Strategies, motivations, and influencing adoption of testing for scientific code

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Bios and Intros

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Slides: https://t.co/antAoj38tD

Aims

Make a case for using tests to improve valuable functional and non-functional attributes of scientific and research code.

Sketch out part of the spectrum of useful unit test related techniques.

Provide some social and organizational strategies to influence adoption.

Science Programming

Science Programming:
A Second Class Citizen?

> *[…] recent studies have found that scientists typically spend 30% or more of their time developing software. However, 90% or more of them are primarily self-taught, and therefore lack exposure to basic software development practices […]*

“Best Practices for Scientific Computing”, Wilson et al, 2012
arXiv:1210.0530 [cs.MS]

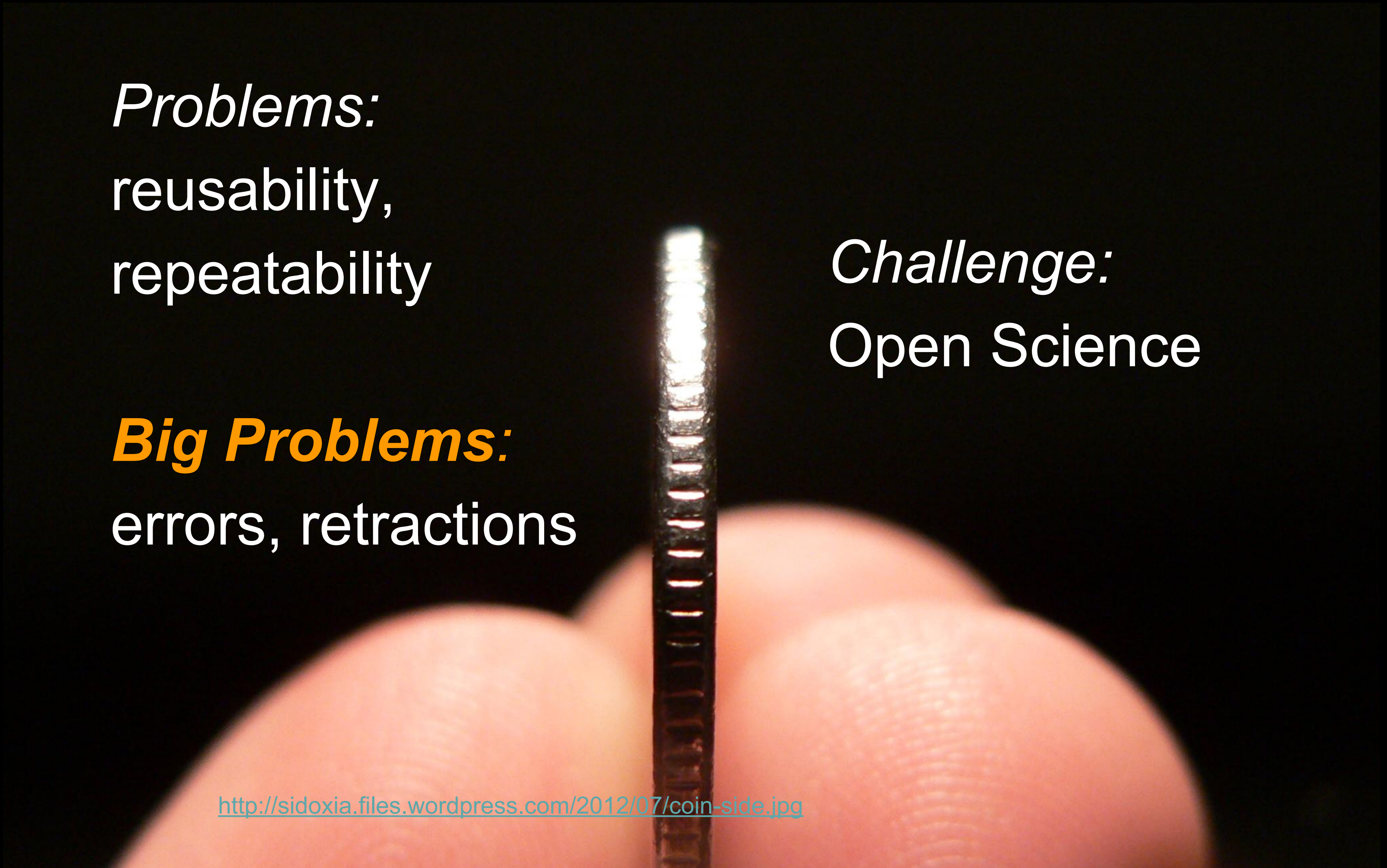
Science Programming = Science

> *An article about computational science in a scientific publication isn't the scholarship itself, it's merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.*

- Jon Claerbout

"The Legal Framework for Reproducible Scientific Research", Stodden, 2009

Science Programming



Problems:

reusability,

repeatability

Big Problems:

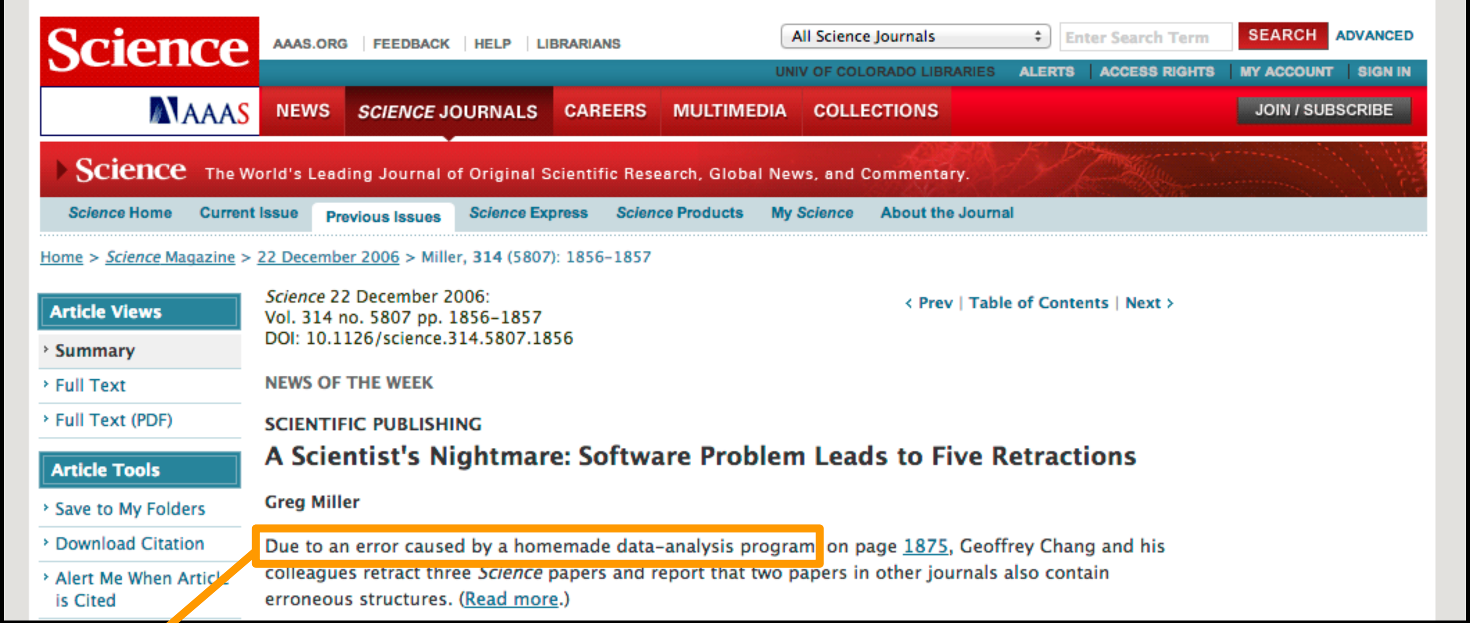
errors, retractions

Challenge:

Open Science

http://sidoxia.files.wordpress.com/2012/07/coin-side.jpg

Your Nightmare?



Home > *Science* Magazine > 22 December 2006 > Miller, **314** (5807): 1856-1857

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

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.)

"Due to an error caused by a *homemade* data-analysis program […]"

http://www.sciencemag.org/content/314/5807/1856

Towards Scientific Software Engineering

“Best Practices for Scientific Computing”

1. Write programs for people, not computers.
2. Automate repetitive tasks.
3. Use the computer to record history.
4. Make incremental changes.
5. Use version control.
6. Don’t repeat yourself (or others).
7. Plan for mistakes.
8. Optimize software only after it works correctly.
9. Document design and purpose, not mechanics.
10. Collaborate.

“Best Practices for Scientific Computing”, Wilson et al, 2012
arXiv:1210.0530 [cs.MS]

Proposed path for improvement: automated tests

Tests are executable specifications: repeatable, independent verification that the code is correct.

Proposed path for improvement: automated tests

Tests are executable specifications: repeatable, independent verification that the code is correct.

Huge spectrum of techniques: unit tests, test driven development, acceptance tests...

Not controversial: Beck, Feathers, Fowler, Hunt & Thomas (PragProg), Martin, Subramaniam, ...

Test Taxonomy

Unit tests primarily concerned with internal quality.

Integration tests, Acceptance tests concerned with external quality.

“Growing Object-Oriented Software, Guided by Tests”, Freeman & Pryce, 2010

About Unit Tests

Small piece of code to test another piece of code.

Expose the behavior of a particular *unit* of code (e.g. a method or function).

Typically written with a framework providing structural and assertion constructs.

Highlights regressions from the contract.

Good Unit Tests

FIRST:

- Fast
- Independent
- Repeatable
- Self-verifying
- Timely

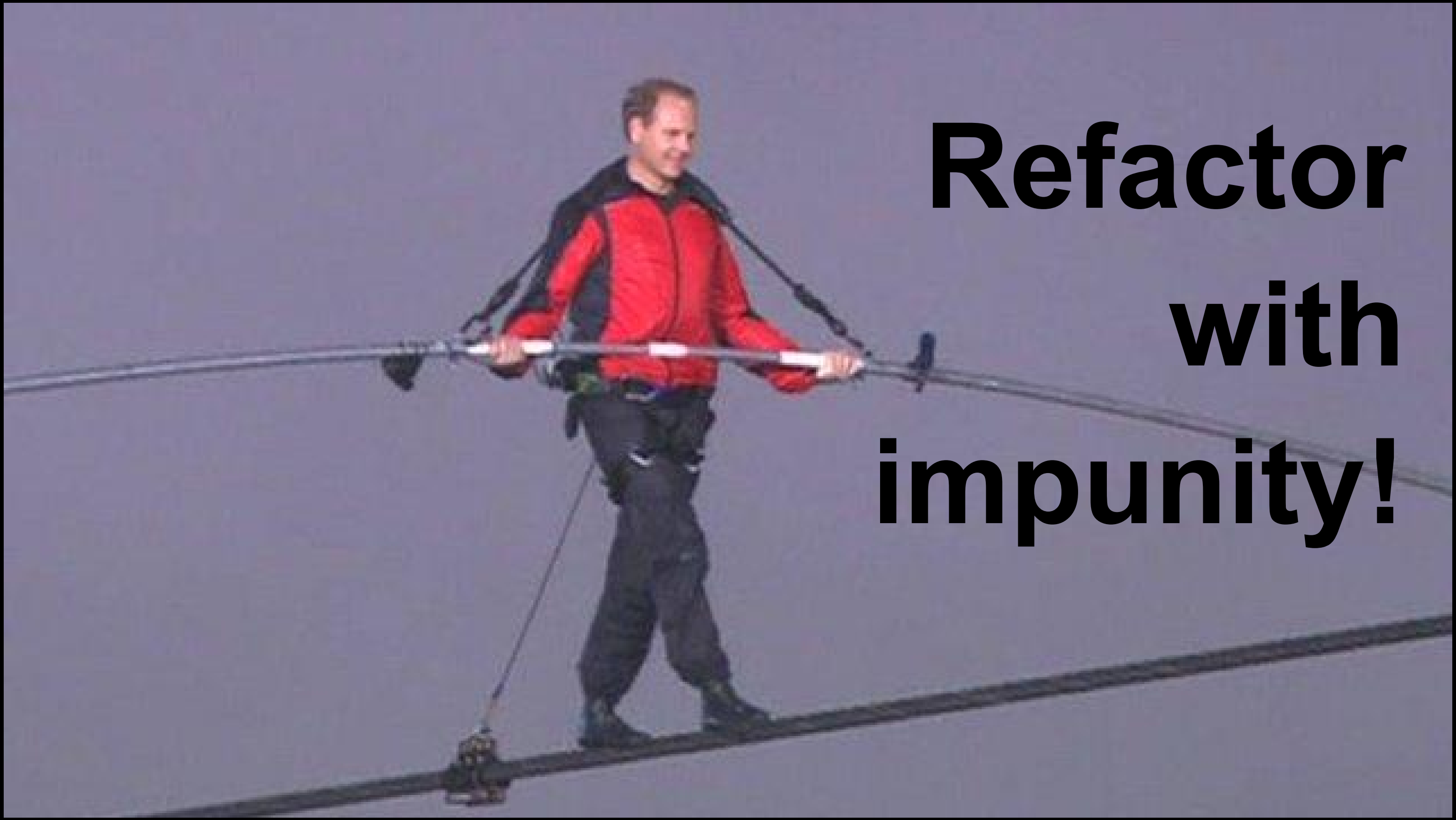
More on Good Unit Tests

Embody good software design

...but with an emphasis on readability.

http://codinghorror.typepad.com/.a/6a0120a85dcdae970b0128776fbe0b970c-pi

Fringe Benefits



Refactor with impunity!

http://news.bbcimg.co.uk/media/images/60949000/jpg/_60949195_jex_1437008_de36-1.jpg

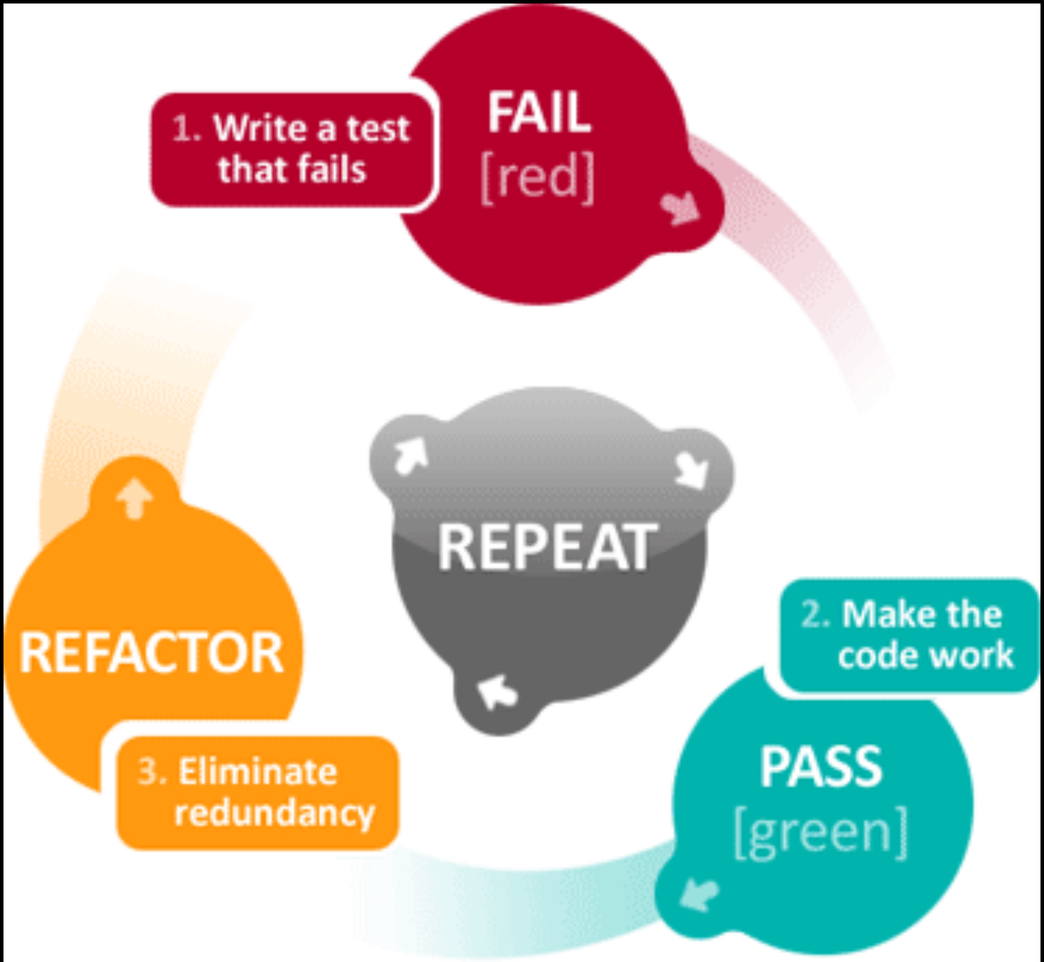
TDD - Test Driven Development

Write the tests for your code ***before*** *writing the code itself*

TDD is a design exercise.

http://farm4.static.flickr.com/3087/2764892330_a8ffb86dcf.jpg

About TDD



http://www.agileapps.co.uk/images/methodology/tdd-red-green-refactor-diagram.gif

About TDD

- Clean code
  - it’s easy to make design or architectural changes
- Readable code
  - ...comes from the constant attention to detail
- Minimal code
  - no more than that which makes the tests pass
- Lots of tests
  - but no more than are needed

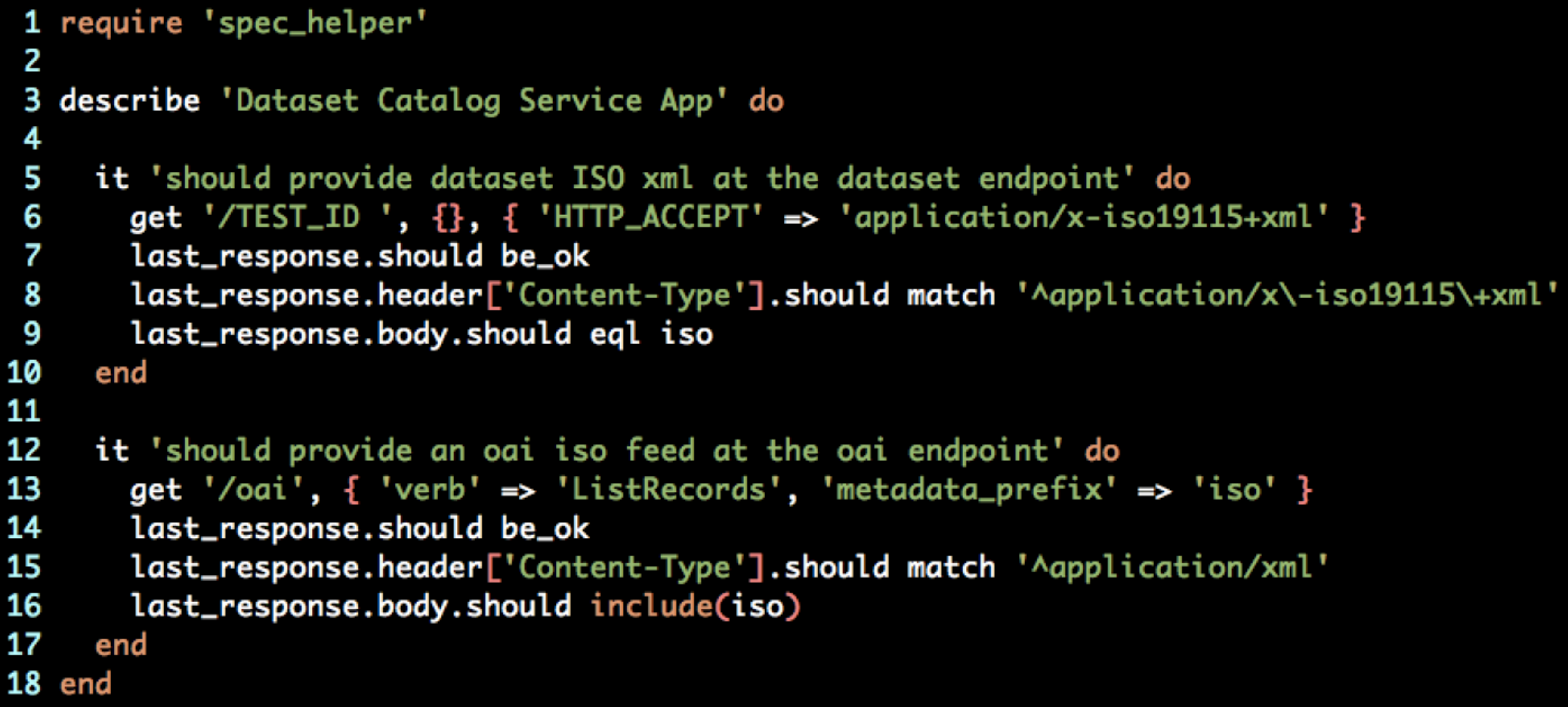
BDD - Behavior Driven Design

a "ubiquitous language" for analysis

Acceptance criteria should be executable

"Introducing BDD", Dan North

BDD: A language of executable specifications



```ruby
require 'spec_helper'

describe 'Dataset Catalog Service App' do

  it 'should provide dataset ISO xml at the dataset endpoint' do
    get '/TEST_ID ', {}, { 'HTTP_ACCEPT' => 'application/x-iso19115+xml' }
    last_response.should be_ok
    last_response.header['Content-Type'].should match '^application/x\-iso19115\+xml'
    last_response.body.should eql iso
  end

  it 'should provide an oai iso feed at the oai endpoint' do
    get '/oai', { 'verb' => 'ListRecords', 'metadata_prefix' => 'iso' }
    last_response.should be_ok
    last_response.header['Content-Type'].should match '^application/xml'
    last_response.body.should include(iso)
  end
end
```

The Extended Test Family

Tests that aren’t unit tests:

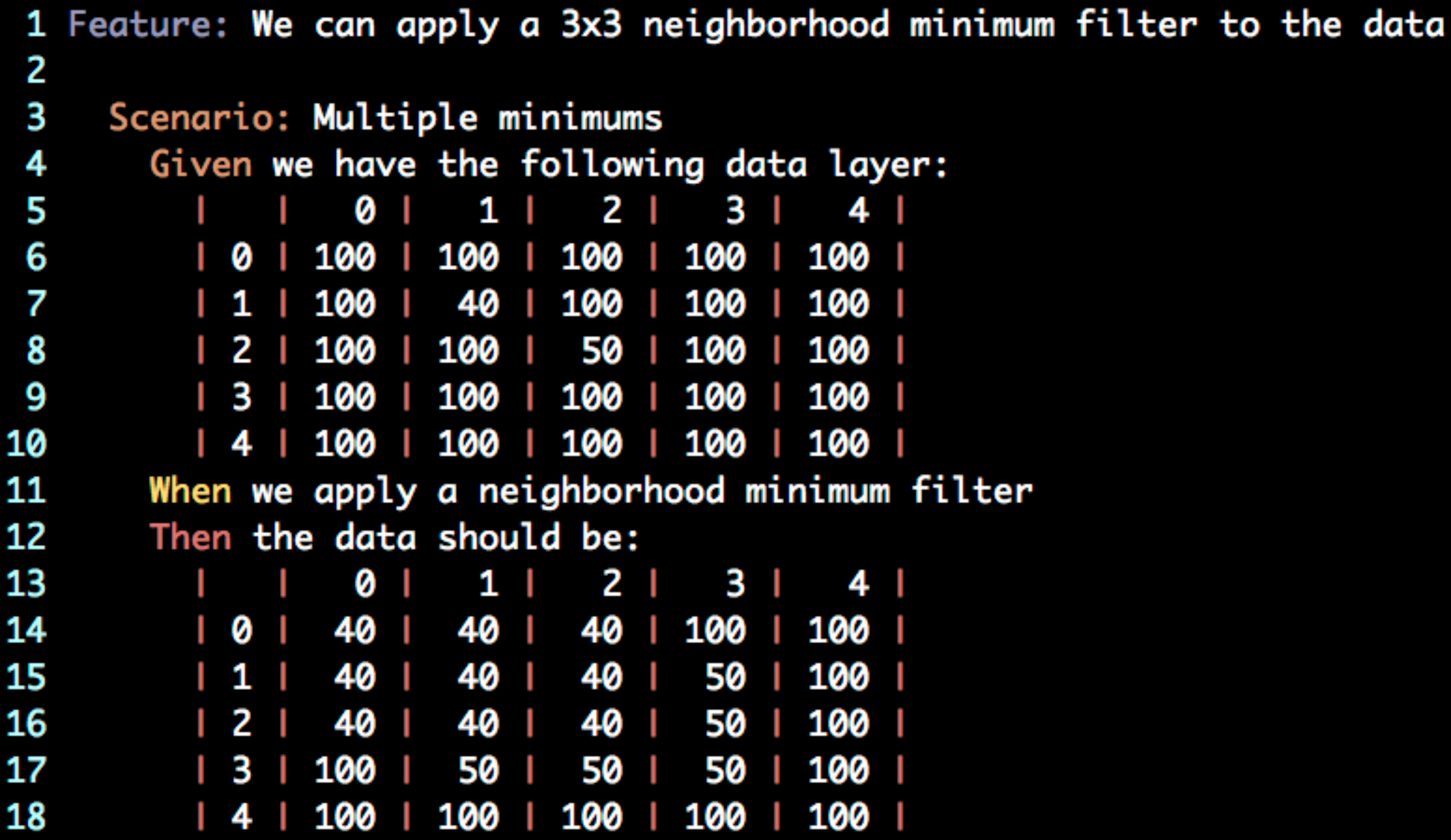
- cover different scopes
- are still valuable
- shouldn’t be conflated with your unit tests!

Also consider stress tests, penetration tests, UI tests, ...

Acceptance Tests

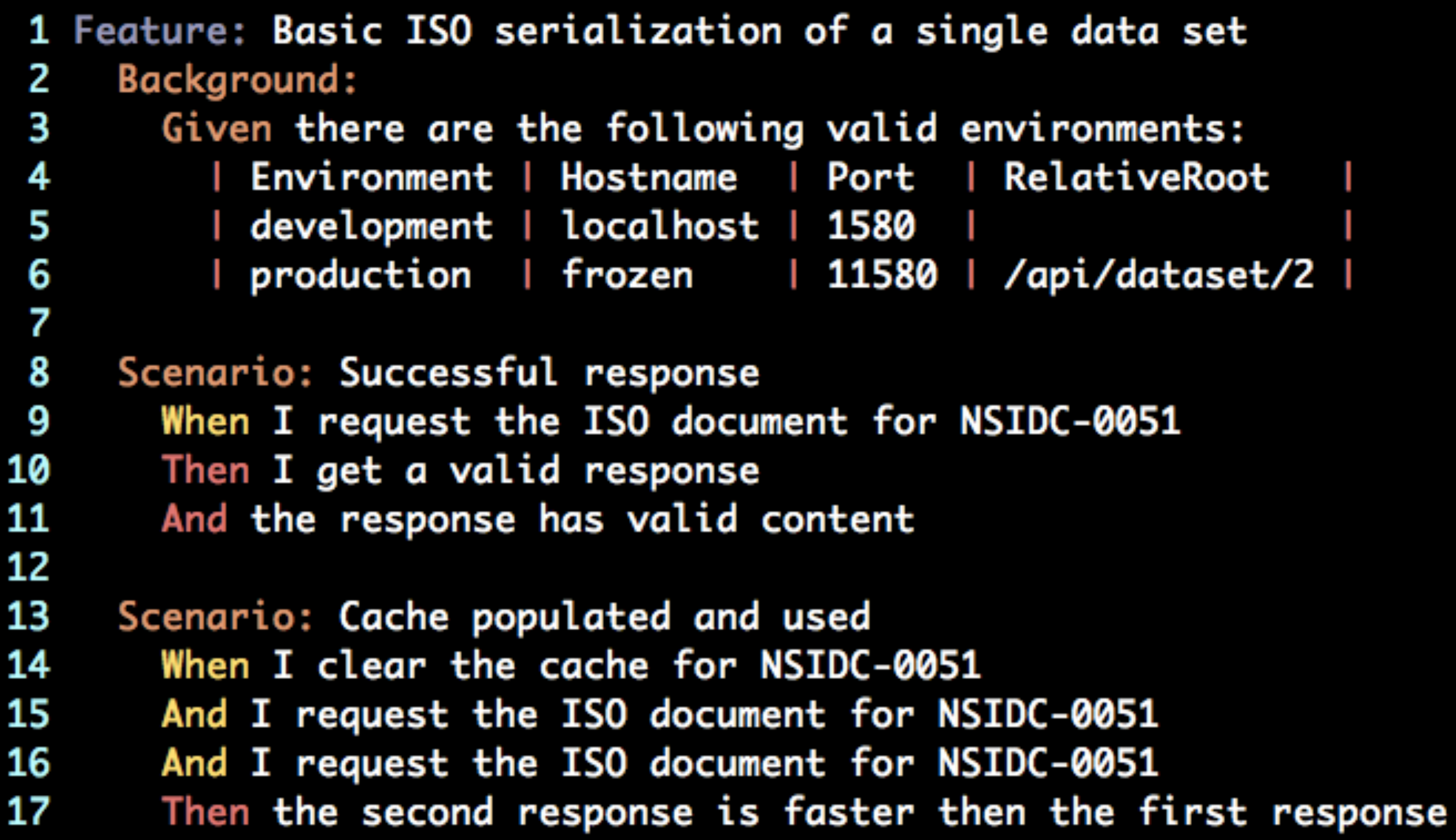
End-to-end tests that verify the code *en bloc* meets the (user-facing) requirements.

Acceptance Tests: A domain-specific language for testing



```
Feature: We can apply a 3x3 neighborhood minimum filter to the data

  Scenario: Multiple minimums
    Given we have the following data layer:
      |   |   0 |   1 |   2 |   3 |   4 |
      | 0 | 100 | 100 | 100 | 100 | 100 |
      | 1 | 100 |  40 | 100 | 100 | 100 |
      | 2 | 100 | 100 |  50 | 100 | 100 |
      | 3 | 100 | 100 | 100 | 100 | 100 |
      | 4 | 100 | 100 | 100 | 100 | 100 |
    When we apply a neighborhood minimum filter
    Then the data should be:
      |   |   0 |   1 |   2 |   3 |   4 |
      | 0 |  40 |  40 |  40 | 100 | 100 |
      | 1 |  40 |  40 |  40 |  50 | 100 |
      | 2 |  40 |  40 |  40 |  50 | 100 |
      | 3 | 100 |  50 |  50 |  50 | 100 |
      | 4 | 100 | 100 | 100 | 100 | 100 |
```

Acceptance Tests: another DSL for a different domain



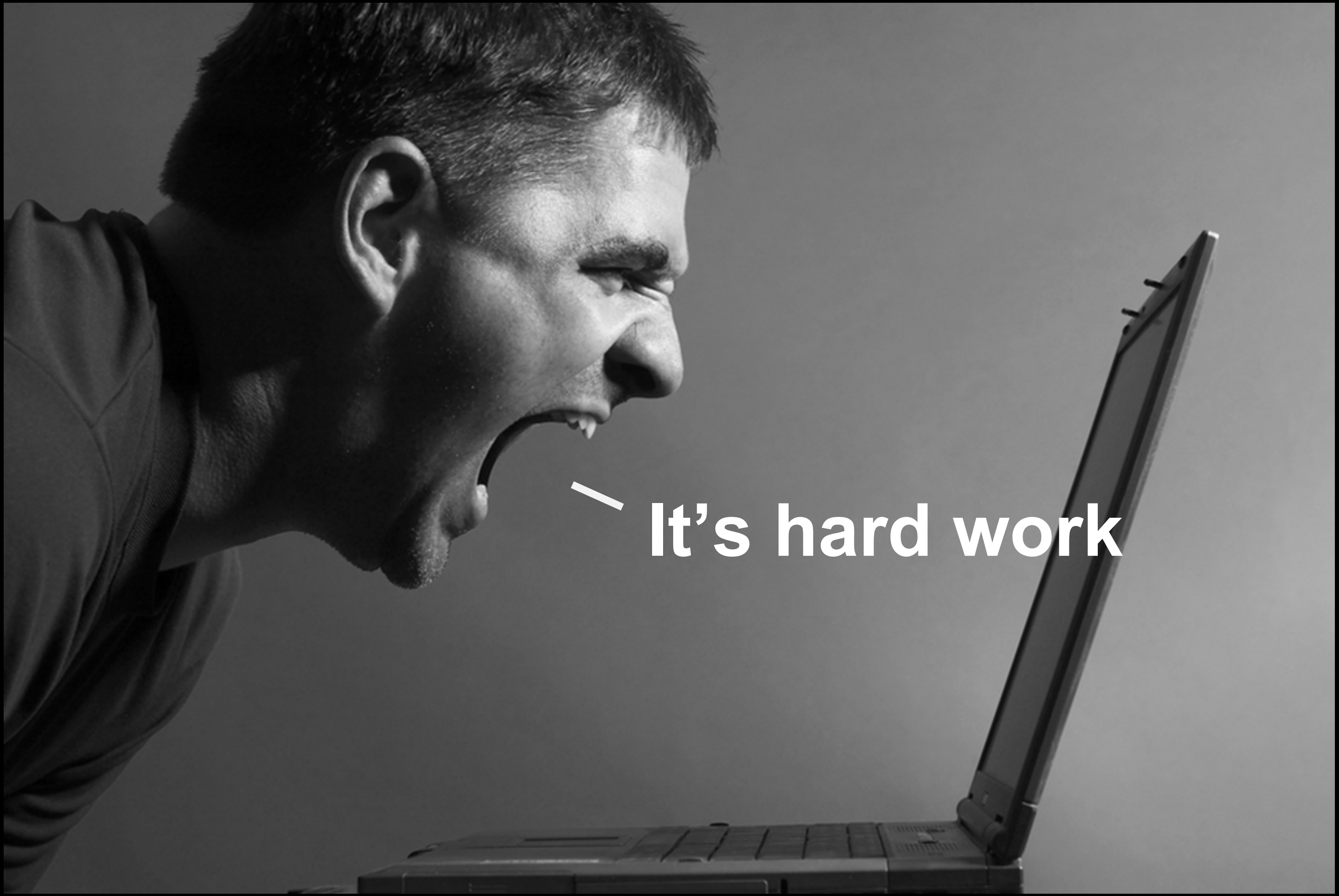
```
Feature: Basic ISO serialization of a single data set
  Background:
    Given there are the following valid environments:
      | Environment | Hostname  | Port  | RelativeRoot   |
      | development | localhost | 1580  |                |
      | production  | frozen    | 11580 | /api/dataset/2 |

  Scenario: Successful response
    When I request the ISO document for NSIDC-0051
    Then I get a valid response
    And the response has valid content

  Scenario: Cache populated and used
    When I clear the cache for NSIDC-0051
    And I request the ISO document for NSIDC-0051
    And I request the ISO document for NSIDC-0051
    Then the second response is faster then the first response
```

Legacy Code

Legacy code = code without unit tests

...but how to get unit tests in?

Un-Legacy Code



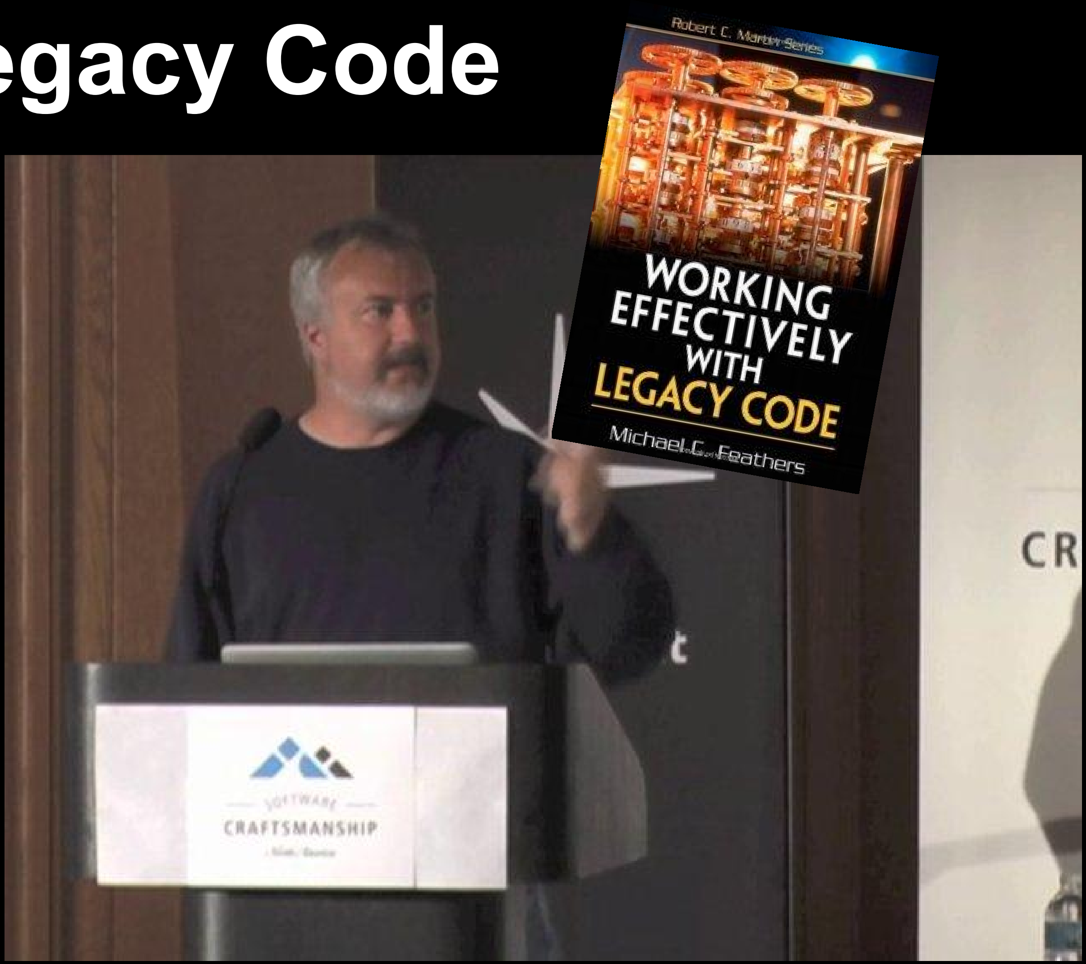
It’s hard work

http://www.menspsychology.com/sites/default/files/facebook-frustration_full.png

Un-Legacy Code

http://worldonline.media.clients.ellingtoncms.com/img/croppedphotos/2011/04/18/trash_pick_up_day_t640.png?a6ea3ebd4438a44b86d2e9c39ecf7613005fe067

Un-Legacy Code



Feathers has great strategies

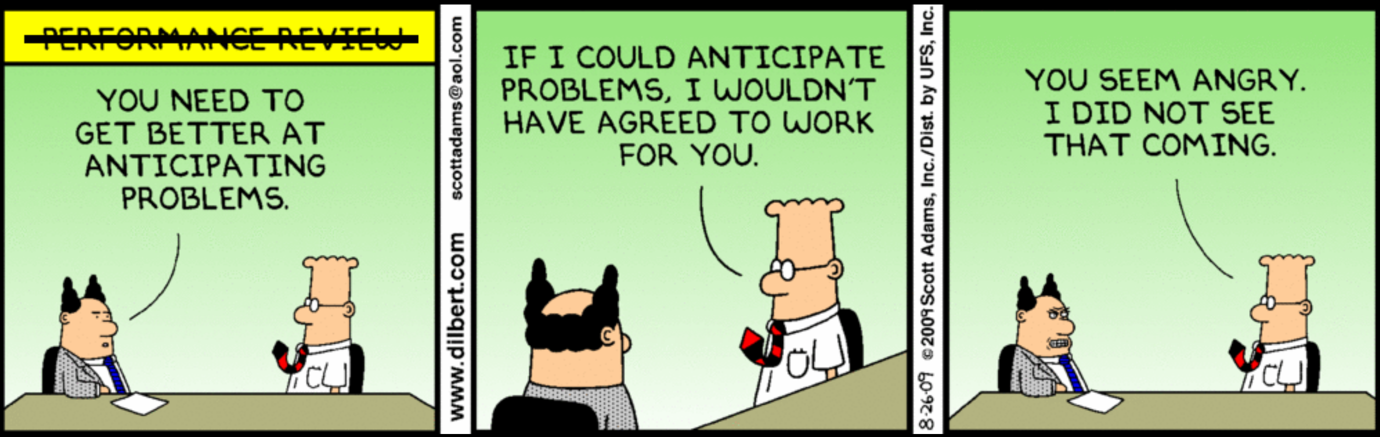
http://b.vimeocdn.com/ts/374/665/374665585_640.jpg

http://ecx.images-amazon.com/images/I/51S2-5n%2BJCL._SY300_.jpg

The Human Side

Cultural and Management Issues

Testing argument #427


~~PERFORMANCE REVIEW~~
YOU NEED TO GET BETTER AT ANTICIPATING PROBLEMS.
scottadams@aol.com
www.dilbert.com
IF I COULD ANTICIPATE PROBLEMS, I WOULDN'T HAVE AGREED TO WORK FOR YOU.
8-26-09 © 2009 Scott Adams, Inc./Dist. by UFS, Inc.
YOU SEEM ANGRY. I DID NOT SEE THAT COMING.

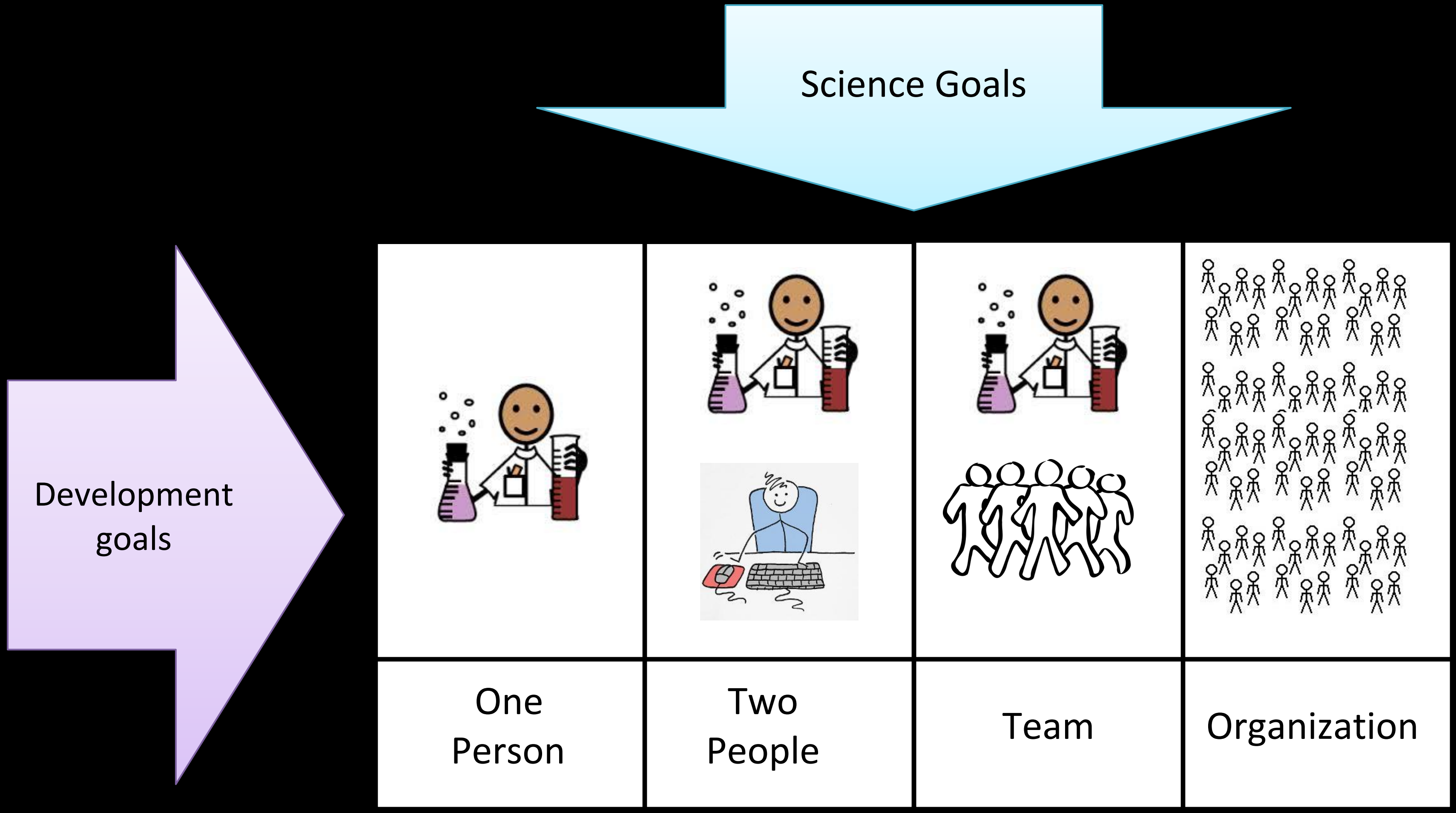
http://dilbert.com/dyn/str_strip/000000000/00000000/0000000/000000/60000/5000/600/65675/65675.strip.zoom.gif (with edits)

“The Farmer and the Engineer”

http://upload.wikimedia.org/wikipedia/commons/e/e7/Farmer_plowing_in_Fahrenwalde,_Mecklenburg-Vorpommern,_Germany.jpg

http://us.123rf.com/400wm/400/400/luislouro/luislouro0905/luislouro090500255/4824342-young-engineer-with-laptop-siting-in-a-tractor-isolated-against-a-white-background.jpg

We are all matrixed



Science Goals

Development goals

One Person

Two People

Team

Organization

* image citations at end

The Arguments Against ~~Testing~~ Anything

"This is going to take longer!"

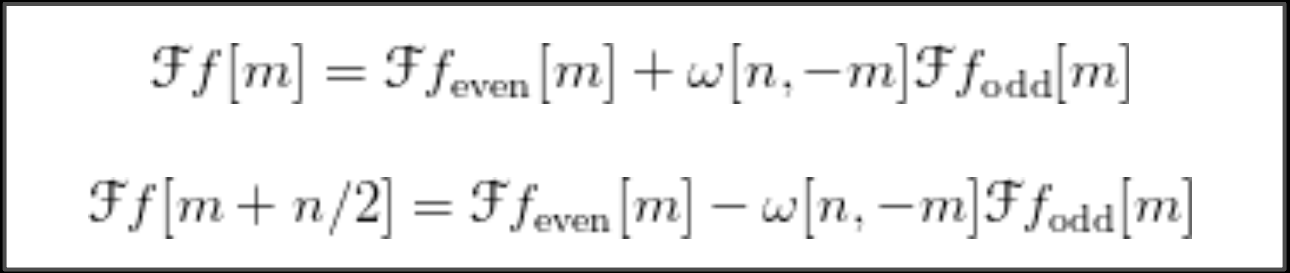
- Nefarious counterpart: "Time writing X lines of code" as a measurement.

"I'm opposed to process mandates."

"Nobody cares about my code but me..."

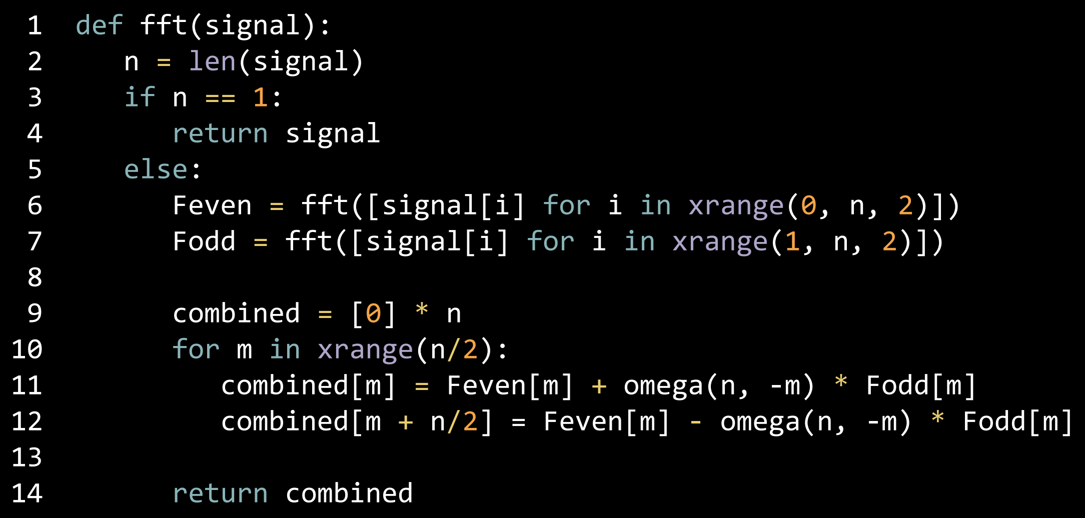
- "...and I'm never going to show anyone anyway."

Complexity in Scientific Software



$$\mathcal{F}f[m] = \mathcal{F}f_{\text{even}}[m] + \omega[n, -m]\mathcal{F}f_{\text{odd}}[m]$$

$$\mathcal{F}f[m + n/2] = \mathcal{F}f_{\text{even}}[m] - \omega[n, -m]\mathcal{F}f_{\text{odd}}[m]$$



```python
def fft(signal):
   n = len(signal)
   if n == 1:
      return signal
   else:
      Feven = fft([signal[i] for i in xrange(0, n, 2)])
      Fodd = fft([signal[i] for i in xrange(1, n, 2)])

      combined = [0] * n
      for m in xrange(n/2):
         combined[m] = Feven[m] + omega(n, -m) * Fodd[m]
         combined[m + n/2] = Feven[m] - omega(n, -m) * Fodd[m]

      return combined
```

http://jeremykun.com/2012/07/18/the-fast-fourier-transform/

The myth of lines of code

- Award winning “best lines of code ever”
- Runs in perl **and** postscript!

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```
/;{}def/#{def}def/$_={/Times-Bold exch selectfont}#/_{rmoveto}#/"{dup}#/*/!/$
;/q{exch}#/x ; {/J q #}#/.{/T q #}#{stringwidth}#{}#{}# 14 string dup dup dup
260 40 moveto 90 rotate ; %/}};$0='"\e[7m \e[0m"';@ARGV=split//,reverse
q(ThePerl). q(Journal) x 220 ; q ; 0 T putinterval exch 7 J putinterval ;
 ; $_= q /m$ pop T($*!$"=!$ " )pop " * true% ? $ " $!" "  !!  !! % !" !"    !
! charpath {!"""}pop $ pop{""!}pop ! neg{!#}pop 220 ! neg _{!!}pop J false %T
charpath  clip " pop 0 " moveto 6{!!}pop $_= 105{!!}pop {$ ! $ " !  #! ##}
pop{dup dup $ ! " pop pop q{"}pop 22{dup show}repeat {"}pop q 22 mul{$ "} pop
neg{!#! $ "}pop ! 8 .65 mul{$ # # $}pop ! neg{"}pop  _ pop{"}pop } repeat pop
" {  $ " ! ! ! $ " ! !" "#"  #"!"""""! #" " # "m/;@ARGV=(@ARGV[-14..-1])x50;q}
 0 "%};s/m[ou]|[-\dA-ln-z.\n_{}]|\$_=//gx;s/(.)(?{$*=''})/('$*.='.(++$#
%2?'':"$0;").'pop;')x(ord($1)-31).'$*'/gee;s/((.(\e\[.m)*|.){77})/$1\n/g;print
; sub showpage {}
```

The myth of lines of code - pt 2

Development effort is not measured in keystrokes.

How much brainpower does my code consume for everyone involved?

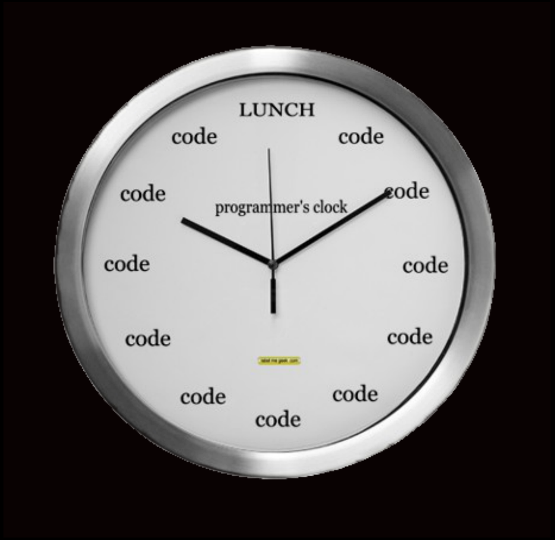
```
if (string.IsNullOrEmpty(filetext) || !filetext.Contains(",")) goto end;

*++b ? (*++b + *(b-1)) 0

getElements( ‘p’, {'class':'statusbar'} )[0].firstChild.innerText
```

The reality of lines of code

The real point: how much time does my code take to create and debug and maintain?



http://www.photoshop3d.com/wp-content/uploads/2007/02/hourglass_00.jpg
http://i1.cpcache.com/product/382140623/programmers_modern_wall_clock.jpg?color=Silver&height=460&width=460&qv=90
http://cdn.homedit.com/wp-content/uploads/2011/02/hwc1.jpg

When is our fft accepted “as given,” and the focus on its application?

```
import unittest

class CoreFFTTests(unittest.TestCase)
  def realNumberTest(self):
     # [Test some real numbers]

  def imaginaryNumberTest(self):
     # [Test some imaginary numbers]

  def complexNumberTests(self):
     # [Test some complex numbers]
```

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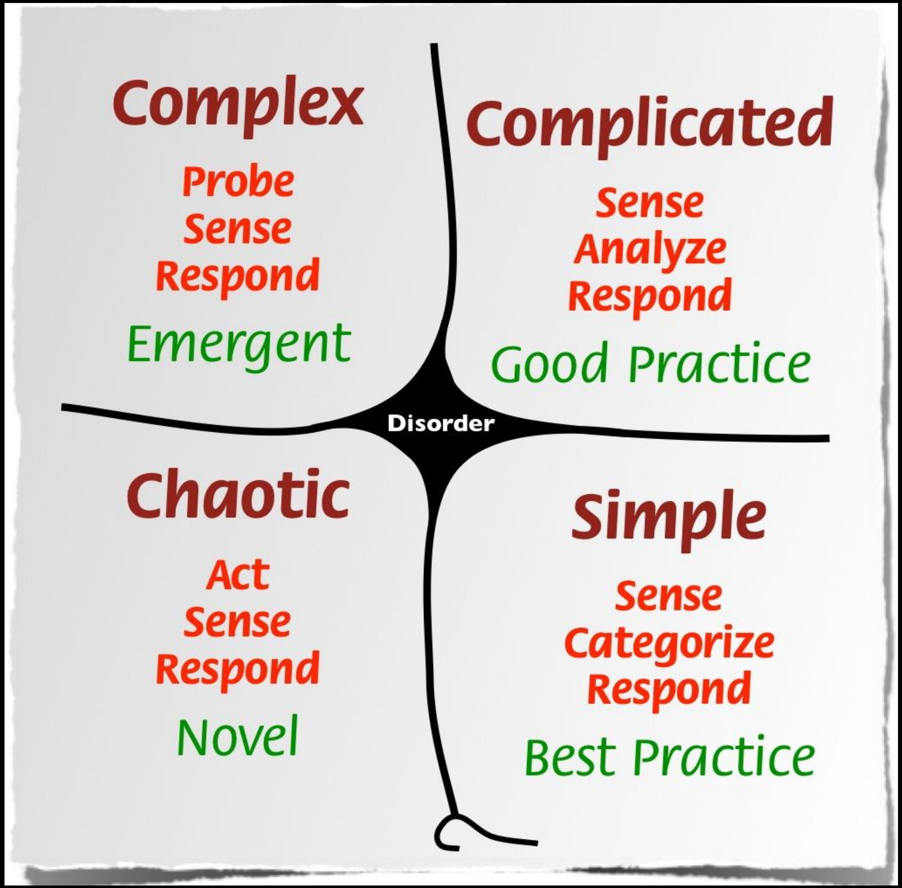
      return combined
```

http://jeremykun.com/2012/07/18/the-fast-fourier-transform/

Process vs good practice



Complex

Probe
Sense
Respond

Emergent

Complicated

Sense
Analyze
Respond

Good Practice

Disorder

Chaotic

Act
Sense
Respond

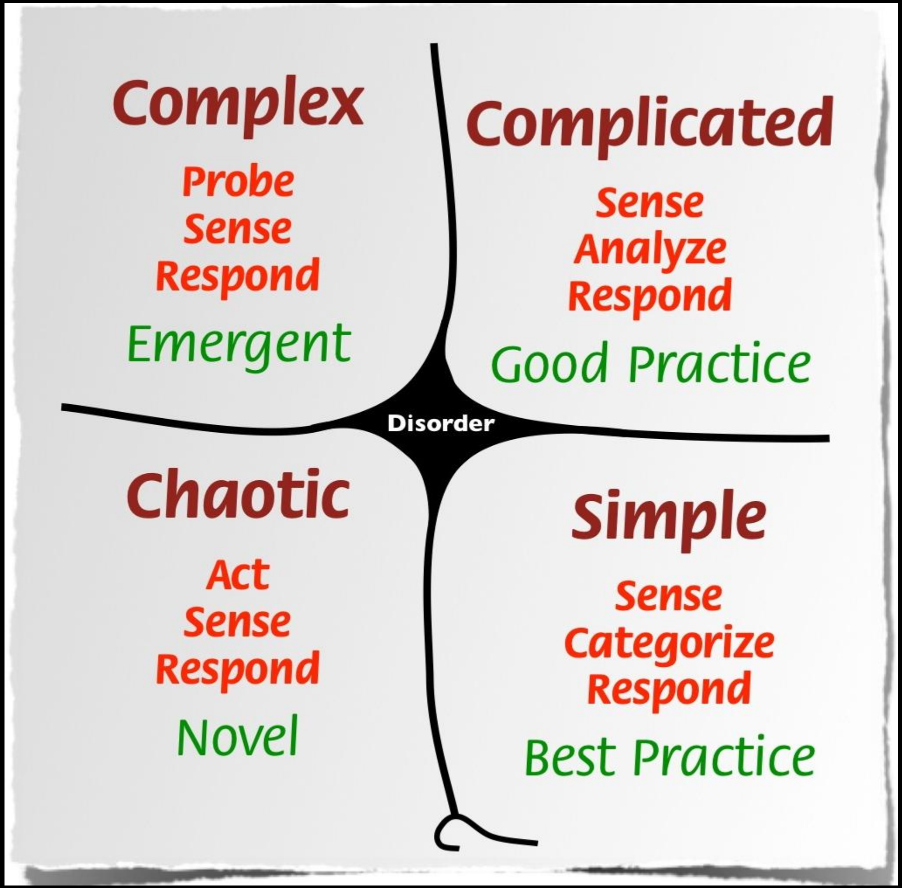
Novel

Simple

Sense
Categorize
Respond

Best Practice

Process vs good practice



Software Engineering

Operational Procedure (Process)

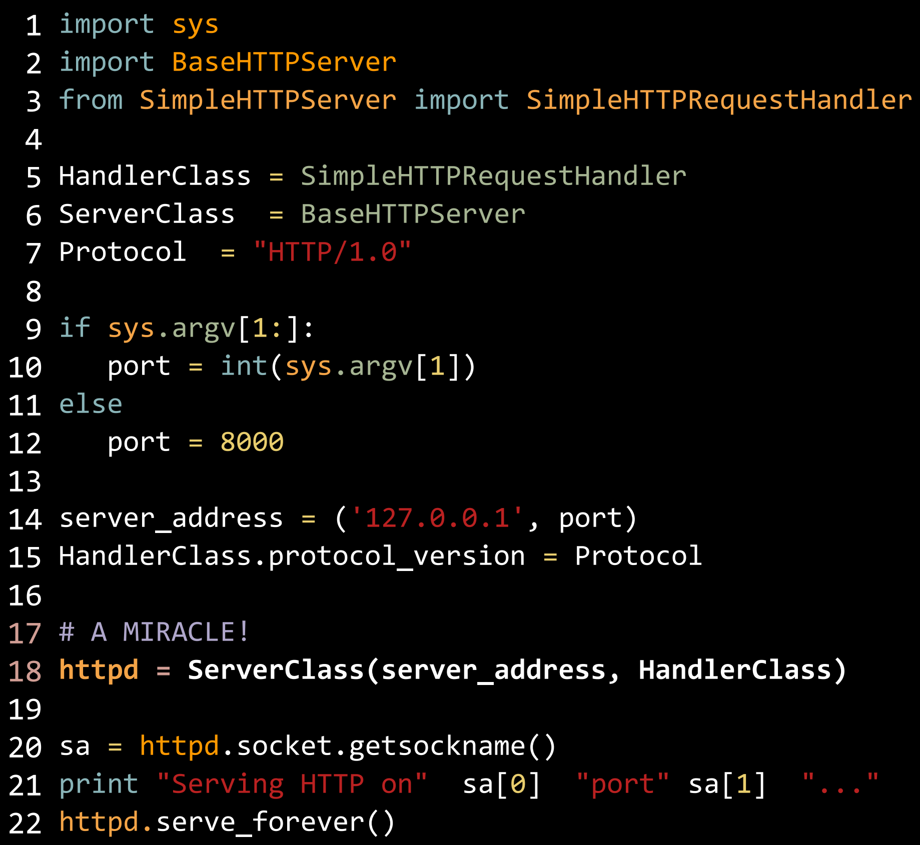
http://en.wikipedia.org/wiki/File:Cynefin_framework_Feb_2011.jpeg

Serving the World Wide Web - 1990

https://github.com/NotTheRealTimBL/WWWDaemon/tree/master/old

http://www.wimklerkx.nl/IN/IN22-14.jpg

Complex -> complicated (but not simple)



```python
import sys
import BaseHTTPServer
from SimpleHTTPServer import SimpleHTTPRequestHandler

HandlerClass = SimpleHTTPRequestHandler
ServerClass  = BaseHTTPServer
Protocol  = "HTTP/1.0"

if sys.argv[1:]:
    port = int(sys.argv[1])
else
    port = 8000

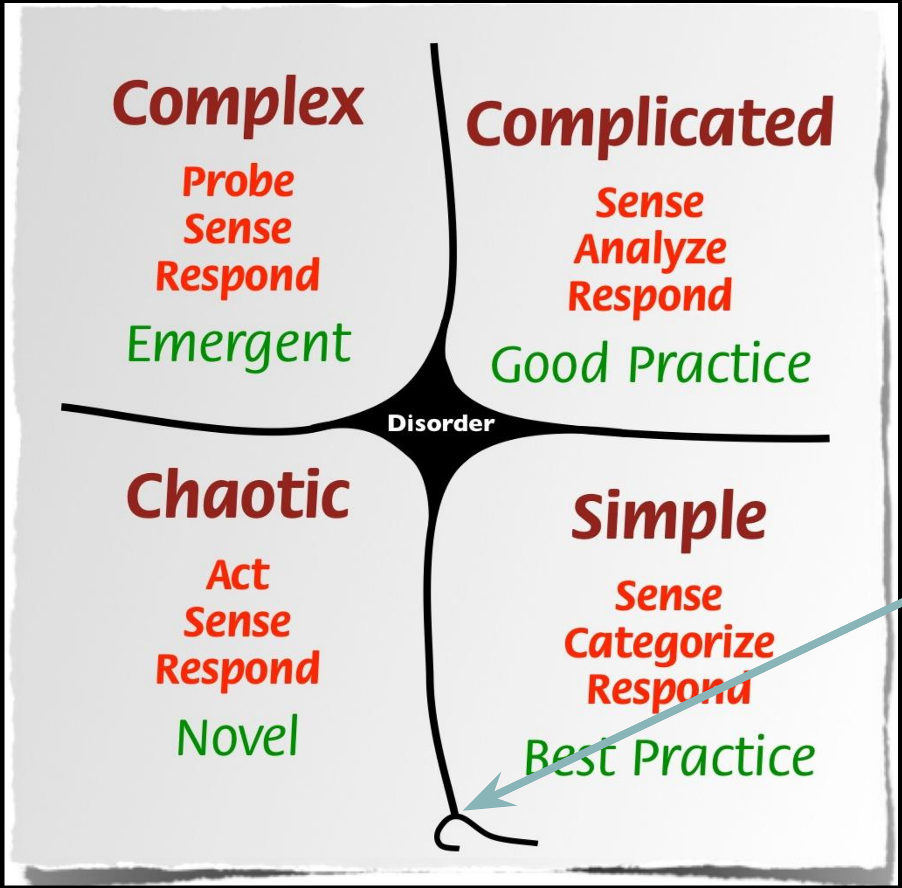
server_address = ('127.0.0.1', port)
HandlerClass.protocol_version = Protocol

# A MIRACLE!
httpd = ServerClass(server_address, HandlerClass)

sa = httpd.socket.getsockname()
print "Serving HTTP on"  sa[0]  "port" sa[1]  "..."
httpd.serve_forever()
```

http://www.linuxjournal.com/content/tech-tip-really-simple-http-server-python

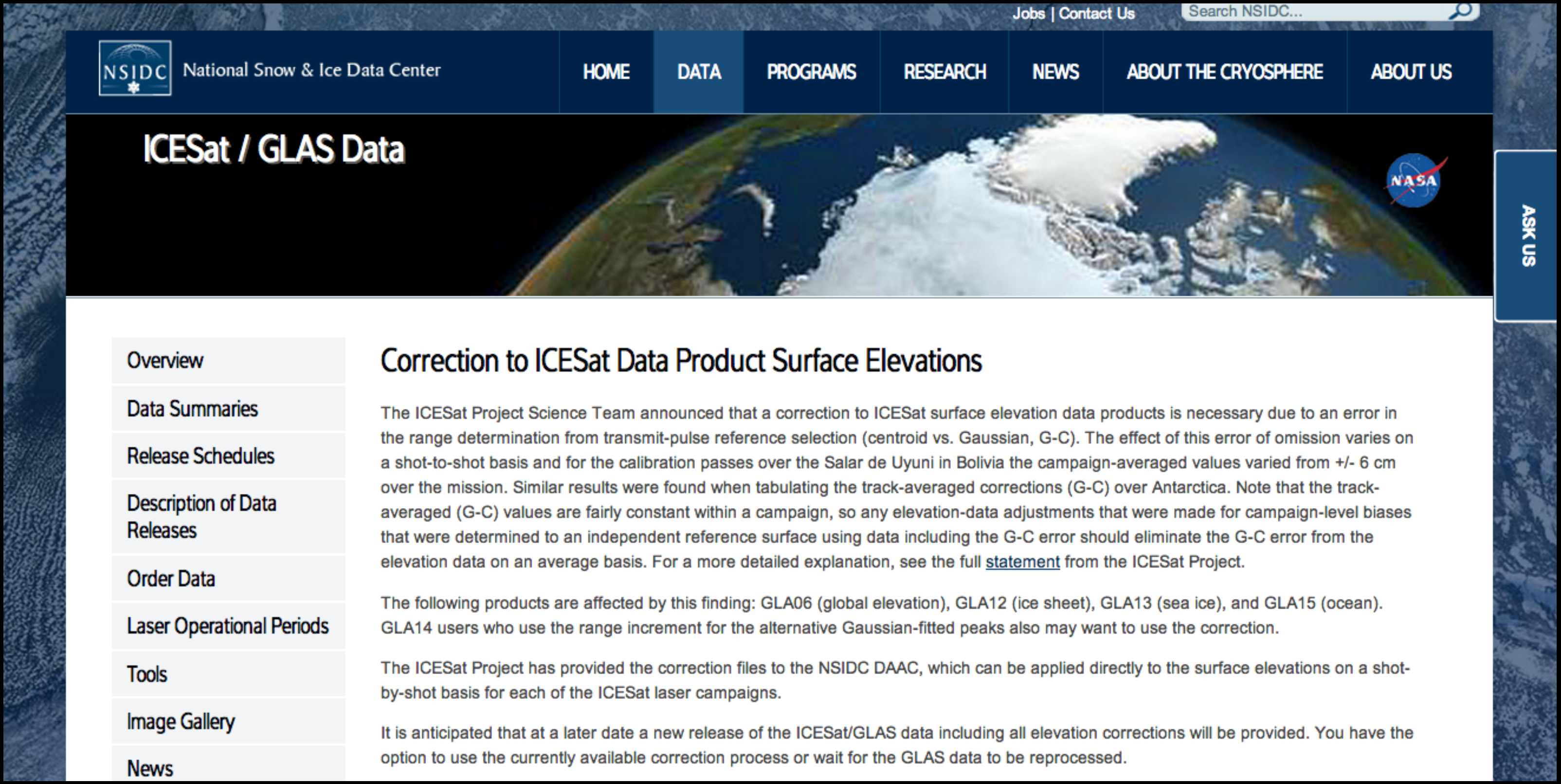
Process vs good practice



The Complexity Cliff (or, why reusing old Fortran will kill you someday.)

http://en.wikipedia.org/wiki/File:Cynefin_framework_Feb_2011.jpeg

My code: mine alone.



Correction to ICESat Data Product Surface Elevations

The ICESat Project Science Team announced that a correction to ICESat surface elevation data products is necessary due to an error in the range determination from transmit-pulse reference selection (centroid vs. Gaussian, G-C). The effect of this error of omission varies on a shot-to-shot basis and for the calibration passes over the Salar de Uyuni in Bolivia the campaign-averaged values varied from +/- 6 cm over the mission. Similar results were found when tabulating the track-averaged corrections (G-C) over Antarctica. Note that the track-averaged (G-C) values are fairly constant within a campaign, so any elevation-data adjustments that were made for campaign-level biases that were determined to an independent reference surface using data including the G-C error should eliminate the G-C error from the elevation data on an average basis. For a more detailed explanation, see the full statement from the ICESat Project.

The following products are affected by this finding: GLA06 (global elevation), GLA12 (ice sheet), GLA13 (sea ice), and GLA15 (ocean). GLA14 users who use the range increment for the alternative Gaussian-fitted peaks also may want to use the correction.

The ICESat Project has provided the correction files to the NSIDC DAAC, which can be applied directly to the surface elevations on a shot-by-shot basis for each of the ICESat laser campaigns.

It is anticipated that at a later date a new release of the ICESat/GLAS data including all elevation corrections will be provided. You have the option to use the currently available correction process or wait for the GLAS data to be reprocessed.

My code: mine alone?

> *Data is a precious thing and will last longer than the systems themselves.*
>
> *Tim Berners-Lee*

- Who owns the results?
- How long will this be around?
- Will your work ever need to be verified?
- Will the data you produce ever need to be expanded upon?

The risk is real
- but the risk is not persuasive!

Google “persuasion” -

- then tell me how often negative methods work

The risk is real
- but the risk is not persuasive!

Be positive (it’s more than just a blood type)

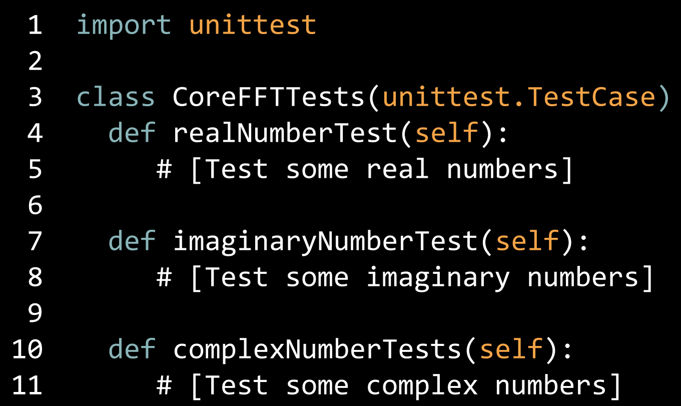
- Humor
- Create a positive experience
- Appeal to order
- Appeal to senses
- Endorsement
- Bandwagon
- [...]

Nuts and bolts technique:

Stroke the (research) ego.

http://images4.wikia.nocookie.net/__cb20130418031554/poohadventures/images/5/5e/Anton_Ego.jpg

Repeat our confidence test



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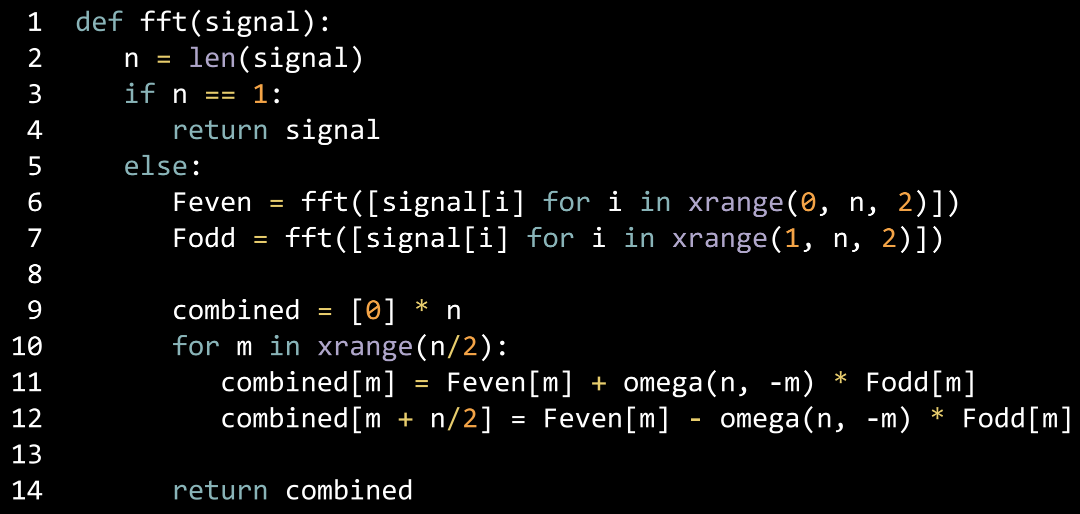

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      return combined
```

http://jeremykun.com/2012/07/18/the-fast-fourier-transform/

Nuts and bolts technique:

Stroke the (research) ego.

"More people will use this!"

- More citations
- More exposure
- More trust

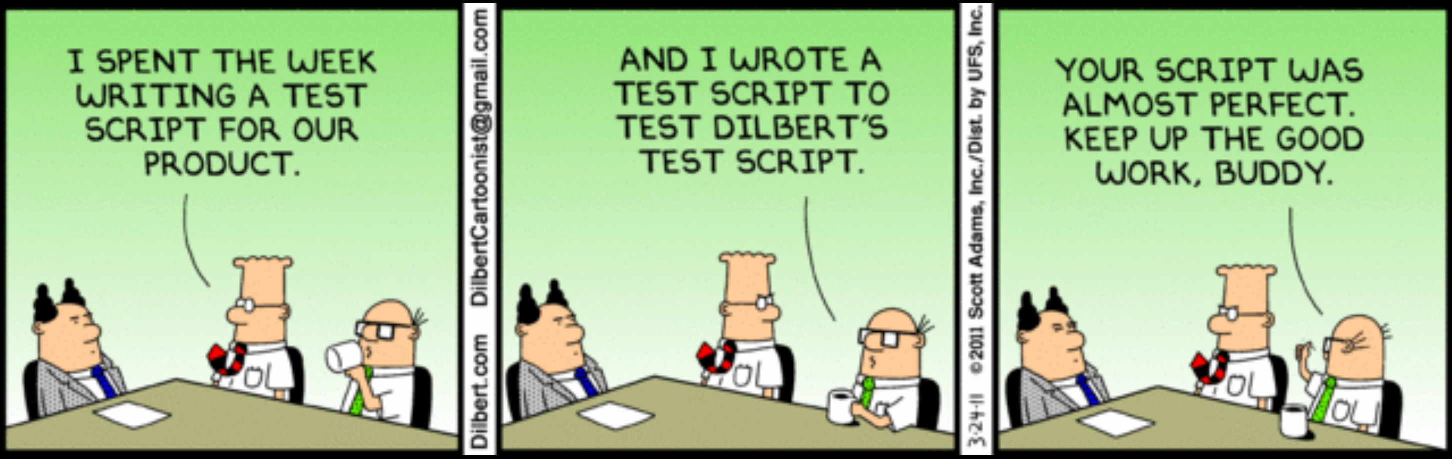
http://images4.wikia.nocookie.net/__cb20130418031554/poohadventures/images/5/5e/Anton_Ego.jpg

Summary: Strategies

- More lines of code: change the argument.
  - It’s about time, maintenance, efficiency
- Opposition to process / mandate: change the argument again.
  - We’re looking to mitigate complexity with good practice, not force another barrier.
- It’s my code; nobody else cares.
  - Carrot: Naked, unbridled flattery of their work.
  - (Stick: call from Bill O’Reilly if errors are found)

What you can do to help

(Hint: don't do this.)


I SPENT THE WEEK WRITING A TEST SCRIPT FOR OUR PRODUCT.
AND I WROTE A TEST SCRIPT TO TEST DILBERT'S TEST SCRIPT.
YOUR SCRIPT WAS ALMOST PERFECT. KEEP UP THE GOOD WORK, BUDDY.
Dilbert.com DilbertCartoonist@gmail.com
3-24-11 ©2011 Scott Adams, Inc./Dist. by UFS, Inc.

http://robwellsblog.files.wordpress.com/2013/08/sci-behind-testing.jpg?w=696

What you can do to help

(Hint: or this.)

FAILURE? MY CODE DOESN'T FAIL! I'M A PRO-FESSIONAL

http://blog.decayingcode.com/image.axd?picture=mycodecantfail_thumb.jpg

Summary of what we do at NSIDC

BDD and TDD in Python, Ruby, JavaScript, Java.

Acceptance testing, including web interfaces.

Continuous integration - all tests are run on every check in.

Continuous delivery: push-button releases.

Further Reading

Anne Wilson (LASP) is also to thank for some of these…

Scholarly articles:

- Wilson et al, "Best Practices for Scientific Computing", highly recommended.
- Merali, "Computational science: ... Error" in Nature. *"As a general rule, researchers do not test or document their programs rigorously, and they rarely release their codes, making it almost impossible to reproduce and verity published results generated by scientific software, say computer scientists."*

Good books for unit testing, TDD, and higher-level tests:

- Freeman and Pryce, Growing Object-Oriented Software, Guided by Tests
- Beck, Test Driven Development: By Example
- Fowler, Mocks Aren't Stubs - Martin Fowler on the terminology and usage of mocks, stubs, test doubles - all those "fake collaborators"
- A couple of Bob Martin's books are particularly noteworthy for covering lots and lots of desirable attributes for code
- Martin, Agile Software Development, Principles, Patterns, and Practices
- Martin, Clean Code: A Handbook of Agile Software Craftsmanship

Also:

- Feathers, Michael C., Working Effectively with Legacy Code , Prentice Hall, 2005, p. xvi.
- Snowden, Cynefin: Wikipedia on Cynefin, David Snowden introducing Cynefin (video) - applicable to knowledge management, cultural change, and community dynamics, and has also involved issues of organizational strategy.
- Snowden, Boone, 2007 "A Leader's Framework for Decision Making" (must pay for access from Harvard Business Review, though perhaps available elsewhere)

Some test frameworks

JUnit - the original (Java)

RSpec (Ruby)

Behave (Python)

Jasmine (JavaScript)

mgunit (IDL)

pfUnit (FORTRAN)

Cucumber (Acceptance tests, lots of languages)

Additional image credits (matrix org slide)

www.simtalk.com/news-2-you/Penguin/Page10.htm

http://images5.cafepress.com/image/31972305_150x150.png

http://uwcpsl.files.wordpress.com/2013/02/teamwork.png

http://morganbeebe.files.wordpress.com/2011/07/stick-figure-group-of-63.jpg

Thank you!

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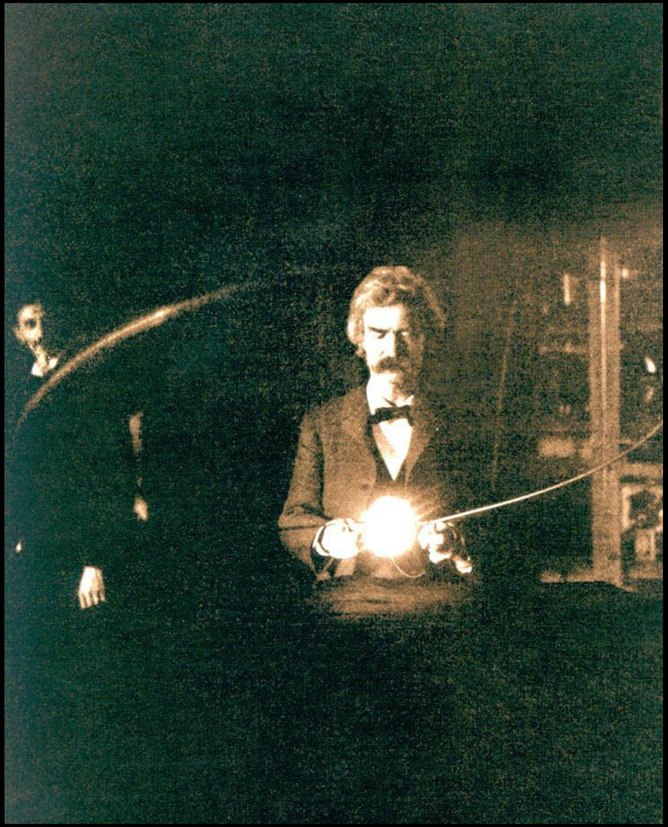

Slides: https://t.co/antAoj38tD

http://www.teslasociety.com/pictures/ntesla4.jpg