

# CAS 741, CES 741 (Development of Scientific Computing Software)

Fall 2020

## 10 Verification and Validation Continued

Dr. Spencer Smith

Faculty of Engineering, McMaster University

October 19, 2020



# Verification and Validation Continued

- Start recording
- Administrative details
- Questions?
- Nonfunctional software testing
- Theoretical foundations of testing
- Complete coverage principle
- White box testing
- Oracle problem
- SCS Specific Ideas
- Overview of template

# Administrative Details

- Drasil projects look at [Learn you a Haskell for Great Good](#)

# Admin Details: VnV Presentations

- Not everyone will do VnV presentations
- Select 1 or 2 of the following:
  - ▶ **Specific** functional system test cases
  - ▶ **Specific** nonfunctional system test cases, such as
    - ▶ Performance profile
    - ▶ Usability testing
  - ▶ SRS verification plan
  - ▶ Automated testing and verification tools
    - ▶ Profiling tools
    - ▶ Continuous integration
    - ▶ Code coverage
    - ▶ Linters
- We would like a variety of topics presented
- If you are uncertain of your specific presentation plan, please ask

# Admin Details: Proof of Concept Presentations

- Deepen your understanding by jumping into implementation
- Identify a risk with your code and implement enough to show you can resolve it
- Looking for an actual demo with running code
- Presentation
  - ▶ Explicitly identify your risk
  - ▶ Run your code
  - ▶ Discuss your implementation
- Simplify as much as necessary
- Do not use this code in your actual implementation

# Administrative Details: Report Deadlines

<b>System VnV Plan</b>	Oct 29
MG + MIS (Traditional)	Nov 19
Drasil Code and Report (Drasil)	Nov 19
Final Documentation	Dec 9

- The written deliverables will be graded based on the repo contents as of 11:59 pm of the due date
- If you need an extension for a written deliverable, please ask
- You should inform your primary and secondary reviewers of the extension
- Two days after each major deliverable, your GitHub issues will be due

# Admin Details: Presentation Schedule

- Syst V&V Plan Present (15 min)
  - ▶ Thurs, Oct 22: Ting-Yu, Mohamed, Naveen, Liz, Salah
- Proof of Concept Demonstrations (15 min)
  - ▶ Mon, Oct 26: Tiago, Mohamed, Xuanming, Parsa, Gaby
  - ▶ Mon, Nov 2: Sid, Shayan, Leila, Xingzhi, Liz
  - ▶ Thurs, Nov 12: Salah, John
- MG Present (10 minutes)
  - ▶ Thurs, Nov 12: John, Tiago, Leila, Xuanming, Andrea
- MIS Present
  - ▶ Mon, Nov 16: Shayan, Parsa, Gaby, Sid, Xingzhi
- Drasil Project Present (20 min each)
  - ▶ Thurs, Nov 26: Andrea, Naveen, Ting-Yu

# Presentation Schedule Continued

- Test or Impl. Present (15 min each)
  - ▶ Mon, Nov 30: John, Salah, Liz, Xingzhi, Leila
  - ▶ Thurs, Dec 3: Shayan, Naveen, Sid, Gaby, Seyed
  - ▶ Mon, Dec 7: Ting-Yu, Xuanming, Mohamed, Andrea, Tiago
- 4 presentations each
- If you will miss a presentation, please trade with someone else



# Questions?

- Questions about V&V?
- Questions about PoC?

# Goals of Testing

- If our code passes all test cases, is it now guaranteed to be error free?
- Are 5000 random tests always better than 5 carefully selected tests?

# Goals of Testing

- To show the **presence** of bugs (Dijkstra, 1972)
- If tests do not detect failures, we cannot conclude that software is defect-free
- Still, we need to do testing - driven by sound and systematic principles
  - ▶ Random testing is often not a systematic principle to use
  - ▶ Need a test plan
- Should help isolate errors - to facilitate debugging

# Goals of Testing Continued

- Should be repeatable
  - ▶ Repeating the same experiment, we should get the same results
  - ▶ Repeatability may not be true because of the effect of the execution environment on testing
  - ▶ Repeatability may not occur if there are uninitialized variables
  - ▶ Repeatability may not happen when there is nondeterminism
- Should be accurate
  - ▶ Accuracy increases reliability
  - ▶ Part of the motivation for formal specification
- Is a successful test case one that passes the test, or one that shows a failure?

# Test (V&V) Plan

- Given that no single verification technique can prove correctness, the practical approach is to use ALL verification techniques. Is this statement True or False?

# Test (V&V) Plan

- Testing can uncover errors and build confidence in the software
- Resources of time, people, facilities are limited
- Need to plan how the software will be tested
- You know in advance that the software is unlikely to be perfect
- You need to put resources into the most important parts of the project
- A risk analysis can determine where to put your limited resources
- A risk is a condition that can result in a loss
- Risk analysis involves looking at how bad the loss can be and at the probability of the loss occurring

# Description Rather Than Specification

- Test cases are often phrased as  $\text{Expected} = \text{Calculated}$
- In scientific software you generally should not test for equality
  - ▶ Absolute error within tolerance
  - ▶ Relative error within tolerance
  - ▶ If comparing matrices or vectors, consider using norms of residual
- Even a specific tolerance often doesn't make sense in a scientific context
- Often your plan should be to **describe** the error rather than **prescribe**
  - ▶ Plot of error versus problem size, or condition number, or ...
  - ▶ Consider summarizing multiple tests with the infinity norm of the relative error (or similar)
- Your description plan is part of your V&V plan!

# White Box Versus Black Box Testing

- Do you know (or can you guess) the difference between white box and black box testing?
- What if they were labelled transparent box and opaque box testing, respectively?



# White Box Versus Black Box Testing

- White box testing is derived from the program's internal structure
- Black box testing is derived from a description of the program's function
- Should perform both white box and black box testing
- Black box testing
  - ▶ Uncovers errors that occur in implementing requirements or design specifications
  - ▶ Not concerned with how processing occurs, but with the results
  - ▶ Focuses on functional requirements for the system
  - ▶ Focuses on normal behaviour of the system

# White Box Testing

- Uncovers errors that occur during implementation of the program
- Concerned with how processing occurs
- Evaluates whether the structure is sound
- Focuses on abnormal or extreme behaviour of the system

# Dynamic Testing

- Is there a dynamic testing technique that can guarantee correctness?
- If so, what is the technique?
- Is this technique practical?

# Dynamic Versus Static Testing

- Another classification of verification techniques, as previously discussed
- Use a combination of dynamic and static testing
- Dynamic analysis
  - ▶ Requires the program to be executed
  - ▶ Test cases are run and results are checked against expected behaviour
  - ▶ Exhaustive testing is the only dynamic technique that guarantees program validity
  - ▶ Exhaustive testing is usually impractical or impossible
  - ▶ Reduce number of test cases by finding criteria for choosing representative test cases

# Static Testing Continued

- Static analysis
  - ▶ Does not involve program execution
  - ▶ Testing techniques simulate the dynamic environment
  - ▶ Includes syntax checking
  - ▶ Generally static testing is used in the requirements and design stage, where there is no code to execute
  - ▶ Document and code walkthroughs (including rubber duck debugging)
  - ▶ Document and code inspections

# Manual Versus Automated Testing

- What is the difference between manual and automated testing?
- What are the advantages of automated testing?
- What is regression testing?

# Manual Versus Automated Testing

- Manual testing
  - ▶ Has to be conducted by people
  - ▶ Includes by-hand test cases, structured walkthroughs, code inspections
- Automated testing
  - ▶ The more automated the development process, the easier to automate testing
  - ▶ Less reliance on people
  - ▶ Necessary for regression testing
  - ▶ Test tools can assist, such as Junit, Cppunit, CuTest etc.
  - ▶ Can be challenging to automate GUI tests
  - ▶ Test suite for Maple has 2 000 000 test cases, run on 14 platforms, every night, automated reporting

# Continuous Integration Testing

- What is continuous integration testing?



# Continuous Integration Testing

- Information available on [Wikipedia](#)
- Developers integrate their code into a shared repo frequently (multiple times a day)
- Each integration is automatically accompanied by regression tests and other build tasks
- Build server
  - ▶ Unit tests
  - ▶ Integration tests
  - ▶ Static analysis
  - ▶ Profile performance
  - ▶ Extract documentation
  - ▶ Update project web-page
  - ▶ Portability tests
  - ▶ etc.
- Avoids potentially extreme problems with integration when the baseline and a developer's code greatly differ

# Continuous Integration Tools

- Gitlab
  - ▶ Example at [Rogue Reborn](#)
  - ▶ [Brasil](#)
    - ▶ Details of Travis CI steps in `.travis.yml` file
    - ▶ Automated case study documentation, code and gen code documentation
    - ▶ Automated build of dependency graphs (bottom of page)
- Jenkins
- Travis
- Docker
  - ▶ Eliminates the “it works on my machine” problem
  - ▶ Package dependencies with your apps
  - ▶ A container for lightweight virtualization
  - ▶ Not a full VM

# Sample Nonfunctional System Testing

- Stress testing - Determines if the system can function when subject to large volumes
- Usability testing
- Performance measurement

# Sample Functional System Testing

- Parallel: Determines the results of the new application are consistent with the processing of the previous application or version of the application

# Theoretical Foundations Of Testing: Definitions

- P (program), D (input domain), R (output domain)
  - ▶  $P: D \rightarrow R$  (may be partial)
- Correctness defined by  $OR \subseteq D \times R$ 
  - ▶ P(d) correct if  $\langle d, P(d) \rangle \in OR$
  - ▶ P correct if all P(d) are correct
- Failure
  - ▶ P(d) is not correct
  - ▶ May be undefined (error state) or may be the wrong result
- Error (Defect)
  - ▶ Anything that may cause a failure
    - ▶ Typing mistake
    - ▶ Programmer forgot to test "x=0"
- Fault
  - ▶ Incorrect intermediate state entered by program

# Definitions Questions

- A test case  $t$  is an element of  $D$  or  $R$ ?
- A test set  $T$  is a finite subset of  $D$  or  $R$ ?
- How would we define whether a test is successful?
- How would we define whether a test set is successful?

# Definitions Continued

- Test case  $t$ : An element of  $D$
- Test set  $T$ : A finite subset of  $D$
- Test is successful if  $P(t)$  is correct
- Test set successful if  $P$  correct for all  $t$  in  $T$

# Theoretical Foundations of Testing

- Desire a test set  $T$  that is a finite subset of  $D$  that will uncover all errors
- Determining an ideal  $T$  leads to several **undecidable problems**
- No algorithm exists:
  - ▶ To state if a test set will uncover all possible errors
  - ▶ To derive a test set that would prove program correctness
  - ▶ To determine whether suitable input exists to guarantee execution of a given statement in a given program
  - ▶ etc.



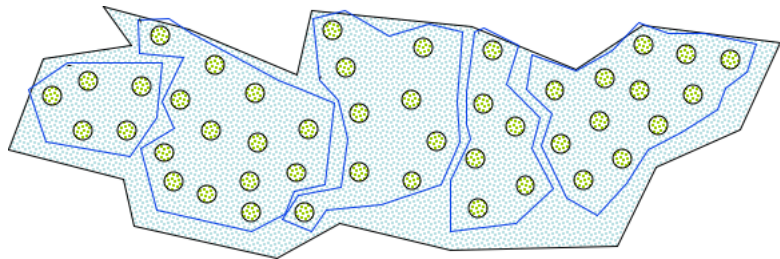
# Empirical Testing

- Need to introduce empirical testing principles and heuristics as a compromise between the impossible and the inadequate
- Find a strategy to select **significant** test cases
- Significant means the test cases have a high potential of uncovering the presence of errors

# Complete-Coverage Principle

- Try to group elements of  $D$  into subdomains  $D_1, D_2, \dots, D_n$  where any element of each  $D_i$  is likely to have similar behaviour
- $D = D_1 \cup D_2 \cup \dots \cup D_n$
- Select one test as a representative of the subdomain
- If  $D_j \cap D_k = \emptyset$  for all  $j \neq k$ , (partition), any element can be chosen from each subdomain
- Otherwise choose representatives to minimize number of tests, yet fulfilling the principle

# Complete-Coverage Principle



# White-box Testing

- Intuitively, after running your test suites, what percentage of the lines of code in your program should be exercised?

# White-box Coverage Testing

- (In)adequacy criteria - if significant parts of the program structure are not tested, testing is inadequate
- Control flow coverage criteria
  - ▶ Statement coverage
  - ▶ Edge coverage
  - ▶ Condition coverage
  - ▶ Path coverage

Examples that follow are from [\[1\]](#)

# Statement-Coverage Criterion

- Select a test set  $T$  such that every elementary statement in  $P$  is executed at least once by some  $d$  in  $T$
- An input datum executes many statements - try to minimize the number of test cases still preserving the desired coverage

## Example

```
read (x); read (y);  
if x > 0 then  
    write ("1");  
else  
    write ("2");  
end if;  
if y > 0 then  
    write ("3");  
else  
    write ("4");  
end if;
```

How would you write a test case?

What is the minimum number of test cases?

## Example

```
read (x); read (y);  
if x > 0 then  
    write ("1");  
else  
    write ("2");  
end if;  
if y > 0 then  
    write ("3");  
else  
    write ("4");  
end if;
```

**$\{\langle x = 2, y = -3 \rangle, \langle x = -13, y = 51 \rangle, \langle x = 97, y = 17 \rangle, \langle x = -1, y = -1 \rangle\}$   
covers all statements**

**$\{\langle x = -13, y = 51 \rangle, \langle x = 2, y = -3 \rangle\}$   
is minimal**



## Weakness of the Criterion

```
if x < 0 then  
    x := -x;  
end if;  
z := x;
```

$\{<x=-3>\}$  covers all  
statements. Why  
is this not enough?

## Weakness of the Criterion

```
if x < 0 then  
    x := -x;  
end if;  
z := x;
```

$\{x < -3\}$  covers all  
statements

it does not exercise the  
case when x is positive  
and the then branch is  
not entered

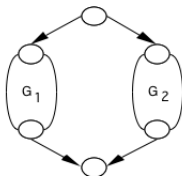
# Edge-Coverage Criterion

- Select a test set  $T$  such that every edge (branch) of the control flow is exercised at least once by some  $d$  in  $T$
- This requires formalizing the concept of the control graph and how to construct it
  - ▶ Edges represent statements
  - ▶ Nodes at the ends of an edge represent entry into the statement and exit

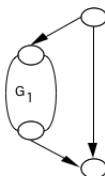
# Control Graph Construction Rules



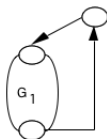
I/O, assignment,  
or procedure call



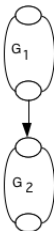
if-then-else



if-then



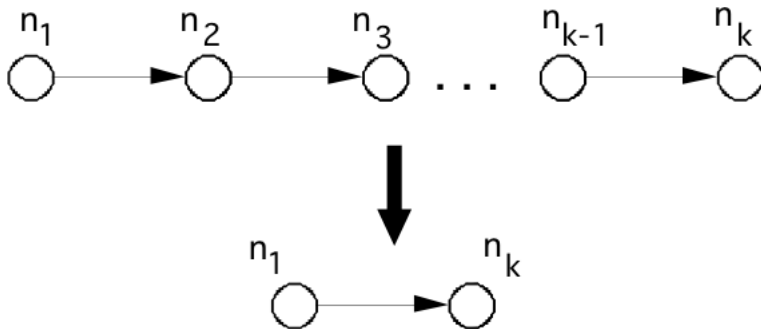
while loop



two sequential  
statements

# Simplification

A sequence of edges can be collapsed into just one edge



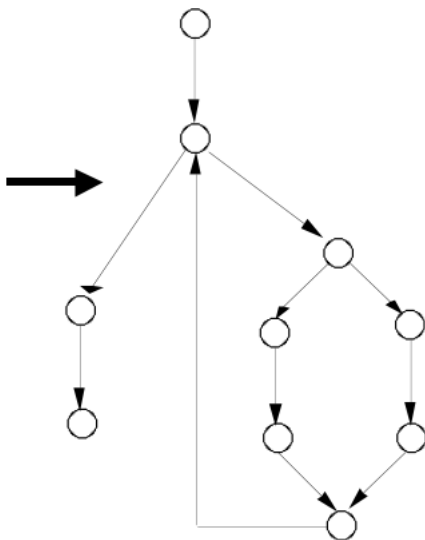
# Example: Euclid's Algorithm

```
begin
  read (x); read (y);
  while  $x \neq y$  loop
    if  $x > y$  then
       $x := x - y$ ;
    else
       $y := y - x$ ;
    end if;
  end loop;
  gcd := x;
end;
```

Draw the control  
flow graph

# Example: Euclid's Algorithm

```
begin
  read (x); read (y);
  while  $x \neq y$  loop
    if  $x > y$  then
       $x := x - y$ ;
    else
       $y := y - x$ ;
    end if;
  end loop;
  gcd := x;
end;
```



# Weakness

```
found := false; counter := 1;
while (not found) and counter < number_of_items loop
    if table(counter) = desired_element then
        found := true;
    end if;
    counter := counter + 1;
end loop;
if found then
    write ("the desired element is in the table");
else
    write ("the desired element is not in the table");
end if;
```

test cases: (1) empty table, (2) table with 3 items, second of which is the item to look for



# Weakness

```
found := false; counter := 1;
while (not found) and counter < number_of_items loop
    if table(counter) = desired_element then
        found := true;
    end if;
    counter := counter + 1;
end loop;
if found then
    write ("the desired element is in the table");
else
    write ("the desired element is not in the table");
end if;
```

test cases: (1) empty table, (2) table with 3 items, second of which is the item to look for

Do not discover the error ( $<$  instead of  $\leq$ )

```
if c1 and c2 then  
    st;  
else  
    sf;
```

*// equivalent to*

```
if c1 then  
    if c2 then  
        st;  
    else  
        sf;  
else  
    sf;
```

# Condition-Coverage Criterion

- Select a test set  $T$  such that every edge of  $P$ 's control flow is traversed and all possible values of the constituents of compound conditions are exercised at least once
- This criterion is finer than edge coverage

# Weakness

```
if  $x \neq 0$  then
     $y := 5$ ;
else
     $z := z - x$ ;
end if;
if  $z > 1$  then
     $z := z / x$ ;
else
     $z := 0$ ;
end if;
```

$\{ \langle x = 0, z = 1 \rangle, \langle x = 1, z = 3 \rangle \}$   
causes the execution of all edges,  
but fails to expose the risk of a  
division by zero

# Path-Coverage Criterion

- Select a test set  $T$  that traverses all paths from the initial to the final node of  $P$ 's control flow
- It is finer than the previous kinds of coverage
- However, number of paths may be too large, or even infinite (see while loops)
- Loops
  - ▶ Zero times (or minimum number of times)
  - ▶ Maximum times
  - ▶ Average number of times

# The Infeasibility Problem

- Syntactically indicated behaviours (statements, edges, etc.) are often impossible
- Unreachable code, infeasible edges, paths, etc.
- Adequacy criteria may be impossible to satisfy
  - ▶ Manual justification for omitting each impossible test case
  - ▶ Adequacy “scores” based on coverage - example 95 % statement coverage

## Further Problem

- What if the code omits the implementation of some part of the specification?
- White box test cases derived from the code will ignore that part of the specification!

# Testing Boundary Conditions

- Testing criteria partition input domain in classes, assuming that behavior is “similar” for all data within a class
- Some typical programming errors, however, just happen to be at the boundary between different classes
  - ▶ Off by one errors
  - ▶  $<$  instead of  $\leq$
  - ▶ equals zero



# Criterion

- After partitioning the input domain  $D$  into several classes, test the program using input values not only “inside” the classes, but also at their boundaries
- This applies to both white-box and black-box techniques
- In practice, use the different testing criteria in combinations
- Use testing tools for coverage metrics

# The Oracle Problem

When might it be difficult to know the “expected” output/behaviour?

# The Oracle Problem

- Given input test cases that cover the domain, what are the expected outputs?
- Oracles are required at each stage of testing to tell us what the right answer is
- Black-box criteria are better than white-box for building test oracles
- Automated test oracles are required for running large amounts of tests
- Oracles are difficult to design - no universal recipe

# The Oracle Problem Continued

- Determining what the right answer should be is not always easy
  - ▶ Scientific computing
  - ▶ Machine learning
  - ▶ Artificial intelligence

# The Oracle Problem Continued

What are some strategies we can use when we do not have a test oracle?

# Strategies Without An Oracle

- Using an independent program to approximate the oracle (pseudo oracle)
- Method of manufactured solutions
- Properties of the expected values can be easier than stating the expected output
  - ▶ Examples?

# Strategies Without An Oracle

- Using an independent program to approximate the oracle (pseudo oracle)
- Method of manufactured solutions
- Properties of the expected values can be easier than stating the expected output
  - ▶ Examples?
  - ▶ List is sorted
  - ▶ Number of entries in file matches number of inputs
  - ▶ Conservation of energy or mass
  - ▶ Expected trends in output are observed (metamorphic testing [5, 4, 6])
  - ▶ etc.

# Challenges Specific to Scientific Computing

- Unknown solution
- Approximation of real numbers
- Nonfunctional requirements
- Parallel computation



# Mutation Testing for SC

- Generate changes to the source code, called mutants, which become code faults
- Mutants include changing an operation, modifying constants, changing the order of execution, etc.
- The adequacy of a set of tests is established by running the tests on all generated mutants
- Need to account for floating point approximations
- See [3]

# Specific SC V&V Approaches

Summary of most points below in [10]

- Compare to closed-form solutions
- Method of manufactured solutions [8]
- Interval arithmetic [2]
- Convergence studies
- Compare to other program (parallel testing)
- Can also consider using code inspection
  - ▶ [7, 9]
  - ▶ Sample checklists

# Specific SC V&V NonFunctional

- Installability, consider VMs
- Portability, consider VMs, Docker, CI
- Describe (rather than specify) impact of changing inputs
  - ▶ Accuracy
  - ▶ Performance
  - ▶ Relative comparison
- Usability
  - ▶ Fairly simple standard survey
  - ▶ Example

# Validation Testing Report for PMGT

- Prepared by Wen Yu ([here](#))
- Do not know the correct solution, but know properties of the correct solution
- Automated correctness validation tests
  - ▶ The area of each element is greater than zero
  - ▶ The boundary of the mesh is closed
  - ▶ Vertices in a clockwise order
  - ▶  $nc + nv - ne = 1$
  - ▶ ...
- Visual correctness verification tests
  - ▶ No vertex outside the input domain
  - ▶ No vertex inside a cell
  - ▶ No dangling edges
  - ▶ All cells connected
  - ▶ The mesh is conformal

# Validation Testing Report for PMGT (Continued)

- List and description of test cases
- Test cases are labelled and numbered
- Traceability to SRS requirements
- Traceability to MG
- Summary of results
- Analysis of results
  - ▶ Focus on nonfunctional requirements
  - ▶ Speed

# Test Plan From BlankProjectTemplate

- Add links to templates
- For Unit VnV plan mention tools
  - ▶ Linters
  - ▶ Coding standard checkers (like flake8)
  - ▶ unit testing frameworks
  - ▶ Performance testing (like Valgrind)

# References I



Carlo Ghezzi, Mehdi Jazayeri, and Dino Mandrioli.

*Fundamentals of Software Engineering.*

Prentice Hall, Upper Saddle River, NJ, USA, 2nd edition, 2003.



Timothy Hickey, Qun Ju, and Maarten H. Van Emden.

Interval arithmetic: From principles to implementation.

*J. ACM*, 48(5):1038–1068, September 2001.



Daniel Hook and Diane Kelly.

Testing for trustworthiness in scientific software.

In *Proceedings of the 2009 ICSE Workshop on Software Engineering for Computational Science and Engineering*, SECSE '09, pages 59–64, Washington, DC, USA, 2009. IEEE Computer Society.

# References II



U. Kanewala and J. M. Bieman.

Techniques for testing scientific programs without an oracle.

*In Software Engineering for Computational Science and Engineering (SE-CSE), 2013 5th International Workshop on*, pages 48–57, May 2013.



Upulee Kanewala, James M. Bieman, and Asa Ben-Hur.

Predicting metamorphic relations for testing scientific software: A machine learning approach using graph kernels.

*Software Testing Verification and Reliability*, preprint, 2015.



# References III



Upulee Kanewala and Anders Lundgren.

Automated metamorphic testing of scientific software.

In Jeffrey C. Carver, Neil Chue Hong, and George Thiruvathukal, editors, *Software Engineering for Science*, Chapman & Hall/CRC Computational Science, chapter Examples of the Application of Traditional Software Engineering Practices to Science, pages 151–174. Taylor & Francis, 2016.



Diane Kelly and Terry Shepard.

Task-directed software inspection technique: an experiment and case study.

In *CASCON '00: Proceedings of the 2000 conference of the Centre for Advanced Studies on Collaborative research*, page 6. IBM Press, 2000.

# References IV



Patrick J. Roache.

*Verification and Validation in Computational Science and Engineering.*

Hermosa Publishers, Albuquerque, New Mexico, 1998.



Terry Shepard and Diane Kelly.

How to do inspections when there is no time.

In *Proceedings of the 23rd International Conference on Software Engineering*, page 718. IEEE Computer Society, 2001.

# References V



W. Spencer Smith.

A rational document driven design process for scientific computing software.

In Jeffrey C. Carver, Neil Chue Hong, and George Thiruvathukal, editors, *Software Engineering for Science*, chapter Section I – Examples of the Application of Traditional Software Engineering Practices to Science, pages 33–63. Taylor & Francis, 2016.