

# Putting it all together

# Why Software Carpentry?



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## ...SCIENTISTS AND THEIR SOFTWARE

A survey of nearly 2,000 researchers showed how coding has become an important part of the research toolkit, but it also revealed some potential problems.

- > **45%** said scientists spend more time today developing software than five years ago."
- > **38%** of scientists spend at least one fifth of their time developing software.

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A survey of nearly 2,000 researchers showed how coding has become an important part of the research toolkit, but it also revealed some potential problems.

- > **45%** said scientists spend more time today developing software than five years ago."
- > **38%** of scientists spend at least one fifth of their time developing software.

> Only **47%** of scientists have a good understanding of software testing.

> Only **34%** of scientists think that formal training in developing software is important.

Images by Greg Wilson and Neil Chue Hong. Data from Hannay et al, “How Do Scientists Develop and Use Scientific Software?

SECSE '09 Proceedings of the 2009 ICSE Workshop on Software Engineering for Computational Science and Engineering, IEEE Computer Society, 2009. DOI: 10.1109/SECSE.2009.5069155

# Software development ≠ research

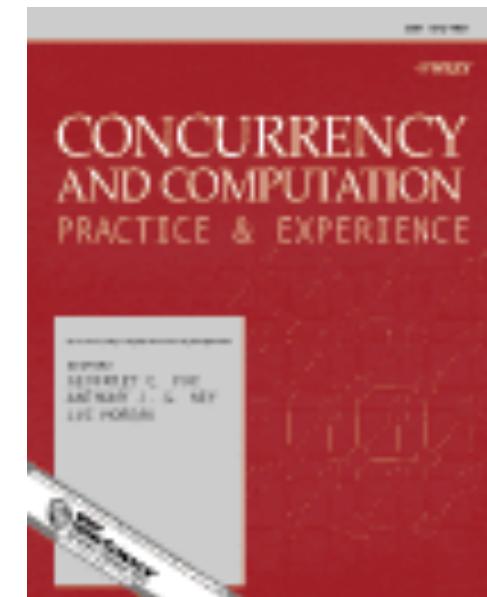
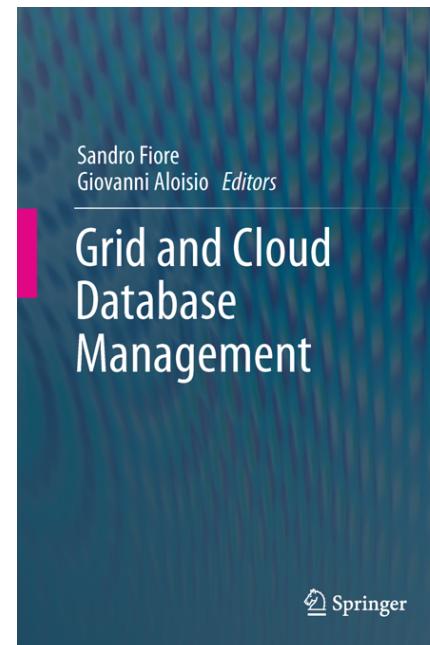


software carpentry

# Software development ≠ research



software carpentry



# Remember Geoffrey Chang!



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# Remember Geoffrey Chang!



We wish to retract our research article ... and both of our Reports...  
An **in-house data reduction program** introduced a **change in sign** for anomalous differences...  
Unfortunately, the use of the multicopy refinement procedure still allowed us to obtain reasonable refinement values for the **wrong** structures.

# Remember Geoffrey Chang!



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An **in-house data reduction program** introduced a **change in sign** for anomalous differences...

Unfortunately, the use of the multicopy refinement procedure still allowed us to obtain reasonable refinement values for the **wrong** structures.

The screenshot shows a Wikipedia page for Geoffrey Chang. At the top, it says "Geoffrey Chang" and "From Wikipedia, the free encyclopedia". Below that, a note states: "This article is an orphan, as few or no other articles link to it. Please introduce links to this page from related articles; suggestions may be available. (February 2009)"

The main text describes Chang as an associate professor at The Scripps Research Institute in La Jolla, California, United States. It mentions his work on the structural biology of integral membrane proteins, particularly exploring X-ray crystallography techniques for solving the tertiary structures of membrane proteins that are notoriously resistant to crystallization. The text also notes that Chang has specialized in structures of multidrug resistance transporter proteins in bacteria.

Further down, it discusses a retraction of their structural papers on EmrE, MsbA, and NorM between 2001 and 2010. The text explains that the initial structures were widely considered puzzling in the field due to their unexpected placement of their ATP binding sites in the assembled dimers.<sup>[2]</sup> The publication of an additional structure in the same protein family indicated that the Chang structures were unlikely to represent the biologically active conformation of the molecules.<sup>[3]</sup> Chang and coauthors issued retractions of their structural papers on EmrE, MsbA, and NorM, citing an error in an internal software utility as the source of the data misinterpretation that led to the appearance of wrongly assembled dimers.<sup>[4][5]</sup> The application of a popular protein structure validation tool to one of the retracted MsbA structures results in scores that indicate severe errors in this structure.<sup>[6]</sup>

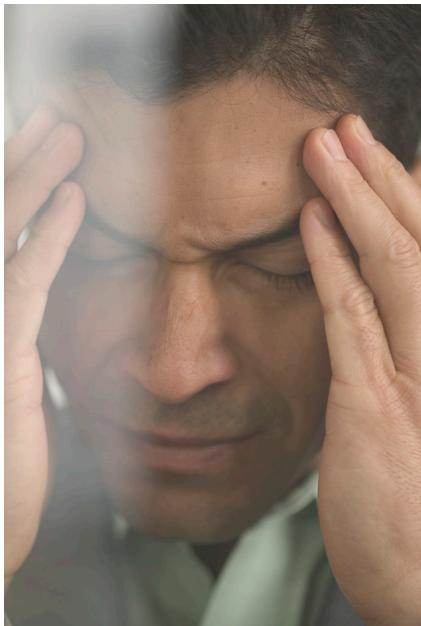
At the bottom of the page, there is a section titled "Retracted papers" which lists:

- 1 Retracted papers
- 2 Recent work
- 3 References
- 4 External links



**Correctness isn't compelling, so...  software carpentry**

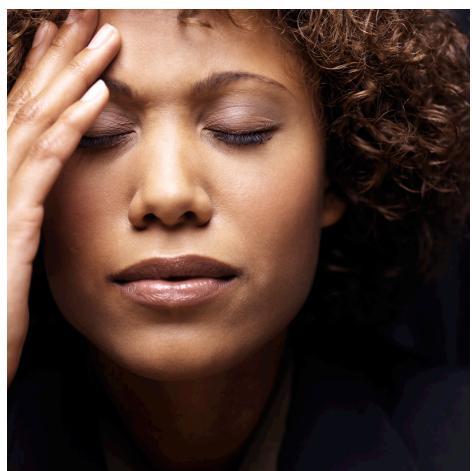
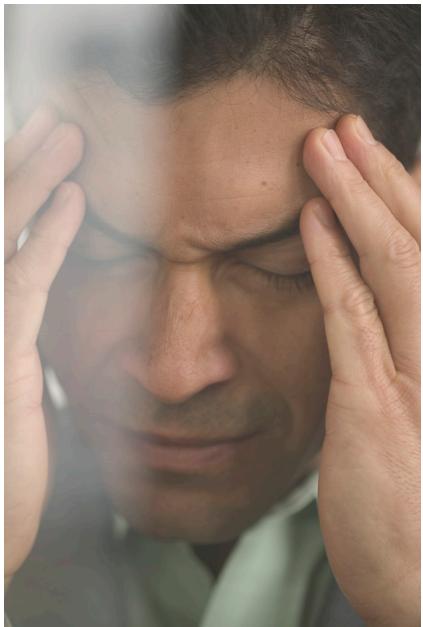
# Correctness isn't compelling, so... software carpentry



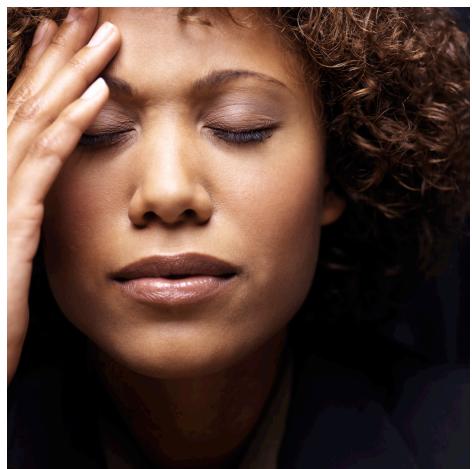
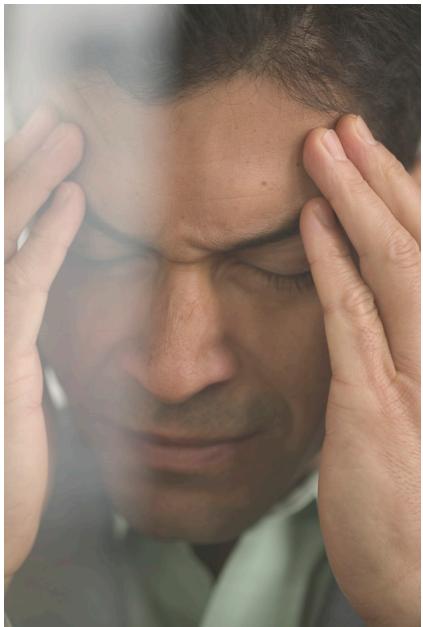
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# Correctness isn't compelling...



software carpentry

# Correctness isn't compelling... software carpentry



# Correctness isn't compelling... software carpentry



```
history  
!123  
history | grep 'ssh'
```

# Correctness isn't compelling...



configure.sh  
build.sh  
install.sh

```
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# Correctness isn't compelling... software carpentry



```
history  
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history | grep 'ssh'
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```
configure.sh  
build.sh  
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```

```
filename = "data.txt"  
source = open(filename, 'r')  
actual_count = 0  
expected_count = None  
# Count number of data records.  
for line in source:  
    if line.startswith('#-'): # Number of records  
        trash, expected_count = line.split()  
        expected_count = int(expected_count)  
    if line.startswith('#'): # Skip comments.  
        pass  
    elif line.startswith('D'): # Skip title line.  
        pass  
    else:  
        actual_count += 1  
source.close()
```

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build.sh  
install.sh

```
class Stack:
    """
    A simple FIFO stack.
    """
    def __init__(self):
        pass
    def push(self, item):
        """
        Add item to stack.
        @param self Stack object
        @param item Item to add
        """
    def pop(self, item):
        pass
    def is_empty(self):
        pass
```

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```
def test_push_pop():
    stack.push(123)
    assert stack.pop() == 123
```

```
class Stack:
```

```
    """
```

```
    A simple FIFO stack.
```

```
    """
```

```
    def __init__(self):
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        def push(self, item):
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            @param self Stack object
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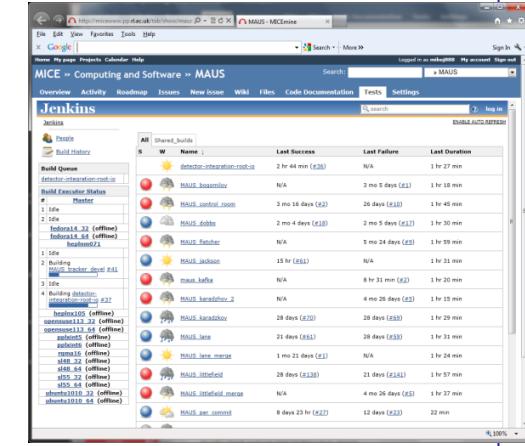
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            @param item Item to add
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```
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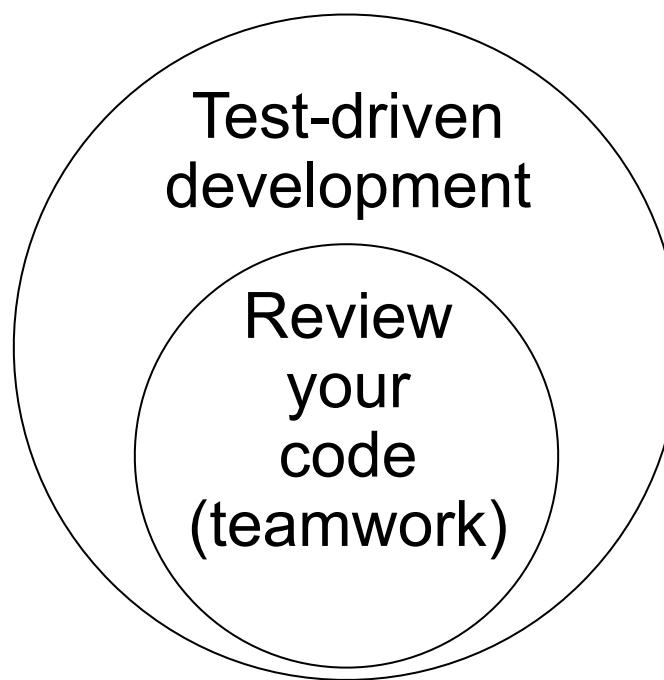
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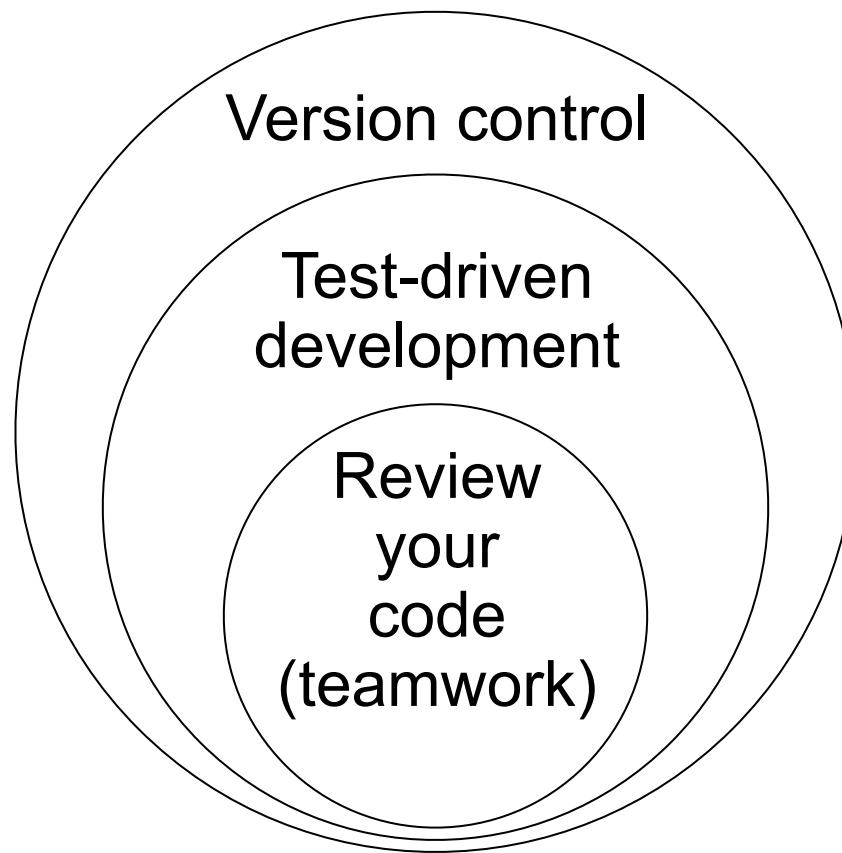
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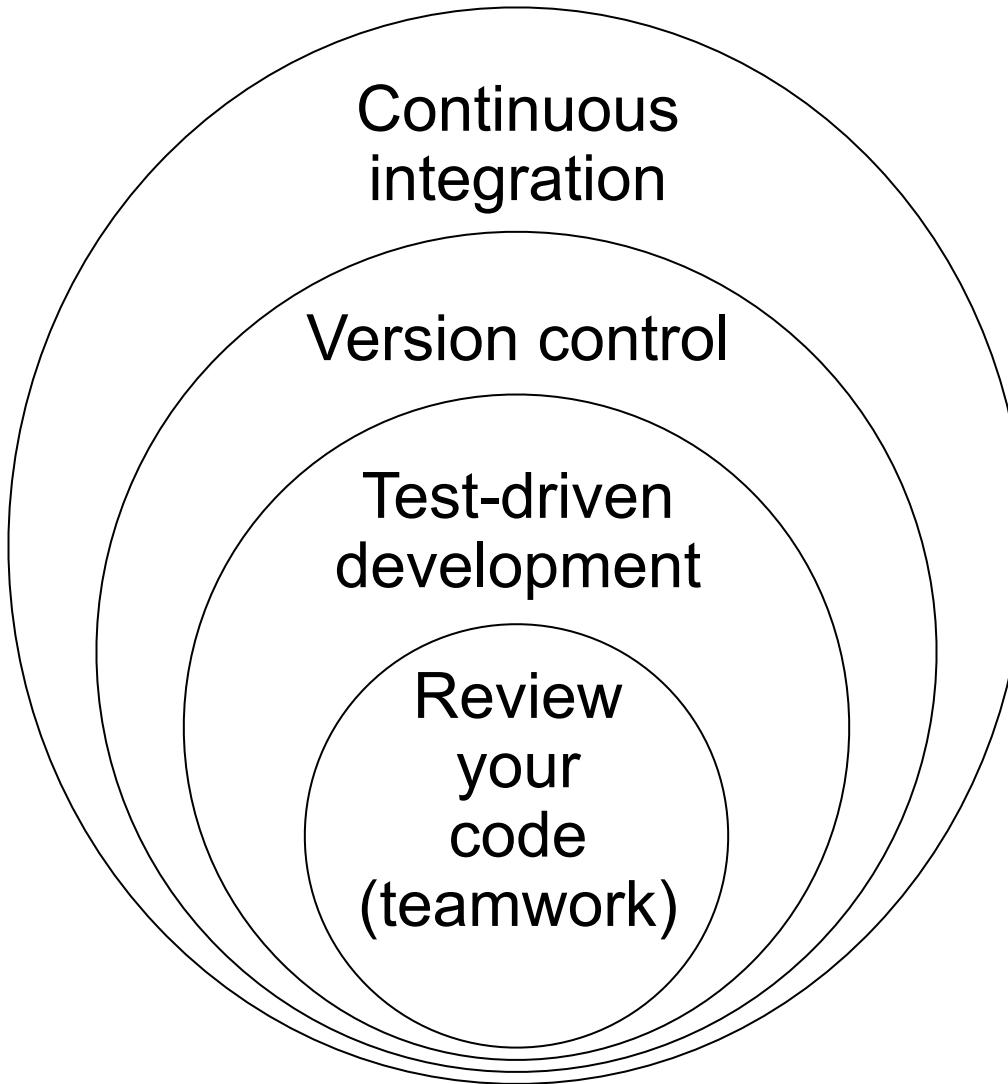


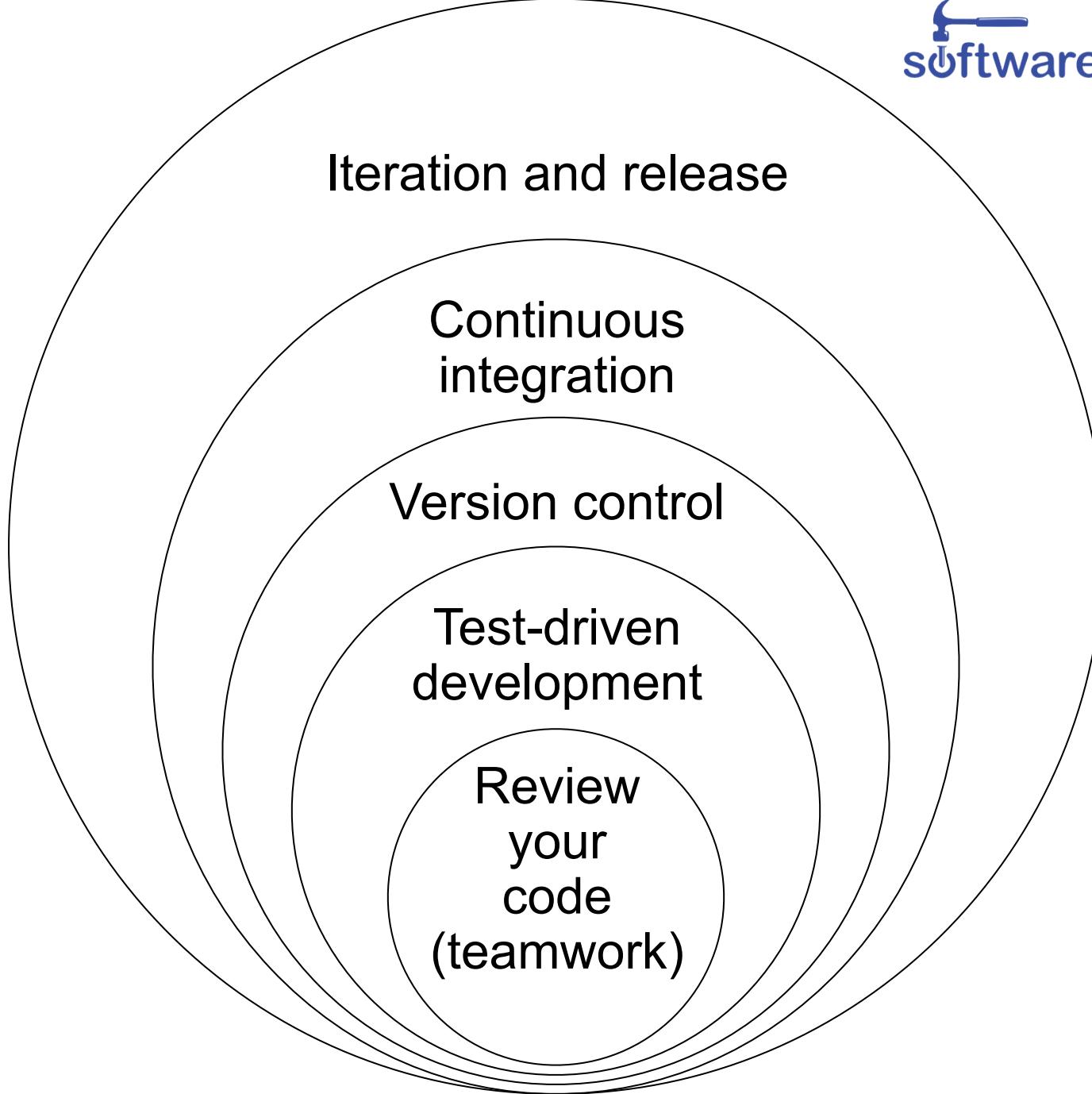


Review  
your  
code  
(teamwork)









# Have your say...



# Have your say...



# Have your say...



Iterative development does not just

# Have your say...



Iterative development does not just  
apply to software

# Have your say...



Iterative development does not just  
apply to software  
so

# Have your say...



Iterative development does not just  
apply to software

so

what did you think of this boot camp?

# current activity:

135 instructors

(30, training)

115 bootcamps

3500 learners



Slide from: <http://www.slideshare.net/kaythaney/upping-our-digital-literacy-okcon>

# Want to get involved?



# Want to get involved?



# Want to get involved?



# Want to get involved?



# Want to get involved?



[admin@software-carpentry.org](mailto:admin@software-carpentry.org)

<http://software-carpentry.org/bootcamps>