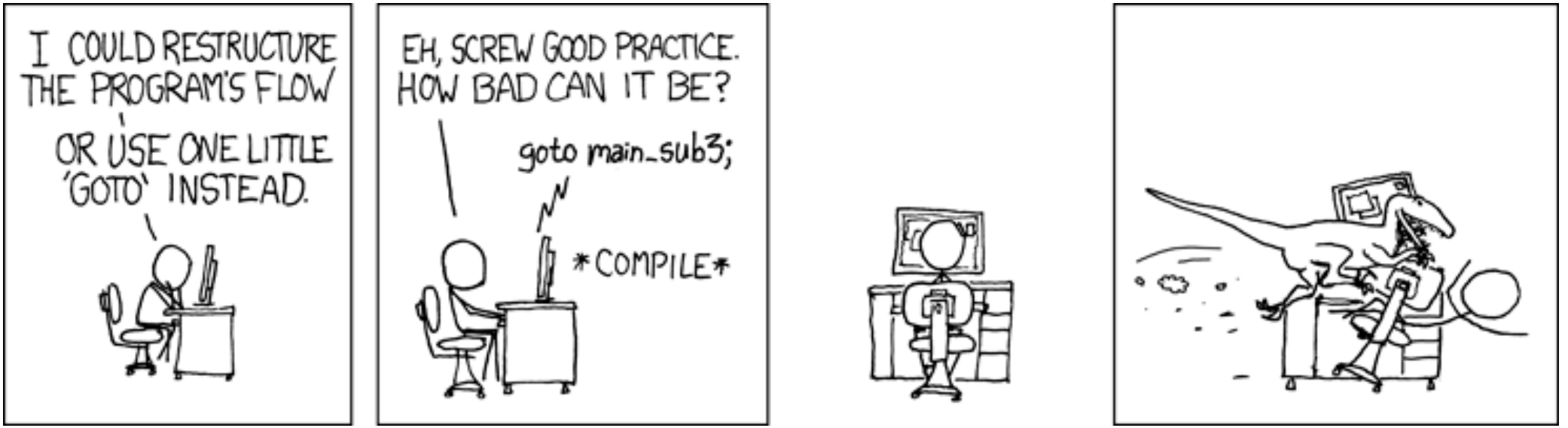
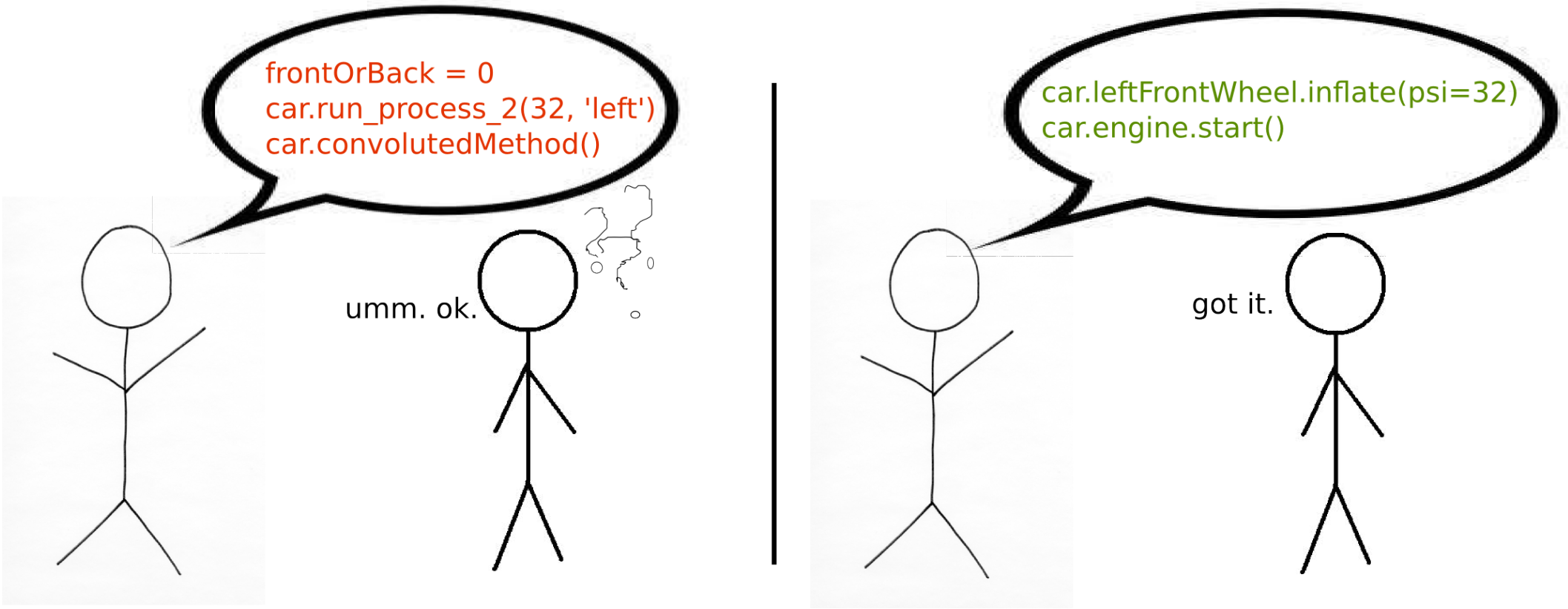
Best Practices for Scientific Coding



DATA SCIENCE BOOTCAMP

Write programs for people, not computers



The reader shouldn’t have to remember tons

Only a handful of facts in their memory

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Only a handful of facts in their memory

Easily understood functions

Each conducts a single, easily understood task

Names should be consistent, distinctive, and meaningful

M. Night Shyamalan

Zach Galifianakis

Irmak Sirer

Names should be consistent, distinctive, and meaningful

What these functions do is very clear:

– bank_account.deposit(20, '$')

– bank_account.withdraw(10, '$')

Aptly named variables:

– current_bank_account_balance

– number_of_bunnies_in_cage

Code style and formatting should be consistent

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Don't use both of these in the same code:

– CamelCaseNaming

– snake_case_naming

Use the same indentation sizes

Keep max line lengths the same

All aspects of software development should be broken down into tasks roughly an hour long

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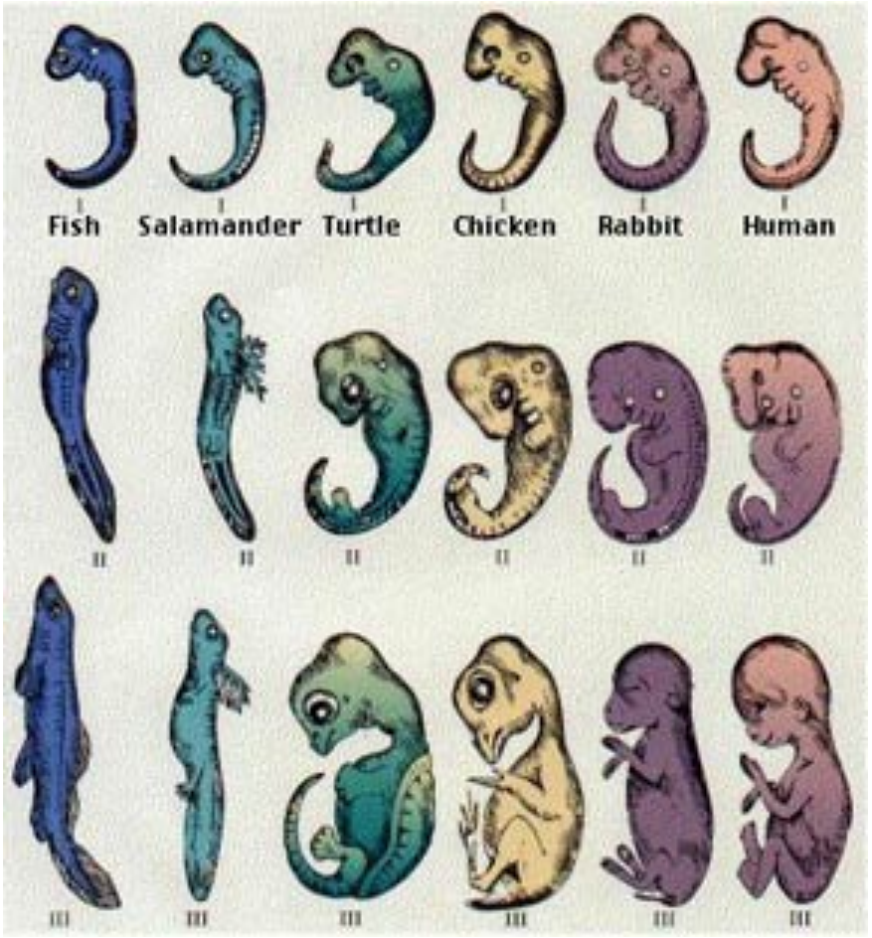
Work in chunks of 50-200 lines of code

Short functions (2-15 lines)

Make incremental changes



Work in small steps

with frequent feedback and course correction

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Hour long coding sessions

Grouped in iterations

Produce working but incomplete code (or results) after each iteration

Use version control

Use a version control system

Everything that's been created manually should be put in version control

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Not data

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Not automatically created stuff like `.pyc` files or emacs backups like `script.py~`

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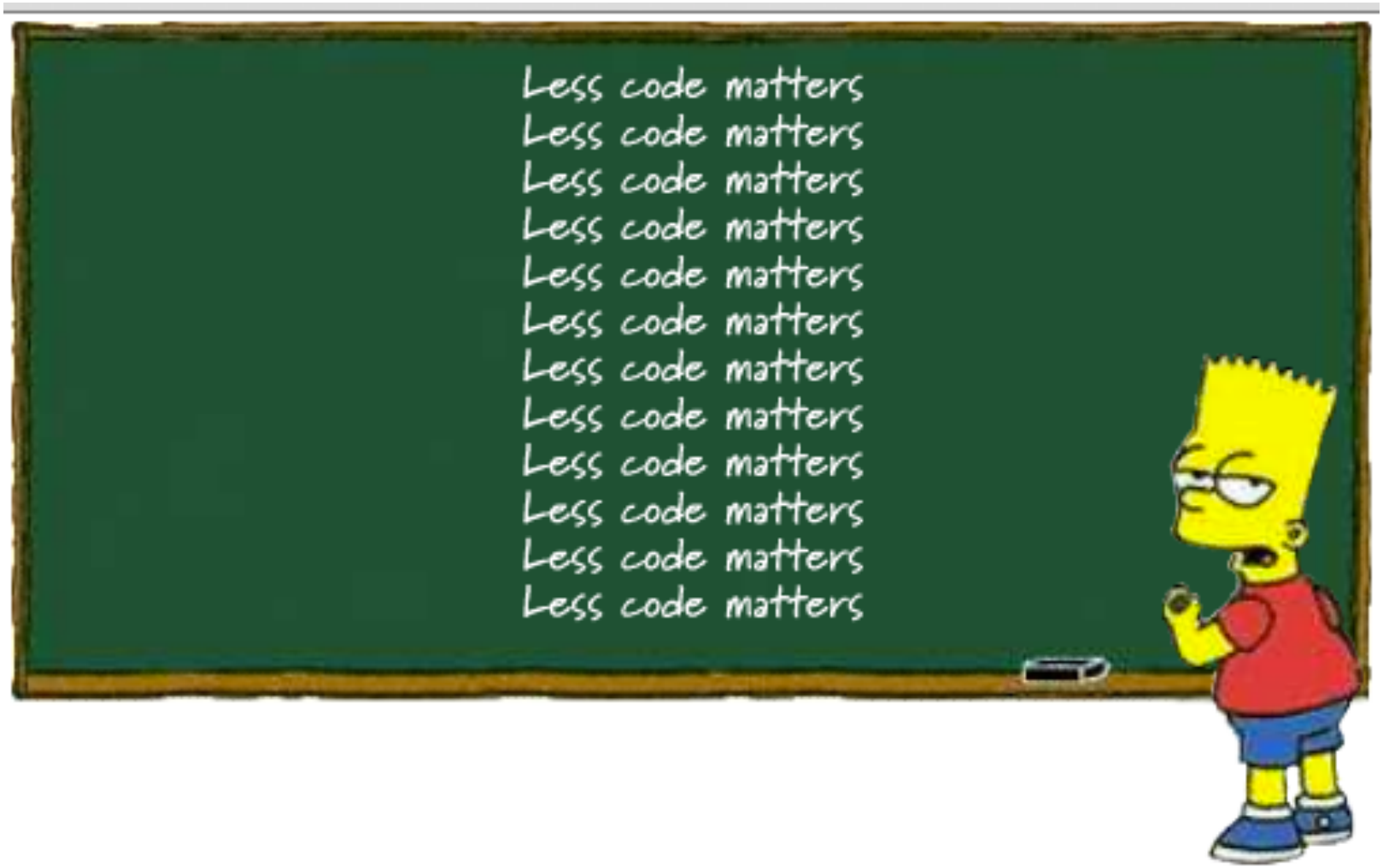
Not tons of big image or text files that don't change

Not automatically created stuff like `.pyc` files or emacs backups like `script.py~`

Commit result graphs

Don't repeat yourself (or others)



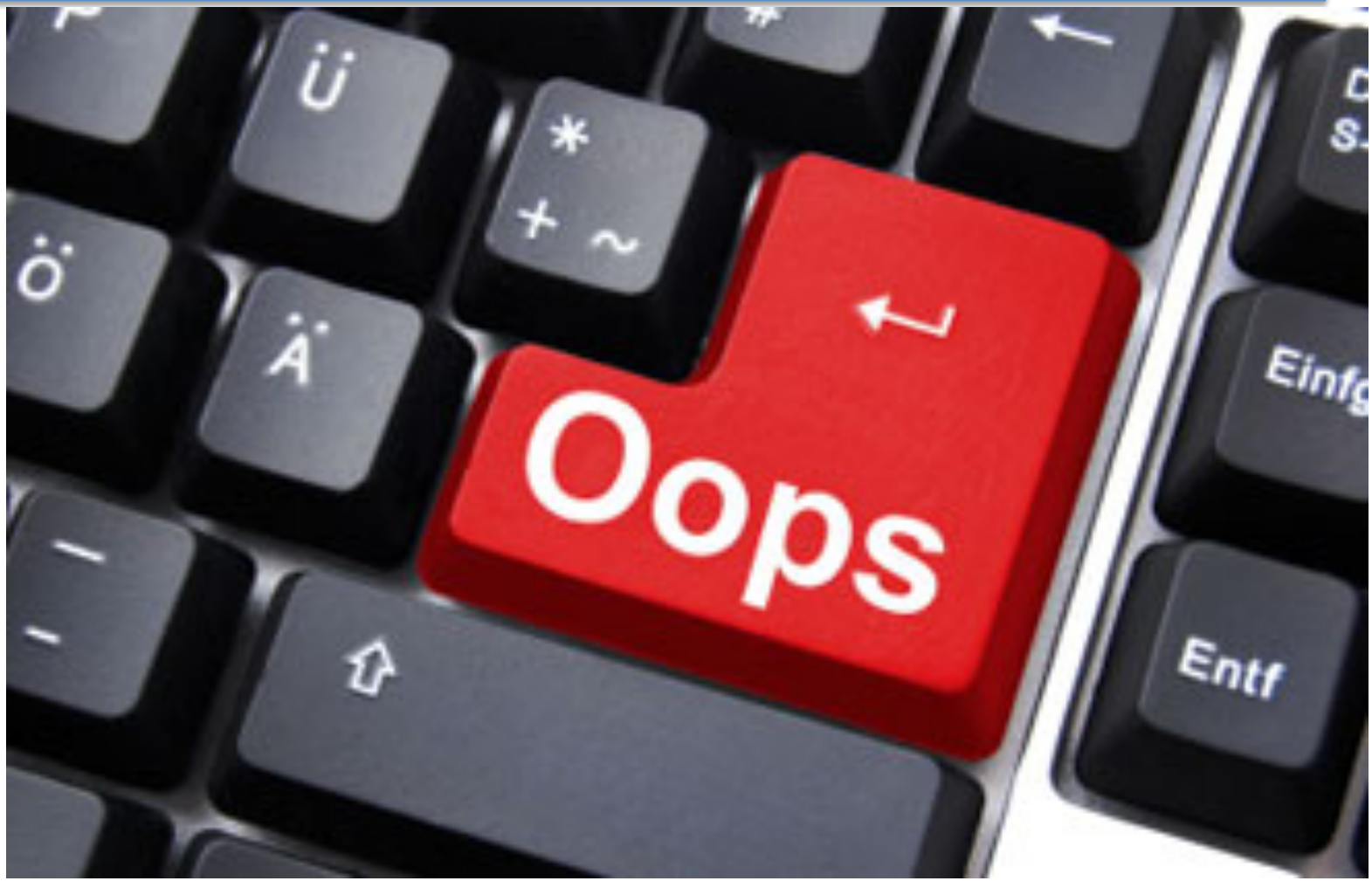
Small scales: don’t copy & paste, modularize

DO NOT copy-paste. I mean it. Stahp.

Large scales: Look for existing packages

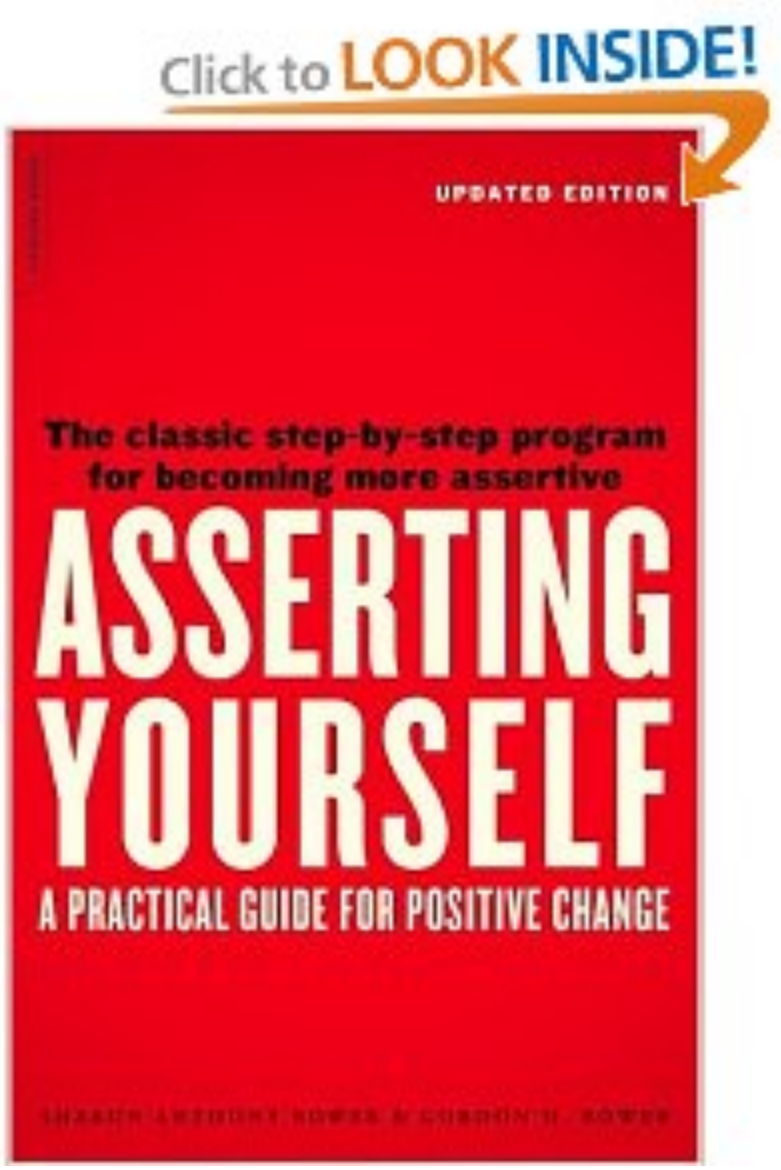
Don’t reinvent the wheel

Plan for mistakes



Defensive programming

Add assertions to programs to check assumptions



Defensive programming

Add assertions to programs to check assumptions

```
def bradford_transfer(grid, point, smoothing):

        assert grid.contains(point), 'Point is not located in grid'
        assert grid.is_local_maximum(point), 'Point is not a local max in grid'

        ...do calculations...

        assert 0.0 < result <= 1.0, 'Bradford transfer value out of legal range'

        return result
```

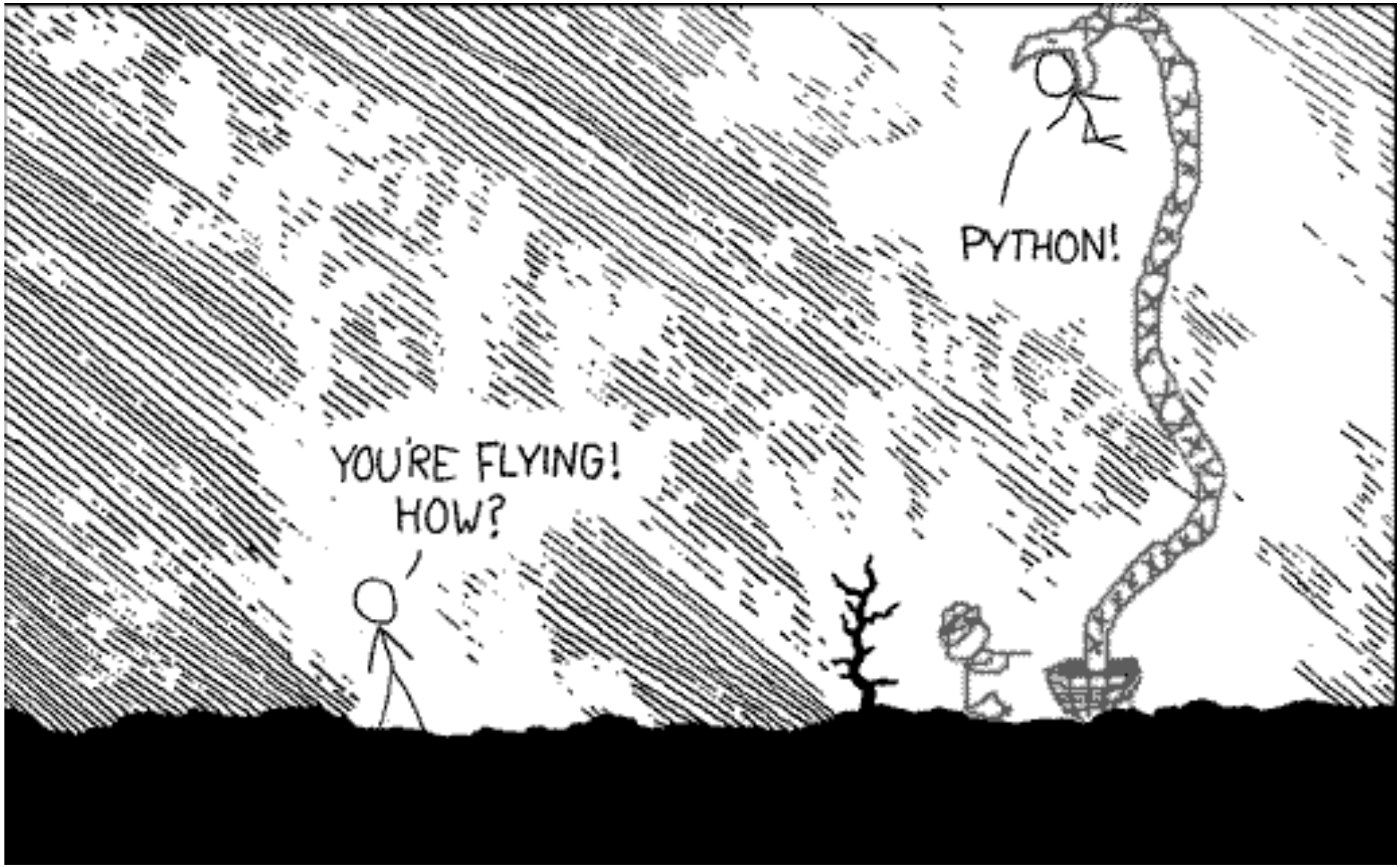
Defensive programming

Add assertions to programs to check assumptions

Turn bugs into test cases

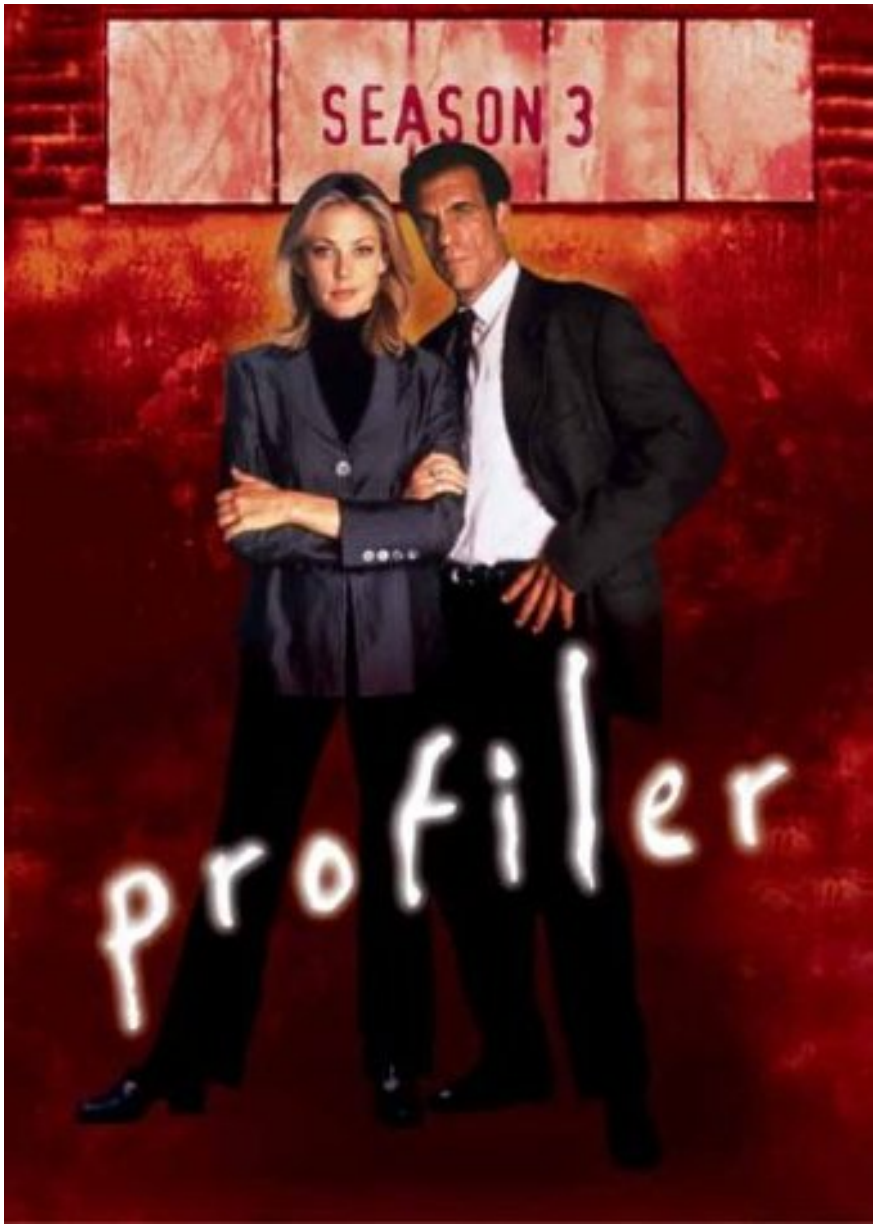
Optimize software only after it works correctly

Develop in the highest-level language possible

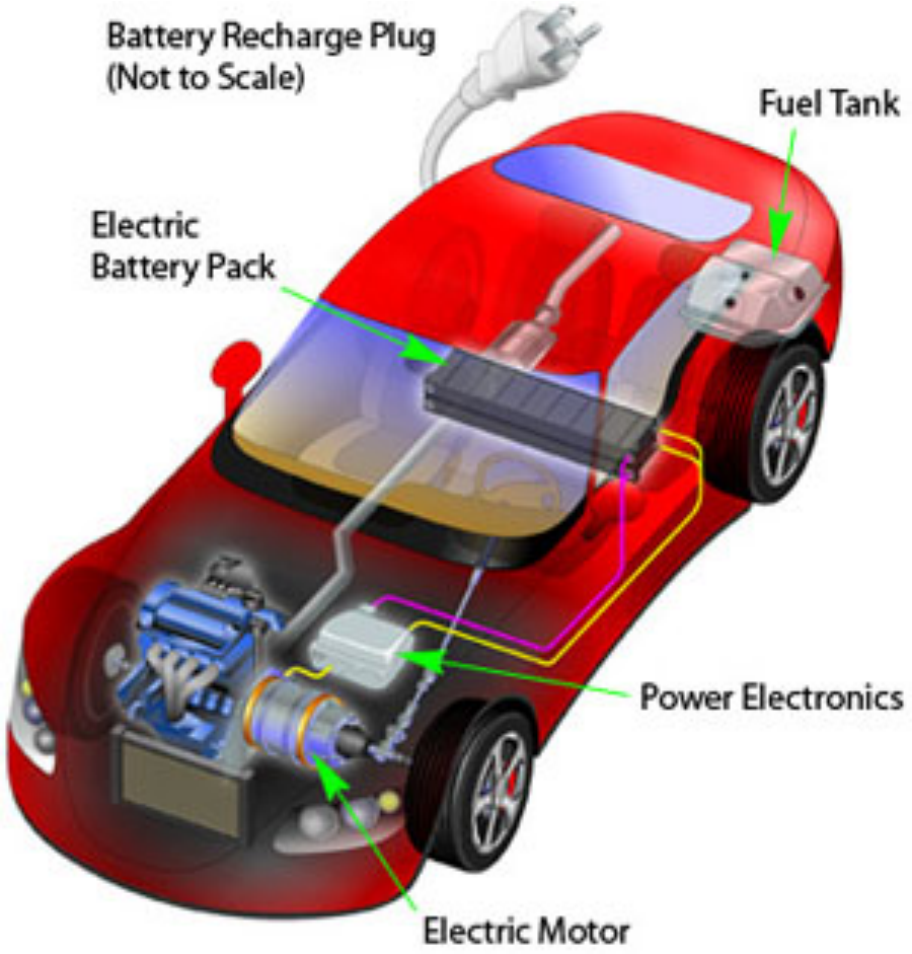


Use a profiler to identify bottlenecks

A profiler times every step of a piece of code

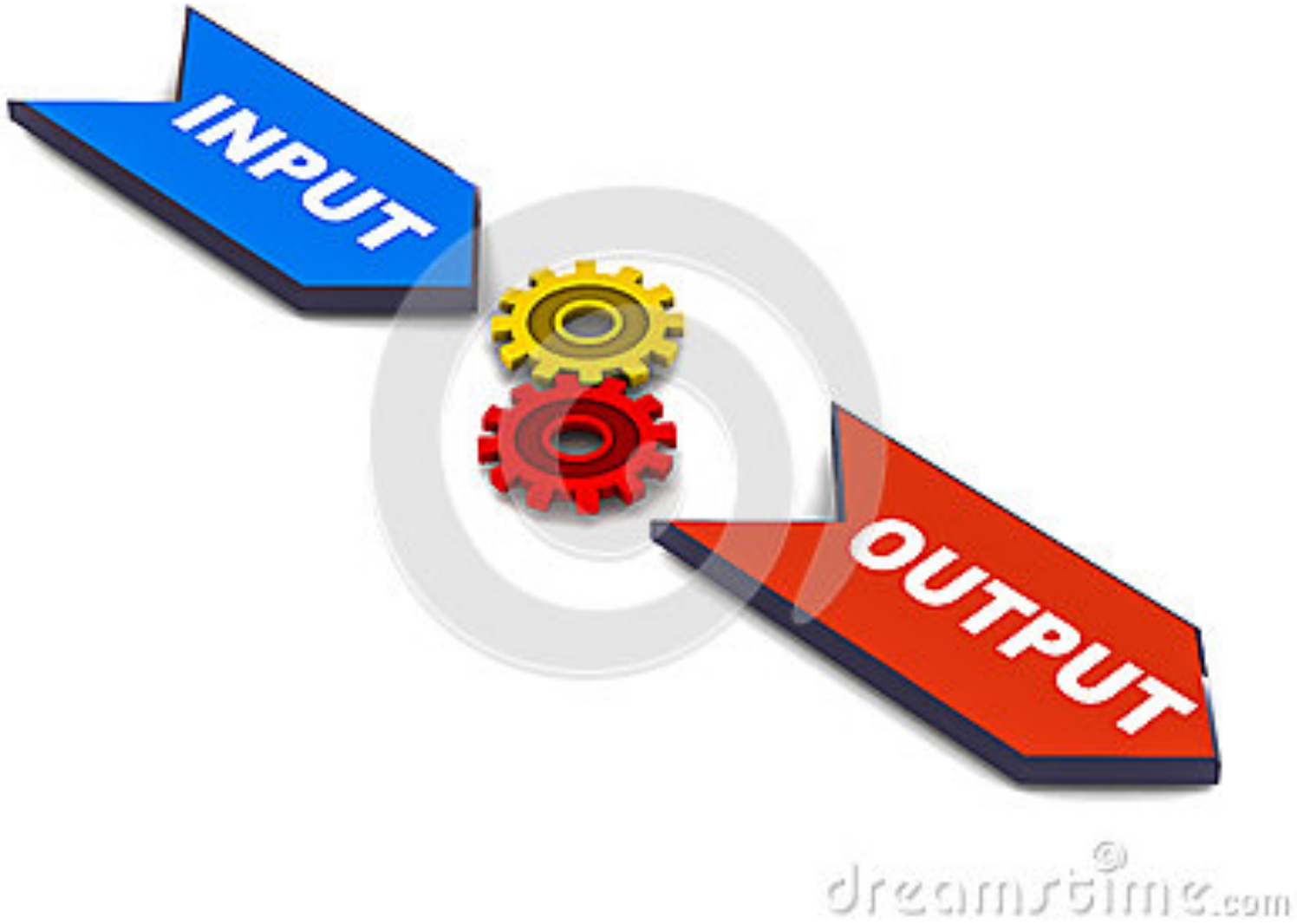


Document design and purpose, not mechanics



Document interfaces and reasons

not implementations



Document interfaces and reasons
not implementations

```
i = i + 1    # Increment the variable i by one.
```

Refactor code instead of explaining how it works

If it needs huge comments, it can be rewritten

Include documentation for code within the code

Comment often

```
1
2  class Point:
3      """ Point class represents and manipulates x,y coords. """
4
5      def __init__(self, x=0, y=0):
6          """ Create a new point at x, y """
7          self.x = x
8          self.y = y
9
10 # Other statements outside the class continue below here.
11
12 q = Point(
```

x=0, y=0
Create a new point at x, y

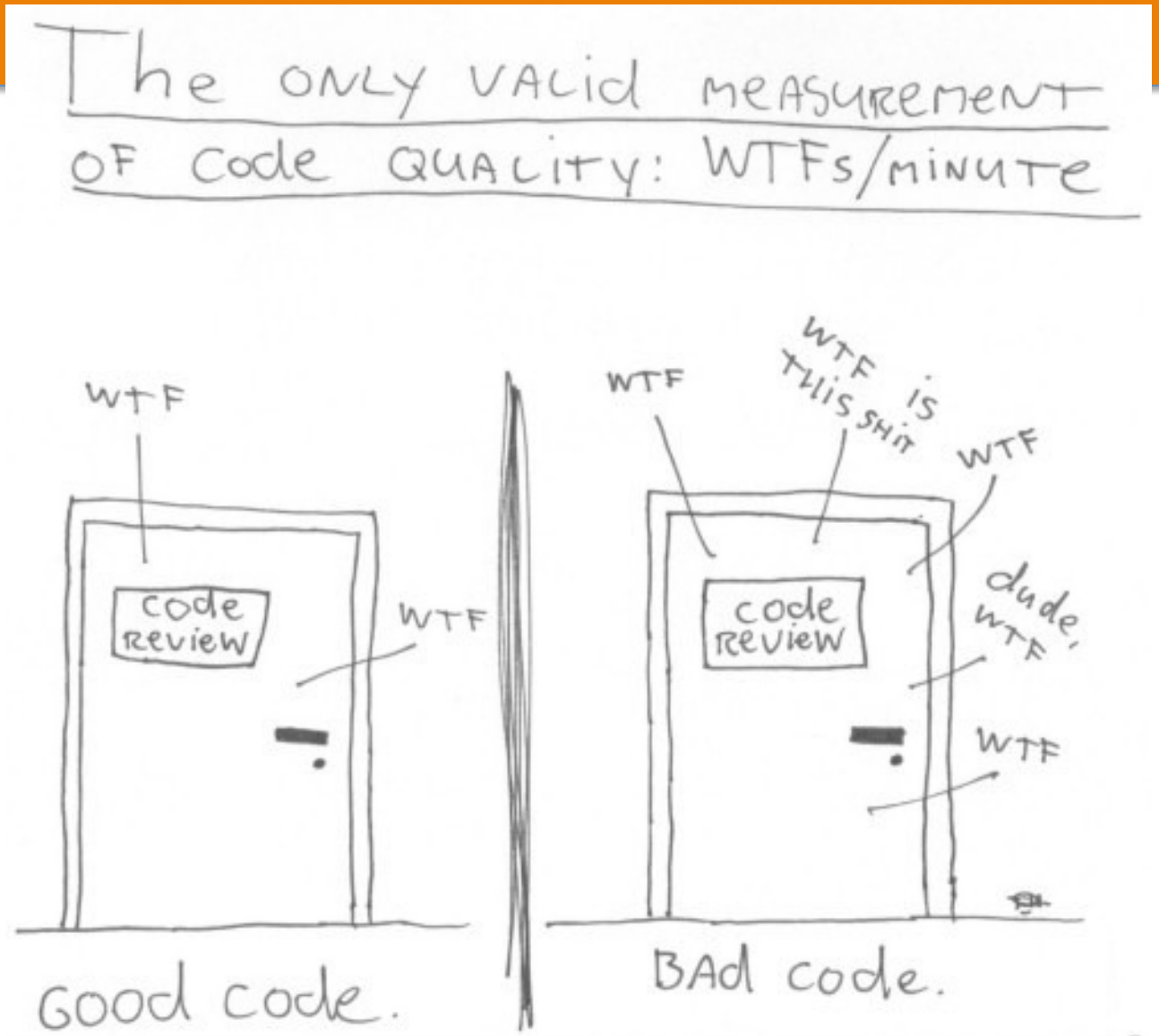
Include documentation for code within the code

Comment often

Docstrings: How to use code

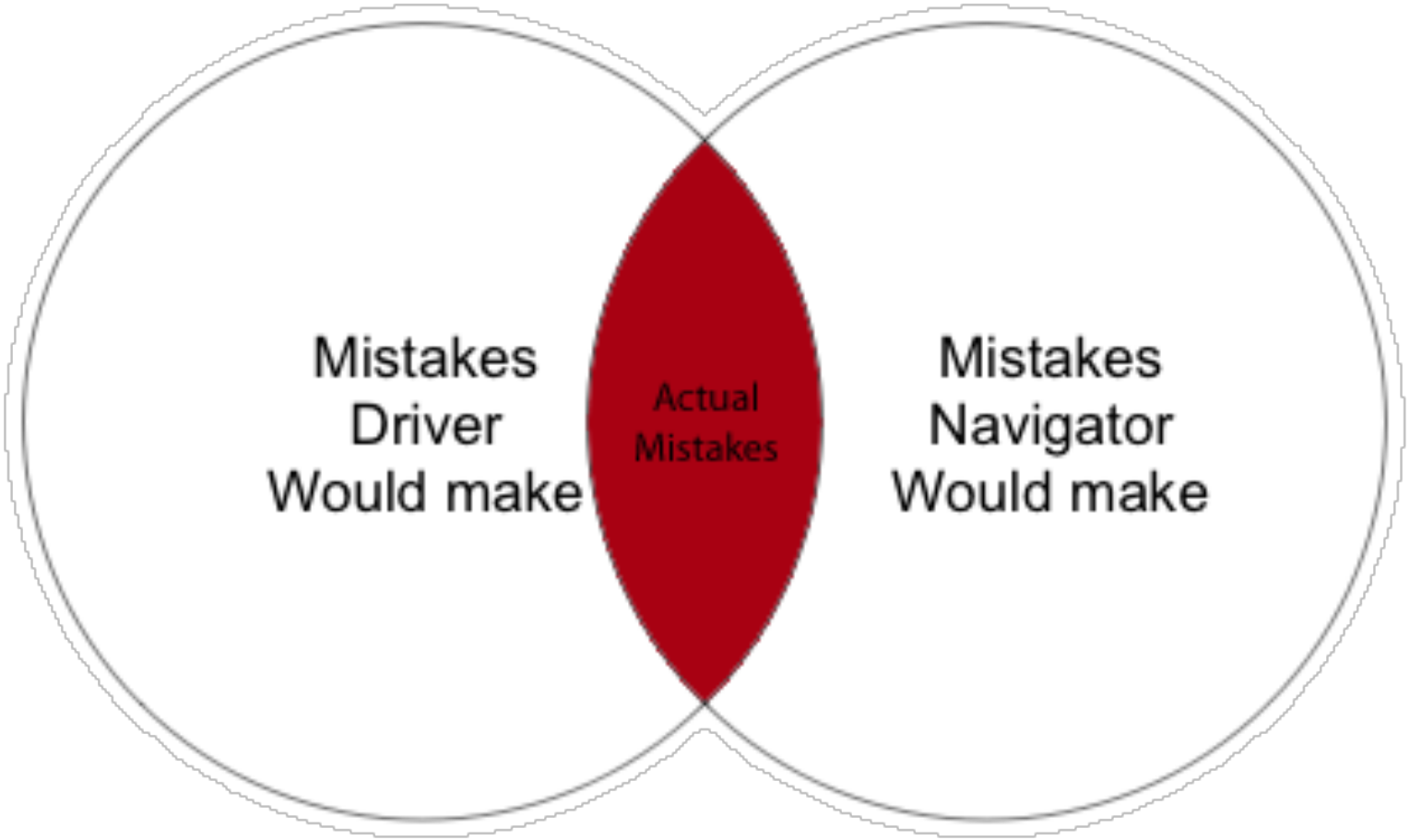
Comments: Why & how code works

Conduct code reviews



Pair Programming

Pair Programming



Pair Programming

Tackling tricky design/coding/debugging

Bringing someone new up to speed

Whenever you can

Python Conventions

Explicit Code No Black Magic

Bad

```
def make_complex(*args):
    x, y = args
    return dict(**locals())
```

Explicit Code No Black Magic

Bad

```
def make_complex(*args):
    x, y = args
    return dict(**locals())
```

Good

```
def make_complex(x, y):
    return {'x': x, 'y': y}
```

One Statement Per Line

One idea at a time

Bad

```
print 'one'; print 'two'

if x == 1: print 'one'

if <complex comparison> and <other complex comparison>:
    # do something
```

One Statement Per Line

One idea at a time

Good

```
print 'one'
print 'two'

if x == 1:
    print 'one'

cond1 = <complex comparison>
cond2 = <other complex comparison>
if cond1 and cond2:
    # do something
```

Naming conventions What to call variables

snake_case for functions, methods, attributes

snake_case or SCREAM_CASE for constants

CapsCamelCase for classes

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regular_attribute
_internal_attribute
__private_attribute

Whitespace Formatting neat code

4 spaces per indentation level

Never mix tabs and spaces

One blank line between functions

Two blank lines between classes

Long Lines

Formatting neat code

Keep lines shorter than 80 characters

Use parentheses to spread over multiple lines

Long Lines Formatting neat code

Keep lines shorter than 80 characters

Use parantheses to spread over multiple lines

Bad:

```
my_very_big_string = """For a long time I used to go to bed early. Sometimes, \
    when I had put out my candle, my eyes would close so quickly that I had not even \
    time to say “I’m going to sleep.”"""

from some.deep.module.inside.a.module import a_nice_function, another_nice_function, \
    yet_another_nice_function
```

Long Lines

Formatting neat code

Keep lines shorter than 80 characters

Use parantheses to spread over multiple lines

Good:

```
my_very_big_string = (
    "For a long time I used to go to bed early. Sometimes, "
    "when I had put out my candle, my eyes would close so quickly "
    "that I had not even time to say “I’m going to sleep.”"
)

from some.deep.module.inside.a.module import (
    a_nice_function, another_nice_function, yet_another_nice_function)
```

Python Idioms

Check if variable equals a constant

No need to explicitly compare to True, None, 0

Bad:

```
if attr == True:
    print 'True!'

if attr == None:
    print 'attr is None!'
```

Check if variable equals a constant

No need to explicitly compare to True, None, 0

Good:

```
# Just check the value
if attr:
    print 'attr is truthy!'

# or check for the opposite
if not attr:
    print 'attr is falsey!'

# or, since None is considered false, explicitly check for it
if attr is None:
    print 'attr is None!'
```

Access a Dictionary Element

Use x in d instead of has_key

Bad:

```
d = {'hello': 'world'}
if d.has_key('hello'):
    print d['hello']    # prints 'world'
else:
    print 'default_value'
```

Access a Dictionary Element

Use x in d instead of has_key

Good:

```
d = {'hello': 'world'}

print d.get('hello', 'default_value') # prints 'world'
print d.get('thingy', 'default_value') # prints 'default_value'

# Or:
if 'hello' in d:
    print d['hello']
```

Manipulating lists

List comprehensions or map() and filter()

Bad:

```
# Filter elements greater than 4
a = [3, 4, 5]
b = []
for i in a:
    if i > 4:
        b.append(i)
```

Manipulating lists

List comprehensions or map() and filter()

Good:

```
a = [3, 4, 5]
b = [i for i in a if i > 4]
# Or:
b = filter(lambda x: x > 4, a)
```

Manipulating lists

List comprehensions or map() and filter()

Bad:

```
# Add three to all list members.
a = [3, 4, 5]
for i in range(len(a)):
    a[i] += 3
```

Manipulating lists

List comprehensions or map() and filter()

Good:

```
a = [3, 4, 5]
a = [i + 3 for i in a]
# Or:
a = map(lambda i: i + 3, a)
```

Read from a file

Use the with statement

Bad:

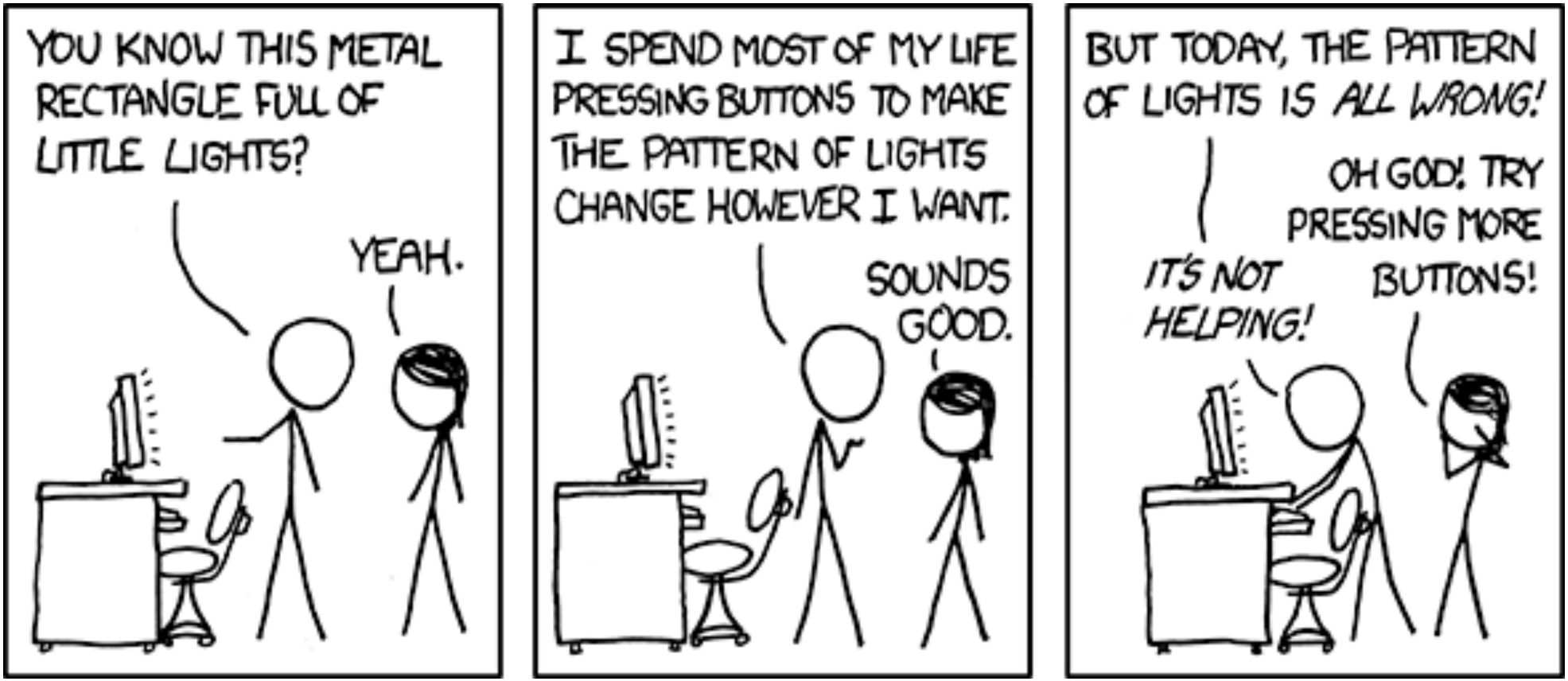
```
f = open('file.txt')
a = f.read()
print a
f.close()
```

Read from a file

Use the with statement

Good:

```
with open('file.txt') as f:
    for line in f:
        print line
```


YOU KNOW THIS METAL RECTANGLE FULL OF LITTLE LIGHTS?
YEAH.
I SPEND MOST OF MY LIFE PRESSING BUTTONS TO MAKE THE PATTERN OF LIGHTS CHANGE HOWEVER I WANT.
SOUNDS GOOD.
BUT TODAY, THE PATTERN OF LIGHTS IS ALL WRONG!
OH GOD! TRY PRESSING MORE BUTTONS!
IT'S NOT HELPING!