Best Practices, Development Methodologies, and the Zen of Python

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Introduction

- Many scientists write code regularly but few have been formally trained to do so
- **Best practices** evolved from programmer's folk wisdom
- They increase productivity and decrease stress
- **Development methodologies**, such as Agile Programming and Test Driven Development, are established in the software engineering industry
- We can learn a lot from them to improve our coding skills
- When programming in Python: Always bear in mind the **Zen of Python**

Outline

1. Introduction
2. Best Practices
   - Style and Documentation
   - Unit Tests
   - Version Control
   - Refactoring
   - Do not Repeat Yourself
   - Keep it Simple
3. Development Methodologies
   - Definition and Motivation
   - Agile Methods
   - Test Driven Development
   - Additional techniques
4. Zen of Python
5. Conclusion

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Coding Style

- Readability counts
- Explicit is better than implicit
- Beautiful is better than ugly

- Give your variables *intention revealing* names
  - For example: `numbers` instead of `nu`
  - For example: `numbers` instead of `list_of_float_numbers`
  - See also: Ottingers Rules for Naming

Example

```
def my_product(numbers):
    """ Compute the product of a sequence of numbers. """
    total = 1
    for item in numbers:
        total *= item
    return total
```

Formatting Code

- Format code to coding conventions
- for example: PEP-8
- OR use a consistent style (especially when collaborating)
- Conventions Specify:
  - variable naming convention
  - Indentation
  - import
  - maximum line length
  - blank lines, whitespace, comments
- Use automated tools to check adherence (aka static checking):
  - pylint
  - pycheker
  - pep8
  - pyflakes
  - flake8 (combination of `pep8` and `pyflakes`)

Documenting Code

- Minimum requirement: at least a single line docstring
- Not only for others, but also for yourself!
- Serves as on-line help in the interpreter

- Document arguments and return objects, including types
- Use the numpy docstring conventions

- Use tools to automatically generate website from docstrings
  - pydoc
  - epydoc
  - sphinx

- For complex algorithms, document every line, and include equations in docstring

- When your project gets bigger: provide a *how-to*, *FAQ* or *quick-start* on your website

Example Docstring

```
def my_product(numbers):
    """ Compute the product of a sequence of numbers.

    Parameters
    ----------
    numbers : sequence
        list of numbers to multiply

    Returns
    -------
    product : number
        the final product

    Raises
    ------
    TypeError
        if argument is not a sequence or sequence contains
        types that can't be multiplied
    """
```

Example Autogenerated Website

Table of Contents

Everything

Modules

my_product_docstring

[hide private]

Everything

All Functions

my_product_docstring.my_

All Variables

my_product_docstring.__p

[hide private]

Home Trees Indices Help

Module my_product_docstring

[hide private]
[frames] | no frames]

Module my_product_docstring

source code

Functions

[hide private]

	my_product(numbers) source code Compute the product of a sequence of numbers.

Variables

[hide private]

	__package__ = None

Function Details

[hide private]

my_product(numbers)

source code

```
Compute the product of a sequence of numbers.

Parameters
----------
numbers : sequence
    list of numbers to multiply

Returns
-------
product : number
    the final product

Raises
------
TypeError
    if argument is not a sequence or sequence contains
    types that can't be multiplied
```

Home Trees Indices Help

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Using Exceptions

- Use the `try except` statements to detect anomalous behaviour:

Example

```
try:
    my_product(['abc', 1])
except TypeError:
    print "'my_product' failed due to a 'TypeError'"
```

- Allow you to recover or fail gracefully
- Resist the temptation to use *special* return values: they will backfire!
  - `(-1, 0, False, None)`
- Fail early, fail often
- Errors should never pass silently...
- Unless explicitly silenced

Appropriate Exceptions

- Python has a built-in Exception hierarchy
- These will suit your needs most of the time, If not, subclass them

```
Exception
+-- StandardError
    +-- ArithmeticError
        +-- FloatingPointError
        +-- OverflowError
        +-- ZeroDivisionError
    +-- AssertionError
    +-- IndexError
    +-- TypeError
    +-- ValueError
```

`import` Pitfalls

- Don't use the *star import*: `import *`
  - Code is hard to read
  - Modules may overwrite each other
  - Where does this function come from?
  - You will import *everything* in a module
  - ...unless you are using the interpreter interactively
- Put all imports at the beginning of the file...
- ...unless you have a very good reason to do otherwise

`import foobar as fb` **VS** `from foo import bar`

Example

```
import my_product as mp
mp.my_product([1,2,3])
```

- \+ origin of `my_product` known
- − slightly more to type
- − fails only on call (late)

Example

```
from my_product import my_product
my_product([1,2,3])
```

- \+ slightly less to type
- \+ fails on import (early)
- − must look at `import` for origin

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Write and Run Unit Tests

- We wish to automate testing of our software
- Instead of testing the whole system we test *units*

Definition of a *Unit*

- The smallest testable piece of code
- Example: `my_product`

Available Packages

- In python we have several packages available:
  - unittest
  - nosetest
  - py.test
  - Mock
- Tests increase the confidence that your code works correctly, not only for yourself but also for your reviewers
- Tests are the only way to trust your code
- It might take you a while to get used to writing them, but it will pay off quite rapidly

Example Unit-Tests

Example

```
import nose.tools as nt
from my_product import my_product

def test_my_product():
    """ Test my_product() on simple case. """
    nt.assert_equal(my_product([1, 2, 3]), 6)

def test_raise_type_error():
    """ Test that my_product raises a type error. """
    nt.assert_raises(TypeError, my_product, ['abc', 1, 2, 3])
```

Running the Tests

```
zsh» nosetests
.F
======================================================================
FAIL: Test that my_product raises a type error.
----------------------------------------------------------------------
Traceback (most recent call last):
  File "/usr/lib/pymodules/python2.6/nose/case.py", line 183, in runTest
    self.test(*self.arg)
  File "/home/valentin/git-working/best-practices-talk/\
       code/my_product_test.py", line 10, in test_raise_type_error
    nt.assert_raises(TypeError, my_product, ['abc', 1, 2, 3])
AssertionError: TypeError not raised

----------------------------------------------------------------------
Ran 2 tests in 0.011s

FAILED (failures=1)
```

Whats going on?

```
>>> my_product(['abc', 1, 2, 3])
    'abcabcabcabcabcabc'
```

A Sneak Preview of Test-Driven Development (TDD)

```
from numbers import Number

def my_product(numbers):
    """ Compute the product of a sequence of numbers. """
    total = 1
    for item in numbers:
        if not isinstance(item, Number):
            raise TypeError("%r unsupported by 'my_product'"
                            %type(item))
        total *= item
    return total
```

But make sure that it works!

Example

```
from my_product_fixed import my_product
```

```
zsh» nosetests my_product_fixed_test.py
..
----------------------------------------------------------------------
Ran 2 tests in 0.001s

OK
```

Goals and Benefits

Goals

- check code works
- check design works
- catch regression

Benefits

- Easier to test the whole, if the units work
- Can modify parts, and be sure the rest still works
- Provide examples of how to use code

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Motivation to use Version Control

Problem 1

"Help! my code worked yesterday, but I can't recall what I changed."

- Version control is a method to track and retrieve modifications in source code

Problem 2

"We would like to work together, but we don't know how!"

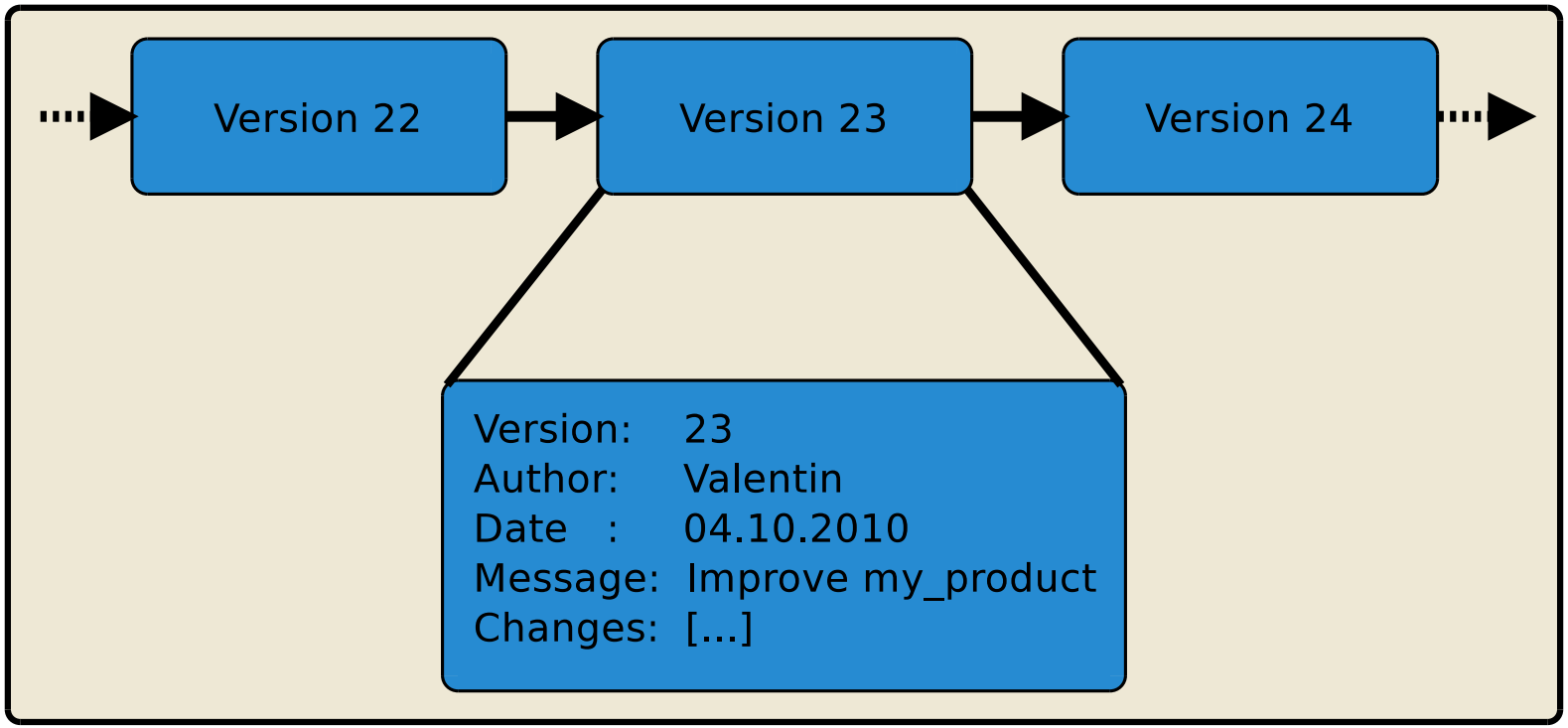
- Concurrent editing by several developers is possible via merging

Features

- Checkpoint significant improvements, for example releases
- Document developer effort
  - Who changed what, when and why?
- Use version control for anything that's text
  - Code
  - Thesis/Papers
  - (Love) letters
- Easy collaboration across the globe

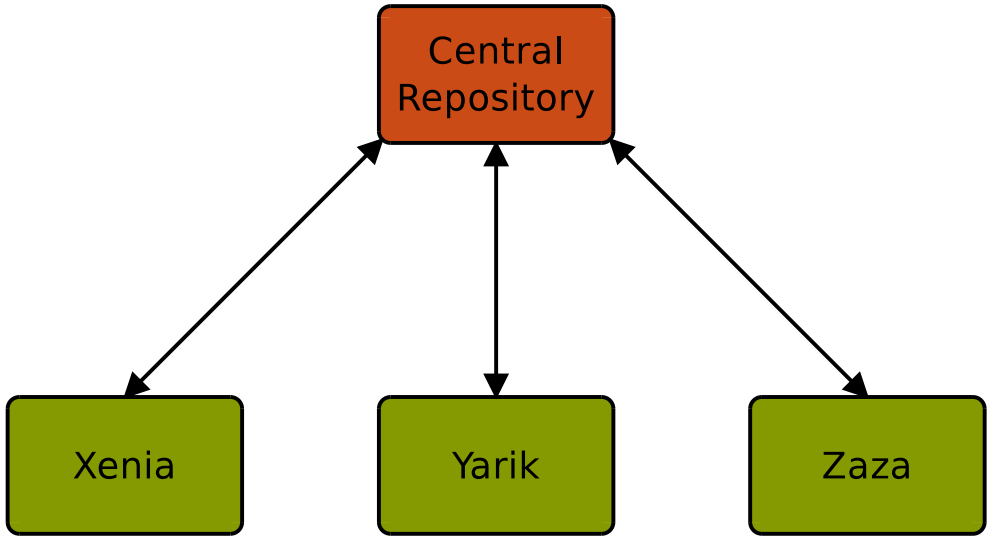
Vocabulary

- Modifications to code are called *commits*
- Commits are stored in a *repository*
- Adding commits is called *committing*



Centralised Version Control

- All developers connect to a single resource over the network
- Any interaction (history, previous versions, committing) require network access



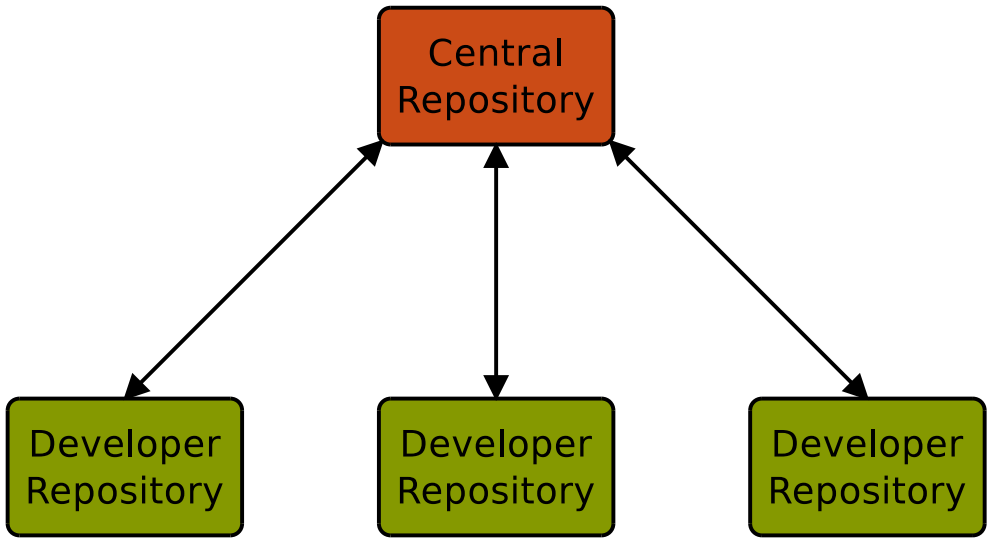
- Example systems: Subversion (svn), Concurrent Version System (cvs)

Distributed Version Control

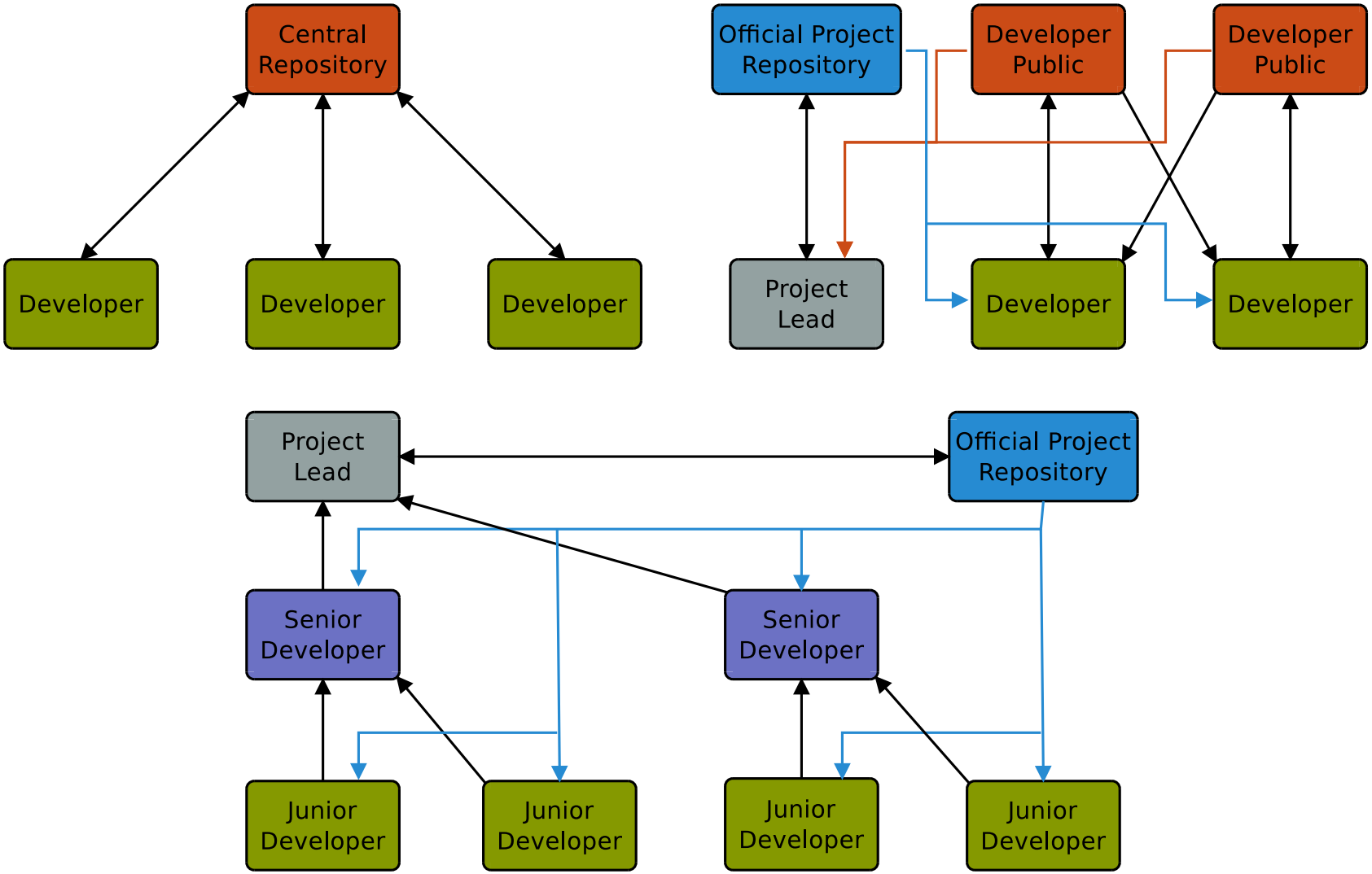
- Several copies of the repository may exist all over the place
- Network access only required when synchronising repositories
- Much more flexible than centralised
- Widely regarded as state-of-the-art
- Example systems: git, Mercurial (hg), Bazaar (bzr)

Distributed like Centralised

- ... except that each developer has a *complete* copy of the entire repository



Distributed Supports any Workflow :-)



What we will use...

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Refactor Continuously

- As a program evolves it may become necessary to rethink earlier decisions and adapt the code accordingly

- Re-organisation of your code without changing its function
- Increase modularity by breaking large code blocks apart
- Rename and restructure code to increase readability and reveal intention

- Always refactor one step at a time, and use the tests to check code still works

- Now is better than never
- Although never is often better than *right* now

Common Refactoring Operations

- Rename class/method/module/package/function
- Move class/method/module/package/function
- Encapsulate code in method/function
- Change method/function signature
- Organize imports (remove unused and sort)

- Generally you will improve the readability and modularity of your code
- Usually refactoring will reduce the lines of code

Refactoring Example

```
def my_func(numbers):
    """ Difference between sum and product of sequence. """
    total = 1
    for item in numbers:
        total *= item
    total2 = 0
    for item in numbers:
        total2 += item
    return total - total2
```

Split into functions, and use built-ins

```
from my_product import my_product

def my_func(numbers):
    """ Difference between sum and product of sequence. """
    product_value = my_product(numbers)
    sum_value = sum(numbers)
    return product_value - sum_value
```

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Do not Repeat Yourself (DRY Principle)

- When developing software, avoid duplication
- No cut&paste!
- Not just lines code, but knowledge of all sorts
- Do not express the same piece of knowledge in two places
- If you need to update this knowledge you will have to update it everywhere
- It is not a question of *how* this may fail, but instead a question of *when*
- Categories of Duplication:
  - Imposed Duplication
  - Inadvertent Duplication
  - Impatient Duplication
  - Interdeveloper Duplication
- If you detect duplication in code thats already written, refactor mercilessly!

Imposed Duplication

- When duplication seems to be forced on us
- We feel like there is no other solution
- The environment or programming language seems to require duplication

Example

- Duplication of a program version number in:
  - Source code
  - Website
  - Licence
  - README
  - Distribution package
- Result: Increasing version number consistently becomes difficult

Inadvertent Duplication

- When duplication happens by accident
- You don't realize that you are repeating yourself

Example

- Variable name: `list_of_numbers` instead of just `numbers`
- Type information duplicated in variable name
- What happens if the set of possible types grows or shrinks?
- Side effect: Type information incorrect, function may operate on any sequence such as tuples

Impatient Duplication

- Duplication due to sheer laziness
- Reasons:
  - End-of-day
  - Deadline
  - Insert `pretext` here

Example

- Copy-and-paste a snippet, instead of refactoring it into a function
- What happens if the original code contains a bug?
- What happens if the original code needs to be changed?

- By far the easiest category to avoid, but requires discipline and willingness
- Be patient, invest time now to save time later! (especially when facing oh so important deadlines)

Interdeveloper Duplication

- Repeated implementation by more than one developer
- Usually concerns utility methods
- Often caused by lack of communication
- Or lack of a module to contain utilities
- Or lack of library knowledge

Interdeveloper Duplication Example

- Product function may already exist in some library
- (Though I admit this may also be classified as impatient duplication)

Example

```
import numpy

def my_product_refactor(numbers):
    """ Compute the product of a sequence of numbers. """
    return numpy.prod(numbers)
```

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Keep it Simple (Stupid) (KIS(S) Principle)

- Resist the urge to over-engineer
- Write only what you need now

- Simple is better than complex
- Complex is better than complicated

- Special cases aren't special enough to break the rules
- Although practicality beats purity

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What is a Development Methodology?

Consists of:

- An attitude that informs the style and approach towards development
- A set of tools and models to support that particular approach

Help answer the following questions:

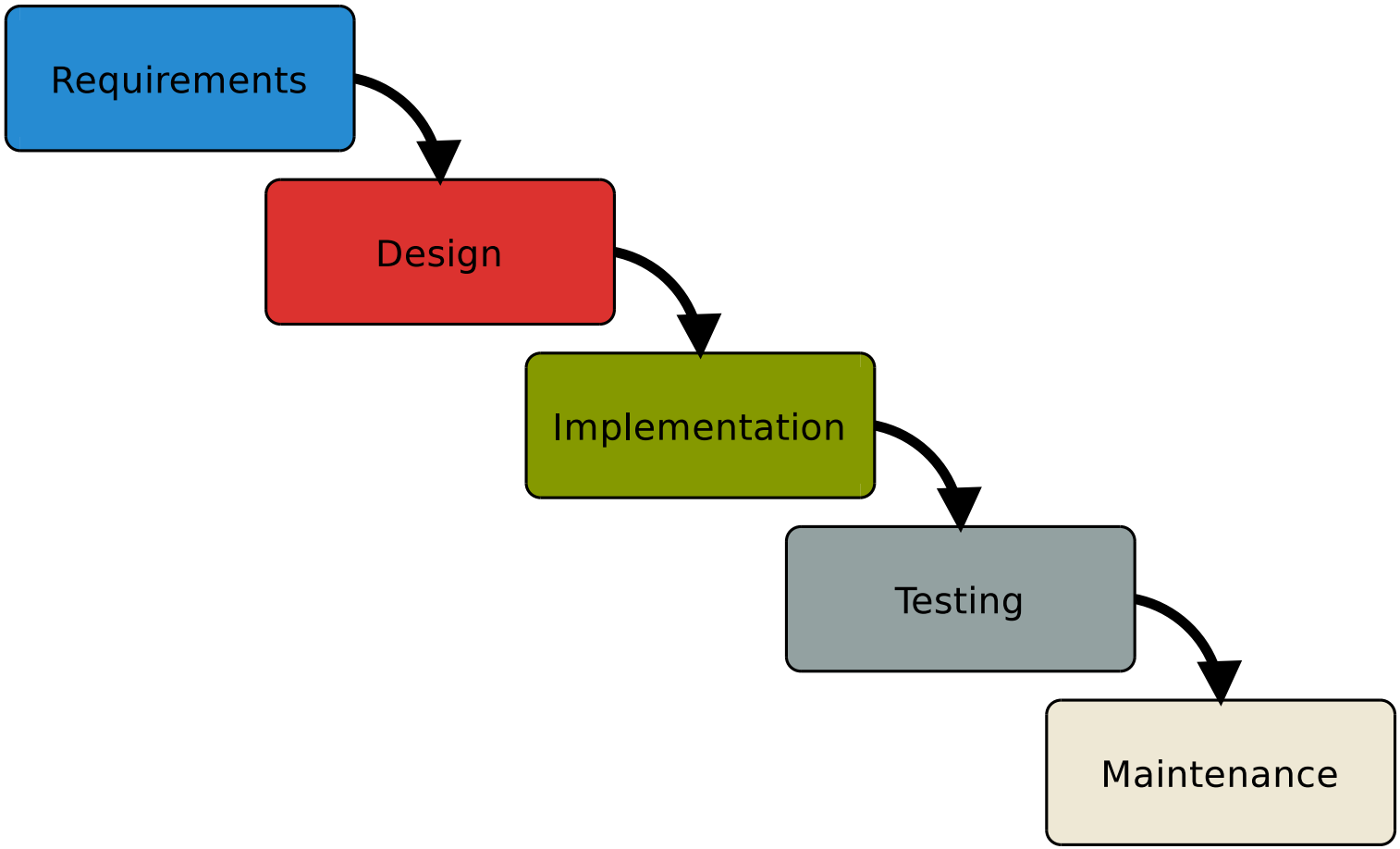
- How far ahead should I plan?
- What should I prioritize?
- When do I write tests and documentation?

Scenarios

- Lone student/scientist

- Small team of scientists, working on a common library
- Speed of development more important than execution speed
- Often need to try out different ideas quickly:
  - rapid prototyping of a proposed algorithm
  - re-use/modify existing code

An Example: The Waterfall Model, Royce 1970



- Sequential software development process
- Originates in the manufacturing and construction industries
- Rigid, inflexible model—focusing on one stage at a time

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Agile Methods

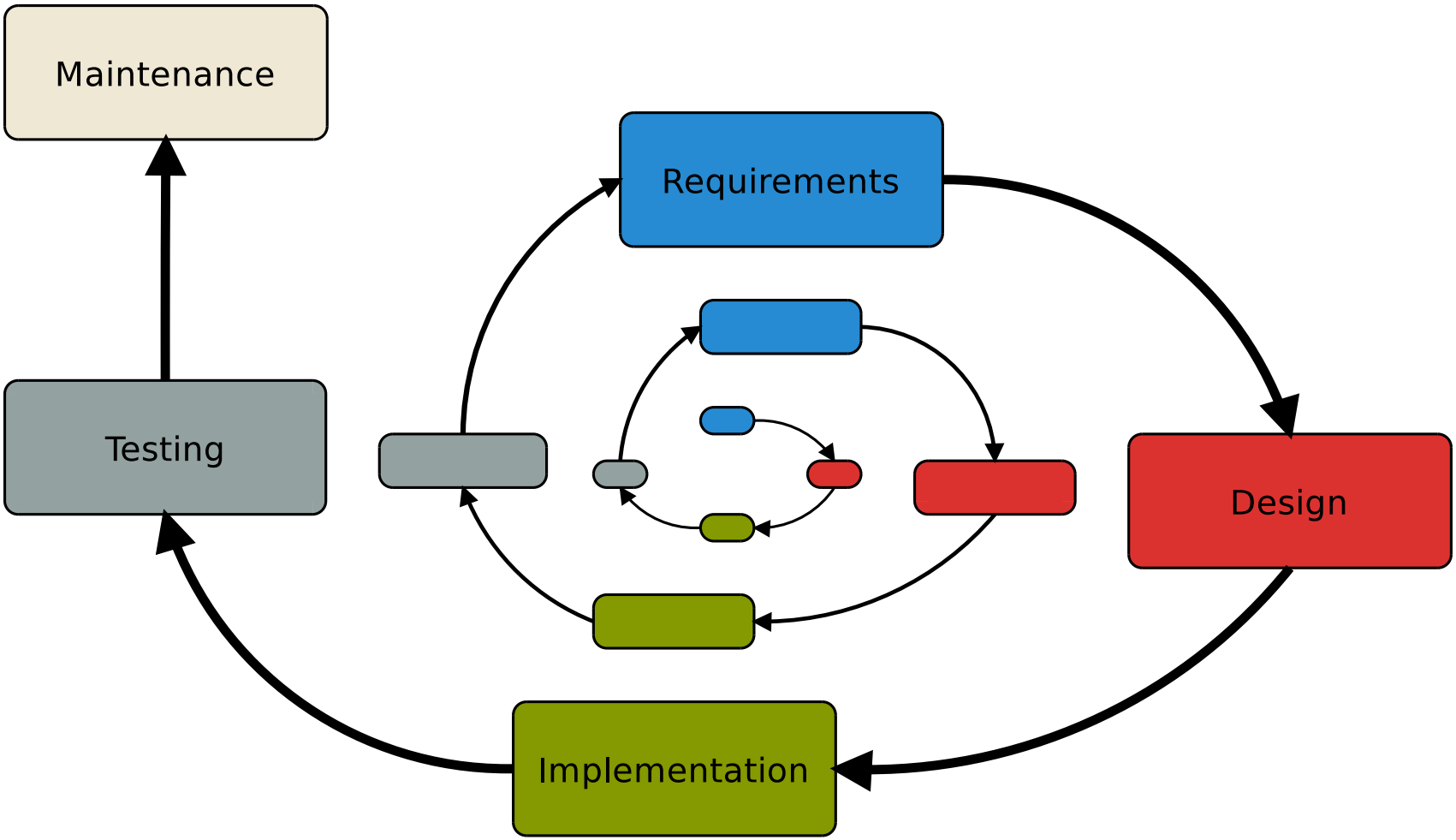
- Agile methods emerged during the late 90's
- Generic name for set of more specific paradigms
- Set of *best practices*

- Particularly suited for:
  - Small teams (Fewer than 10 people)
  - Unpredictable or rapidly changing requirements...
  - ... isn't this what science is all about?

Prominent Features of Agile methods

- Minimal planning, small development iterations
- Design/implement/test on a modular level
- Rely heavily on testing
- Promote collaboration and teamwork, including frequent input from customer/boss/professor
- Very adaptive, since nothing is set in stone

The Agile Spiral



Agile methods

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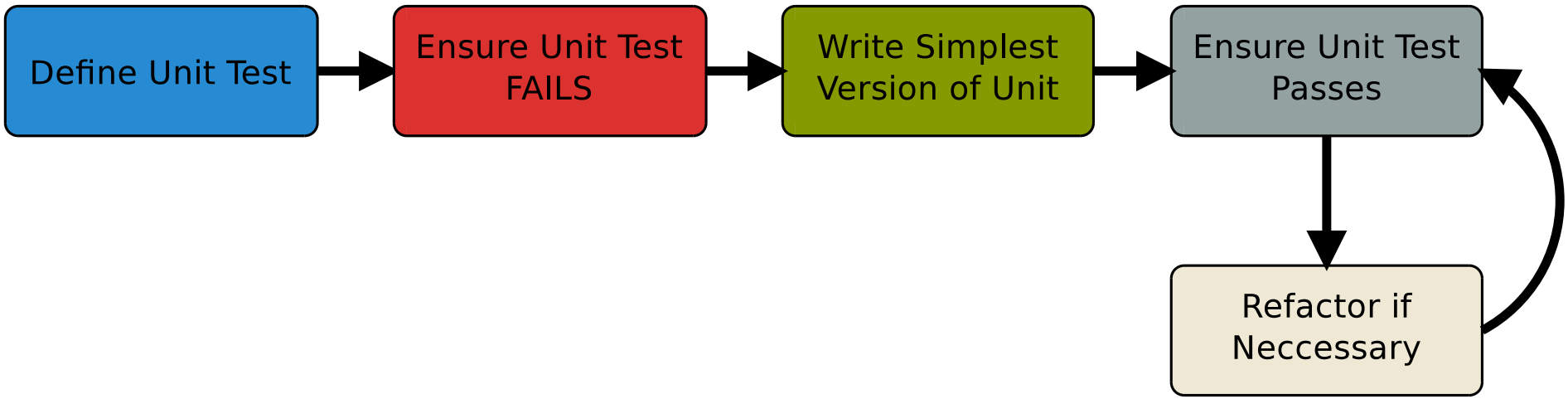
Test Driven Development (TDD)



- Define unit tests first!
- Develop one unit at a time!

Benefits of TDD

- Encourages simple designs and inspires confidence
- No one ever *forgets* to write the unit tests
- Helps you design a good API, since you are forced to use it when testing (*dog fooding*)
- Perhaps you may want to even write the documentation first?

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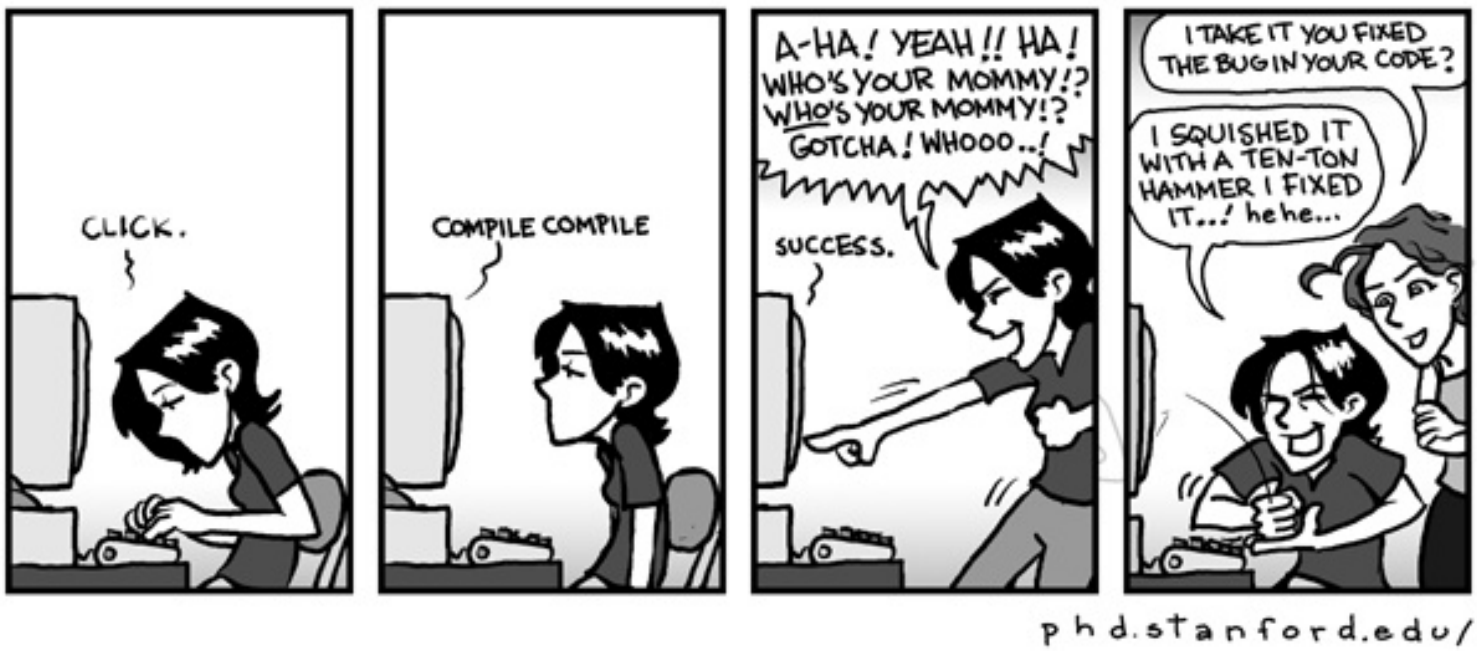
Dealing with Bugs — The Agile Way

- Write a unit test to expose the bug
- Isolate the bug using a debugger
- Fix the code, and ensure the test passes
- Use the test to catch the bug should it reappear (regression)

Debugger

- A program to run your code one step at a time, and giving you the ability to inspect the current state
- For example:
  - pdb
  - ipdb (IPython enhanced pdb)
  - winpdb
  - pudb
  - pydb|pydbgr

Dealing with Bugs?



Design by Contract

- Functions carry their specifications around with them:
  - Keeping specification and implementation together makes both easier to understand
  - ...and improves the odds that programmers will keep them in sync
- A function is defined by:
  - pre-conditions: what must be true in order for it to work correctly
  - post-conditions: what it guarantees it will be true if pre-conditions are met
- Pre- and post-conditions constrain how the function can evolve:
  - can only ever relax pre-conditions (i.e., take a wider range of input)...
  - ...or tighten post-conditions (i.e., produce a narrower range of output)
  - tightening pre-conditions, or relaxing post-conditions, would violate the function's contract with its callers

Defensive Programming

- Specify pre- and post-conditions using assertion:
  - `assert len(numbers) > 0`
  - `raise AssertionError`
- Use assertions liberally
- Program as if the rest of the world is out to get you!
- Fail early, fail often, fail better!
- The less distance there is between the error and you detecting it, the easier it will be to find and fix
- It's never too late to do it right
  - Every time you fix a bug, put in an assertion and a comment
  - If you made the error, the right code can't be obvious
  - You should protect yourself against someone "simplifying" the bug back in

Pair Programming

- Two developers, one computer
- Two roles: driver and navigator
- Driver sits at keyboard
  - Can focus on the tactical aspects
  - See only the “road” ahead
- Navigator observes and instructs
  - Can concentrate on the “map”
  - Pay attention to the big picture
- Switch roles every so often!

- In a team: switch pairs every so often!

Pair Programming — Benefits

- Know-How is shared/transfered:
  - Specifics of the system
  - Tool usage (editor, interpreter, debugger, version control)
  - Coding style, idioms, knowledge of library
- Less likely to:
  - Surf the web, read personal email
  - Be interrupted by others
  - Cheat themselves (being impatient, taking shortcuts)
- Pairs produce code which:[1]
  - Is shorter
  - Incorporates better designs
  - Contains fewer defects...
  - ... $1+1 > 2$!

[1] Cockburn, Alistair, Williams, Laurie (2000). *The Costs and Benefits of Pair Programming*

Optimization for Speed — My Point of View

- Readable code is usually better than fast code
- Programmer/Scientist time is more valuable than computer time
- Don't optimize early, ensure code works, has tests and is documented...
- *before* starting to optimize
- Only optimize if it is absolutely necessary
- Only optimize your bottlenecks
- ...and identify these using a profiler

Profilers and Viewers

Profiler

- A tool to measure and provide statistics on the execution of code.
  - timeit
  - cProfile
  - line profiler
  - Memory profiler

Viewer

- Viewers display the profiler output, usually a call-graph
  - gprof2dot
  - run snake run
  - kcachegrind

Quick Example

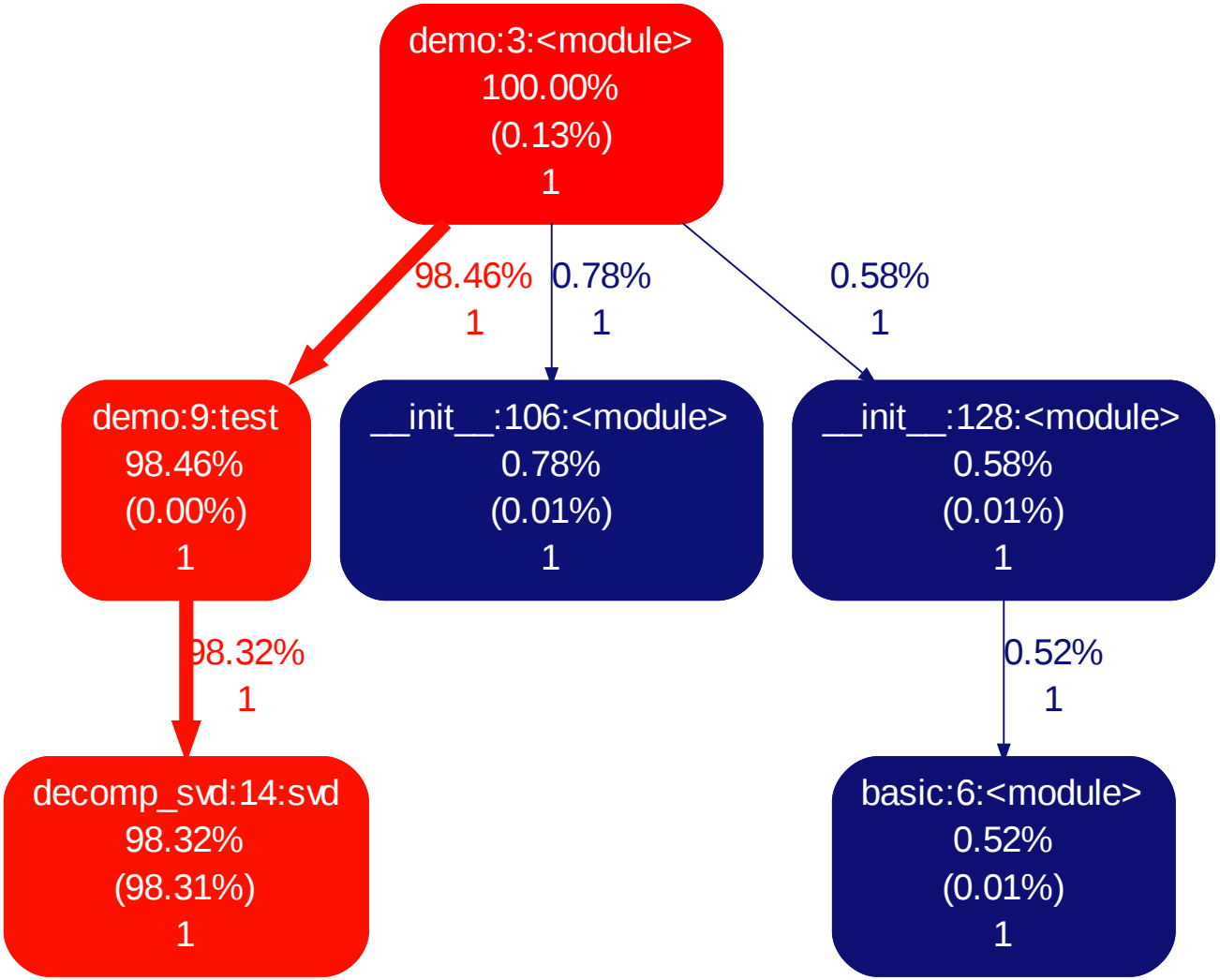
Call the Profiler

```
zsh» python -m cProfile -o profile-stats \
    ./wiki2beamer-0.9.2 slides.wiki > /dev/null
```

Generate the Call-Graph

```
zsh» gprof2dot.py -f pstats profile-stats |
    dot -Tpdf -o profile_stats.svg
```

Call-Graph


demo:3:<module>
100.00%
(0.13%)
1
98.46%
1
0.78%
1
0.58%
1
demo:9:test
98.46%
(0.00%)
1
__init__:106:<module>
0.78%
(0.01%)
1
__init__:128:<module>
0.58%
(0.01%)
1
98.32%
1
0.52%
1
decomp_svd:14:svd
98.32%
(98.31%)
1
basic:6:<module>
0.52%
(0.01%)
1

Prototyping

- Ever tried to hit a moving target?

- If you are unsure how to implement something, write a prototype
- Hack together a proof of concept quickly
- No tests, no documentation, keep it simple (stupid)
- Use this to explore the feasibility of your idea
- When you are ready, scrap the prototype and start with the unit tests

- In the face of ambiguity, refuse the temptation to guess

Quality Assurance

- The techniques I have mentioned above help to assure high quality of the software
- Quality is not just testing:
  - Trying to improve the quality of software by doing more testing is like trying to lose weight by weighing yourself more often
- Quality is designed in (For example, by using the DRY and KISS principles)
- Quality is monitored and maintained through the whole software life cycle

Outline

1. Introduction
2. Best Practices
   - Style and Documentation
   - Unit Tests
   - Version Control
   - Refactoring
   - Do not Repeat Yourself
   - Keep it Simple
3. Development Methodologies
   - Definition and Motivation
   - Agile Methods
   - Test Driven Development
   - Additional techniques
4. Zen of Python
5. Conclusion

The Zen of Python

```
>>>import this
The Zen of Python, by Tim Peters

Beautiful is better than ugly.
Explicit is better than implicit.
Readability counts.
Simple is better than complex.
Complex is better than complicated.
Flat is better than nested.
Sparse is better than dense.
Readability counts.
Special cases aren't special enough to break the rules.
Although practicality beats purity.
Errors should never pass silently.
Unless explicitly silenced.
In the face of ambiguity, refuse the temptation to guess.
There should be one-- and preferably only one --obvious way to do it.
Although that way may not be obvious at first unless you're Dutch.
Now is better than never.
Although never is often better than *right* now.
If the implementation is hard to explain, it's a bad idea.
```

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Results

- Every scientific result (especially if important) should be independently reproduced at least internally before publication. (German Research Council 1999)
- Increasing pressure to make the source code (and data?) used in publications available
- With unit tested code you need not be embarrassed to publish your code
- Using version control allows you to share and collaborate easily
- In this day and age there is **absolutely no excuse** to not use them!
- If you can afford it, hire a developer :-)

The Last Slide

- Slides based on:
  - Material by Pietro Berkes and Tiziano Zito
  - *The Pragmatic Programmer* by Hunt and Thomas,
  - *The* Course on Software Carpentry by Greg Wilson
- Open source tools used to make this presentation:
  - Wiki2beamer
  - LaTeXbeamer
  - Dia
  - Pygments
  - Minted
  - Solarized theme for pygments

Questions ?

https://github.com/esc/best-practices-talk

http://krzz.de/u