Test, Debug, Profile

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Based on a talk by Pietro Berkes

Scientific Programming

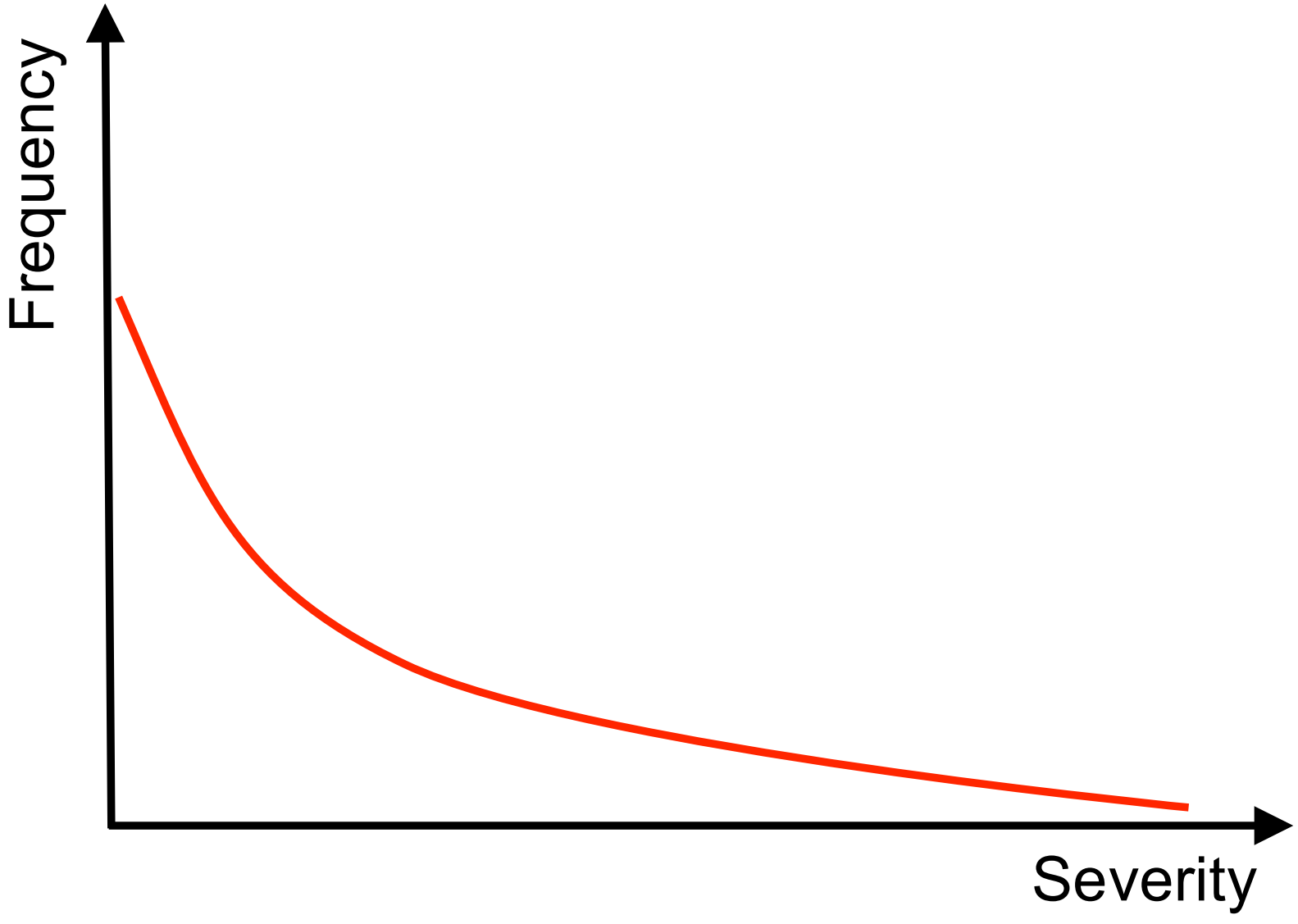
Goal

- allow exploring many different approaches
- allow frequent changes and adjustments
- produce correct and reproducible results

Requirements

- bugs most be noticed
- code can be modify easily
- others can run code too
- scientist's time is used optimally

Effect of Software Errors



Effect of Software Errors: Retractions

Science 22 December 2006:
Vol. 314 no. 5807 pp. 1856-1857
DOI: 10.1126/science.314.5807.1856

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NEWS OF THE WEEK

SCIENTIFIC PUBLISHING

A Scientist's Nightmare: Software Problem Leads to Five Retractions

Greg Miller

Due to an error caused by a homemade data-analysis program, on page 1875, Geoffrey Chang and his colleagues retract three *Science* papers and report that two papers in other journals also contain erroneous structures. (Read more.)

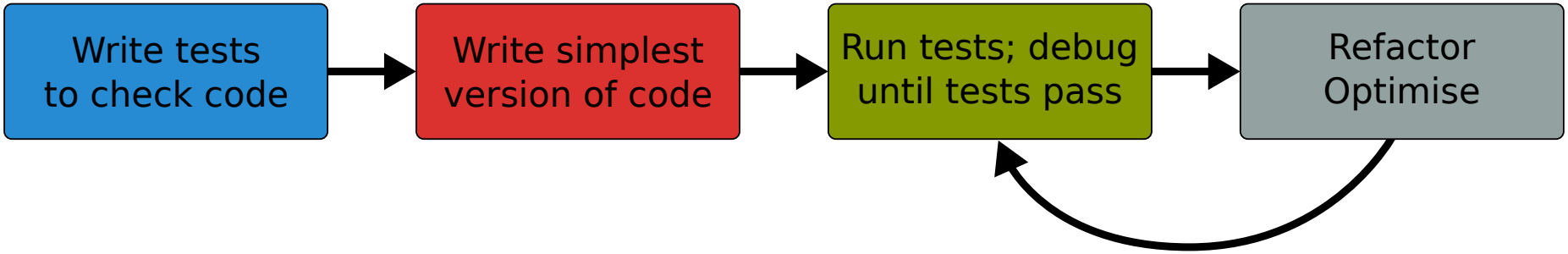
Retraction Watch

Error in one line of code sinks cancer study

without comments

Authors of a 2016 cancer paper have retracted it after finding an error in one line of code in the program used to calculate some of the results.

Outline



`unittest`	`pdb`	`timeit`
`doctest`		`cProfile`
`coverage`		`pstats`

- standard python tools
- ipython magic commands
- mostly command line

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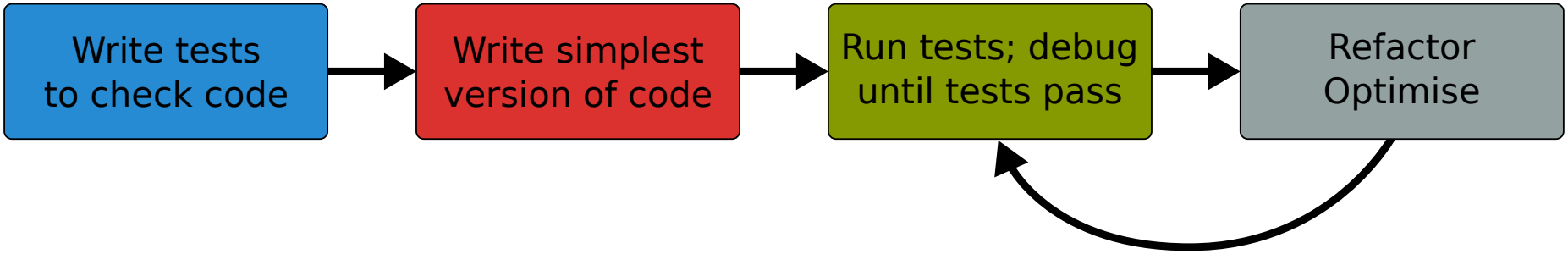

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Testing

Something you do anyway.

- run code and see if it crashes
- check if output makes sense
- run code with trivial input
- ...

Formal Testing

- important part of modern software development
- unittest and integration tests
- tests written in parallel with code
- tests run frequently/automatically
- generate reports and statistics

```
[...]
replace predefined histogram ... ok
add a legend; change line color of last histogram to red ... ok
put title and axis labels ... ok

----------------------------------------------------------------------
Ran 18 tests in 5.118s

OK
GoodBye!
```

Benefits

- only way to trust your code
- faster development
  - know where your bugs are
  - fixing bugs will not (re)introduce others
  - change code with out worrying about consistency
- encourages better code
- provides example/documentation

```
FAIL: test_result (test_fibonacci.FiboTest)
test 7th fibonacci number
----------------------------------------------------------------------
Traceback (most recent call last):
  File "test_fibonacci.py", line 18, in test_result
    self.assertEqual(result, expect)
AssertionError: 21 != 13
```

An Example

```
def remove(thelist, entry):
    """ remove entry object from list """
    for idx, item in enumerate(thelist):
        if entry is item:
            del thelist[idx]
            break
    else:
        raise ValueError("Entry not in the list")
```

Assume we find this code in an old library of ours.

An Example

```
def remove(thelist, entry):
    """ remove entry object from list """
    thelist.remove(entry)
```

We prefer to keep it simple! Everything fine, right?

An Example

```
def remove(thelist, entry):
    """ remove entry object from list """
    thelist.remove(entry)
```

```
ERROR: test_remove_array (__main__.RemoveTest)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "list_tests.py", line 19, in test_remove_array
    lrm.remove(l, x)
  File ".../examples/list_removal.py", line 3, in remove
    thelist.remove(entry)
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

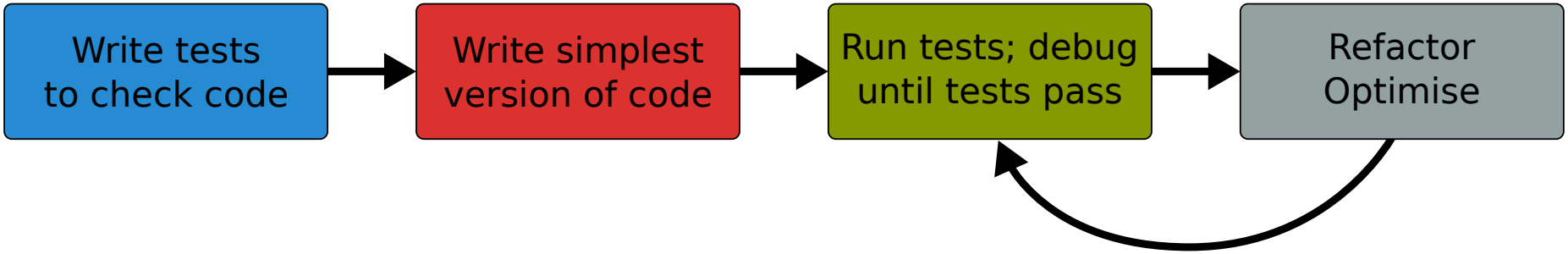
Start Testing

At the beginning, testing feels weird:

1. It's obvious that this code works
2. The tests are longer than the code
3. The test code is a duplicate of the real code

$\rightarrow$ it might take a while to get used to testing,
but it will pay off quiet rapidly.

Outline



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unittest

- library for unittests
- part of standard python
- at the level of other modern tools

Alternatives

- pytest

Anatomy of a TestCase

```
import unittest

class DemoTests(unittest.TestCase):

    def test_boolean(self):
        """ tests start with 'test' """
        self.assertTrue(True)
        self.assertFalse(False)

    def test_add(self):
        """ docstring can be printed """
        self.assertEqual(2+1, 3)

if __name__ == "__main__":
    """ execute all tests in module """
    unittest.main()
```

Summary on Anatomy

Test Cases

- are subclass of `unittest.TestCase`
- group test units

Test Units

- methods, whose names **start** with `test`
- should cover **one** aspect
- check behaviour with "assertions"
- rise exception if assertion fails

Running Tests

Option 1 execute all test units in all test cases of this file

```
if __name__ == "__main__":
    unittest.main(verbosity=1)
```

```
python3 test_module.py
```

Option 2 Execute all tests in one file

```
python3 -m unittest [-v] test_module
```

Option 3 Discover all tests in all submodules

```
python3 -m unittest discover [-v]
```

TestCase.assertSomething

- check boolean value

```
assertTrue('Hi'.islower())                    # fail
assertFalse('Hi'.islower())                   # pass
```

- check equality

```
assertEqual(2+1, 3)                           # pass
""" assertEqual can compare all sorts of objects """
assertEqual([2]+[1], [2, 1])                  # pass
```

- check numbers are close

```
from math import sqrt, pi
assertAlmostEqual(sqrt(2), 1.414, places=3) # pass
""" values are rounded, not truncated """
assertAlmostEqual(pi, 3.141, 3)               # fail
assertAlmostEqual(pi, 3.142, 3)               # pass
```

TestCase.assertRaises

- most convenient with context managers

```
with self.assertRaises(ErrorType):
    do_something()
    do_some_more()
```

- Important: use most specific exception class

```
bad_file = "inexistent"
with self.assertRaises(FileNotFoundError):    # raises NameError
    open(bad_fil, 'r')

with self.assertRaises(Exception):
    open(bad_fil, 'r')                        # pass
```

TestCase.assertMoreThings

```
assertGreater(a, b)
assertLess(a, b)

assertRegex(text, regexp)

assertIn(value, sequence)

assertIsNone(value)

assertIsInstance(my_object, class)

assertCountEqual(actual, expected)
```

complete list at
https://docs.python.org/3/library/unittest.html

TestCase.assertNotSomething

Most of the `assert` methods have a `Not` version

```
assertEqual
assertNotEqual

assertAlmostEqual
assertNotAlmostEqual

assertIsNone
assertIsNotNone
```

Testing with numpy

numpy arrays have to be compared elementwise

```
class SpecialCases(unittest.TestCase):
    def test_numpy(self):
        a = numpy.array([1, 2])
        b = numpy.array([1, 2])
        self.assertEqual(a, b)
```

```
======================================================================
ERROR: test_numpy (__main__.SpecialCases)
----------------------------------------------------------------------
Traceback (most recent call last):
  [..]
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

numpy.testing

- defines appropriate function

```
numpy.testing.assert_array_equal(x, y)
numpy.testing.assert_array_almost_equal(x, y, decimal=6)
```

- use numpy functions for more complex tests

```
numpy.all(x)          # True if all elements of x are true
numpy.any(x)          # True if any of the elements of x is true
numpy.allclose(x, y)  # True if element-wise close
```

Example

```
""" test that all elements of x are between 0 and 1 """
assertTrue(all(logical_and(x > 0.0, x < 1.0))
```

Strategies for Testing

- What does a good test look like?
- What should I test?
- What is special for scientific code?

What does a good test look like?

Given put system in right state

- create objects, initialise parameters, . . .
- define expected result

When action(s) of the test

- one or two lines of code

Then compare result with expectation

- set of assertions

What does a good test look like? – Example

```
import unittest

class LowerTestCase(unittest.TestCase):

    def test_lower(self):
        # given
        string = 'HeLlO wOrld'
        expected = 'hello world'

        # when
        result = string.lower()

        # then
        self.assertEqual(result,expected)
```

What should I test?

- simple, general case

```
string = 'HeLlO wOrld'
```

- corner cases

```
string = ''
string = 'hello'
string = '1+2=3'
```

  often involves design decisions

- any exception you raise explicitly
- any special behaviour you rely on

Reduce Overhead 1: Loops

```
import unittest

class LowerTestCase(unittest.TestCase):

    def test_lower(self):
        # given
        # Each test case is a tuple (input, expected)
        test_cases = [('HeLlO wOrld', 'hello world'),
                      ('hi', 'hi'),
                      ('123 ([?', '123 ([?'),
                      ('', '')]
        for string, expected in test_cases:
            # run several subtests
            # when
            output = string.lower()
            # then
            self.assertEqual(output, expected)
```

Reduce Overhead 1: Subtests

```
import unittest

class LowerTestCase(unittest.TestCase):

    def test_lower(self):
        # given
        # Each test case is a tuple (input, expected)
        test_cases = [('HeLlO wOrld', 'hello world'),
                      ('hi', 'hi'),
                      ('123 ([?', '123 ([?'),
                      ('', '')]
        for string, expected in test_cases:
            with self.subTest(config = string):
                # when
                output = string.lower()
                # then
                self.assertEqual(output, expected)
```

Reduce Overhead 2: Fixtures

- allow to use same setup/cleanup for several tests
- useful to
  - create data set at runtime
  - load data from file or database
  - create mock objects
- available for test case as well as test unit

```
class FixureTestCase(unittest.TestCase):

    @classmethod
    def setUpClass(self):       # called at start of TestCase

    def setUp(self):            # called before each test

    def tearDown(self):         # called at end of each test
```

What is special for scientific code?

often deterministic test cases very limited/impossible

Numerical Fuzzing

- generate random input (print random seed)
- still need to know what to expect

Know What You Expect

- use inverse function
- generate data from model
- add noise to known solutions
- test general routine with specific ones
- test optimised algorithm with brute-force approach

Automated Fuzzying: Hypothesis (not in standard library)

hypothesis generates test inputs according to given properties.

```
import unittest, numpy
from hypothesis import given, strategies as st

class SumTestCase(unittest.TestCase):

    @given(st.lists(st.integers(), min_size=2, max_size=2))
    def test_sum(self, vals):
        self.assertEqual(vals[0]+vals[1], numpy.sum(vals))
```

Why?

- cover large search-space (default 100 inputs)
- good for finding edge cases
- less manual work

Test Driven Development (TDD)

Tests First

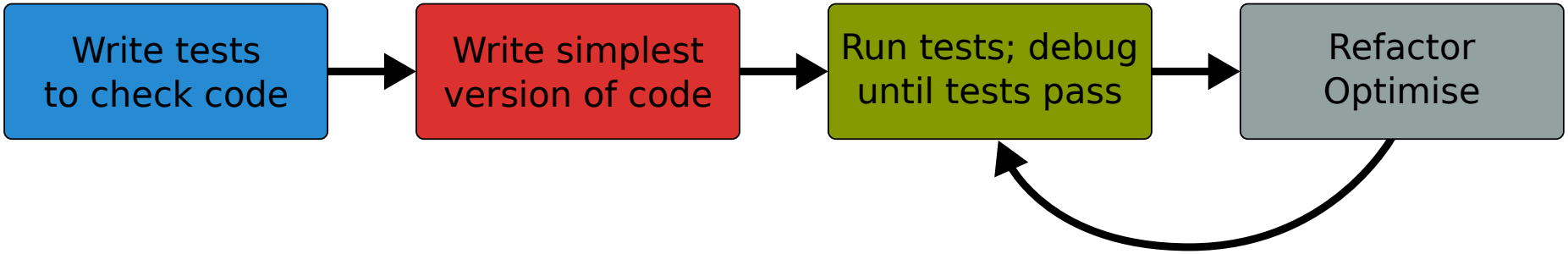
- choose next feature
- write test(s) for feature
- write simplest code

Benefits

- forced to think about design before coding
- code is decoupled and easier to maintain
- you will notice bugs

DEMO

Outline



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doctest

- poor man's unittest
- ensure docstrings are up-to-date

```python
def add(a,b):
    """ add two numbers

    Example
    -------
    >>> add(40,2)
    42

    """
    return a+b
```

```
python3 -m doctest [-v] my_doctest.py

Trying:
    add(40,2)
Expecting:
    42
ok
1 items had no tests:
    my_doctest
1 items passed all tests:
   1 tests in my_doctest.add
1 tests in 2 items.
1 passed and 0 failed.
Test passed.
```

Code Coverage

- it's easy to leave part untested
  - features activated by keyword
  - code to handle exception
- coverage tools track the lines executed

coverage.py

- python script
- produces text and HTML reports

```
python3 -m coverage run test_file.py
python3 -m coverage report [-m] [--omit="/usr*"]
```

- not in standard library
  get from https://coverage.readthedocs.io/en/latest/

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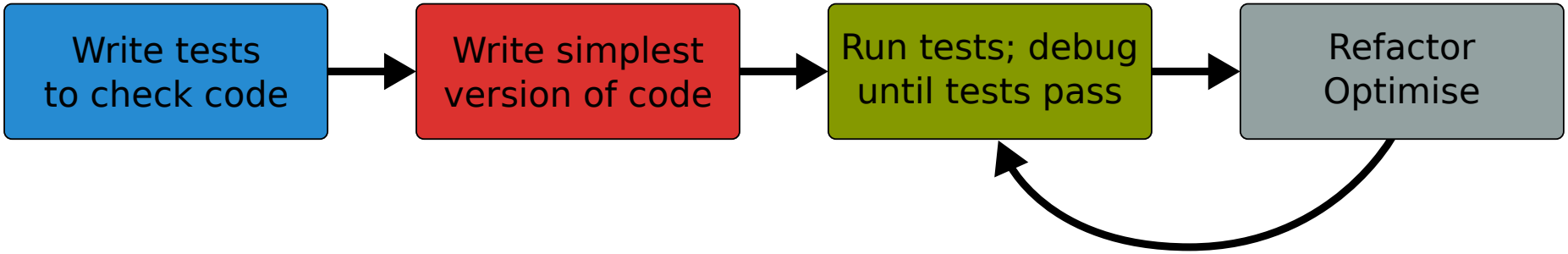

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Debugging

- use tests to avoid bugs and limit „search space”
- avoid `print` statements
- use debugger

pdb – the Python debugger

- command line based
- opens an interactive shell
- allows to
  - stop execution anywhere in your code
  - execute code step by step
  - examine and change variables
  - examine call stack

Entering pdb

- enter at start of file

```
python3 -m pdb myscript.py
```

- enter at statement/function

```
import pdb
# your code here
pdb.run(expression_string)
```

- enter at point in code

```
# some code here
# the debugger starts here
import pdb; pdb.set_trace()
# rest of the code
```

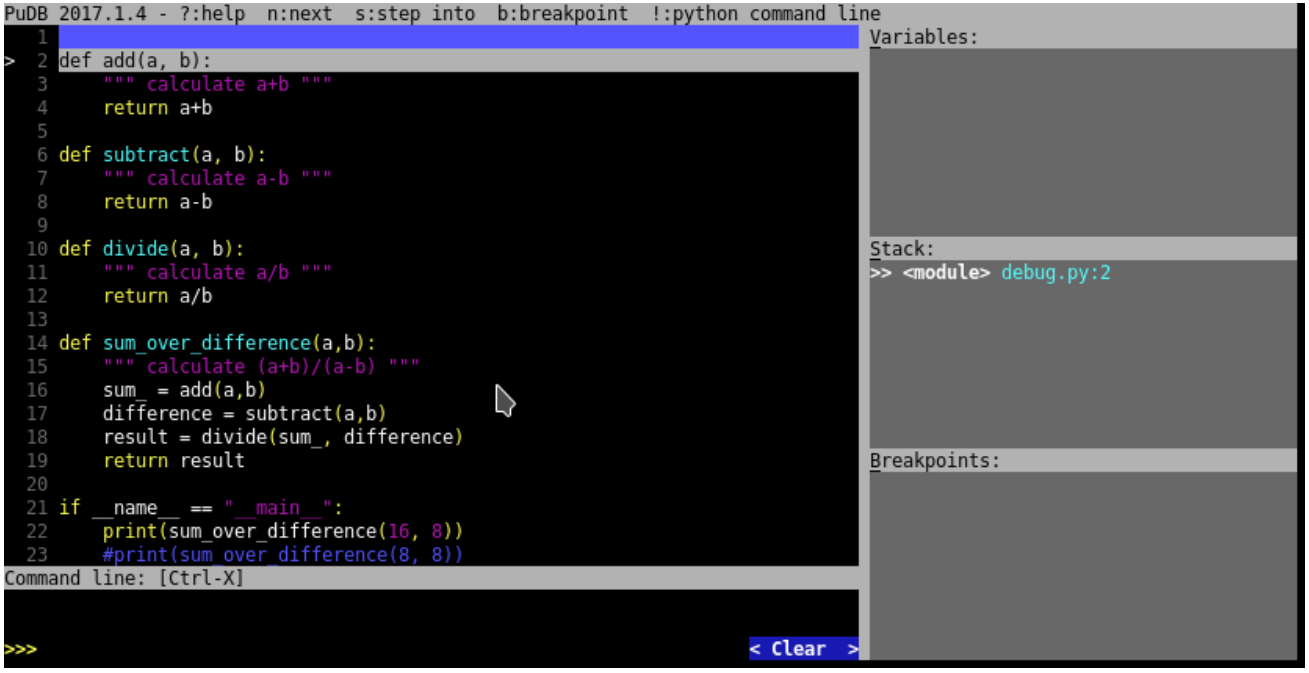
- from ipython

```
%pdb      # enter pdb on exception
%debug    # enter pdb after exception
```

Alternatives

If you prefere graphical tools

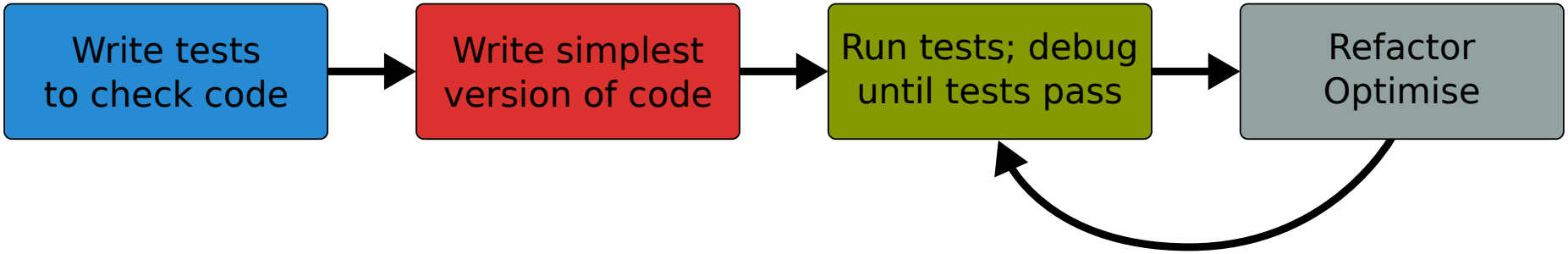
- take a look at PuDB



- or use the debugger in your development environment (Spyder, PyCharm)

DEMO

Outline



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Optimising

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2. identify time-consuming parts of code
3. only optimise those parts
4. keep running tests
5. stop as soon as possible

Optimising

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timeit

- precise timing for function/expression
- test different versions of a code block
- easiest with ipython's magic command

`a**2` or `pow(a,2)`?

```
In [1]: a = 43563

In [2]: %timeit pow(a,2)
10000000 loops, best of 5: 268 ns per loop

In [3]: %timeit a**2
10000000 loops, best of 5: 209 ns per loop
```

cProfile & Pstats

Profiling identify where most time is spent

cProfile standard python module for profiling

pstats tool to look at profiling data

- run cProfile

```
python3 -m cProfile [-s cumtime] myscript.py
python3 -m cProfile [-o myscript.prof] myscript.py
```

- analyse output from shell

```
python3 -m pstats myscript.prof

stats      # print statistics
sort       # change sort order
callers    # print callers
callees    # print callees
```

Non-Standard Tools

- pyprof2calltree and kcachegrind: open cProfile output in GUI

```
python3 -m cProfile -o myscript.prof myscript.py
. ~/school_venv/bin/activate  # on school laptops activate venv
pyprof2calltree -i myscript.prof -k
```

- pprofile: line-granularity profiler

```
pprofile3 myscript.py

pprofile3 -f callgrind -o myscript.prof myscript.py
kcachegrind myscript.prof
```

- line_profiler: original line-granularity profiler
(needs code change)

DEMO

Final Thoughts

- testing, debugging and profiling can help you a lot
- using the right tools makes life a lot easier
- python comes with good tools included
- it's as easy as it gets – there are no excuses