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Better Scientific Software tutorial @ ISC 2022

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- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software tutorial, ISC, 2022 ...

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## **Software Testing - Outline**

# **Testing Introduction**

- What is testing?
- Challenges of testing
- Simple Examples

# **Testing Examples**

Walk Through Testing Example

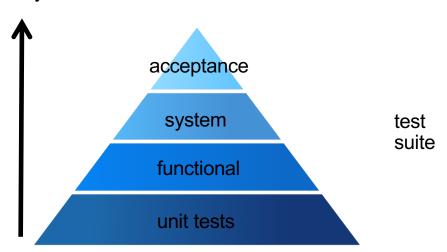




# **General Categories of Testing**

- Development tests
  - Tests run to protect stability while making changes to the code
  - Can include: unit, functional, integration, system, regression, verification, performance, etc.
- Post-installation "smoke" tests
  - Simple tests to ensure the build/install process has succeeded
  - Typically take only a few minutes
  - Could be a subset of development tests
- Continuous integration tests
  - Rapid feedback aimed at preventing changes from breaking key branches of the code
  - Run quickly, fail fast, catch problems that would impact other developers
  - Usually associated with automation

Code coverage, Complexity







# **Example types of testing**

- Unit testing verify the execution of a single routine
- Integration testing verify that modules or components execute correctly
- System testing verify that the program operates correctly as a whole
- Regression testing comparison with previous output to determine if unintended changes have been introduced
- Acceptance testing verify that the program meets customer requirements or not

Note that this is neither a complete nor prescriptive list of testing types. There are many other types of tests. Sometimes it can be beneficial to combine testing strategies, such as testing the interoperability of modules and components at the system level.





#### What about Verification and Validation?

Scientific computing and software engineering use different definitions

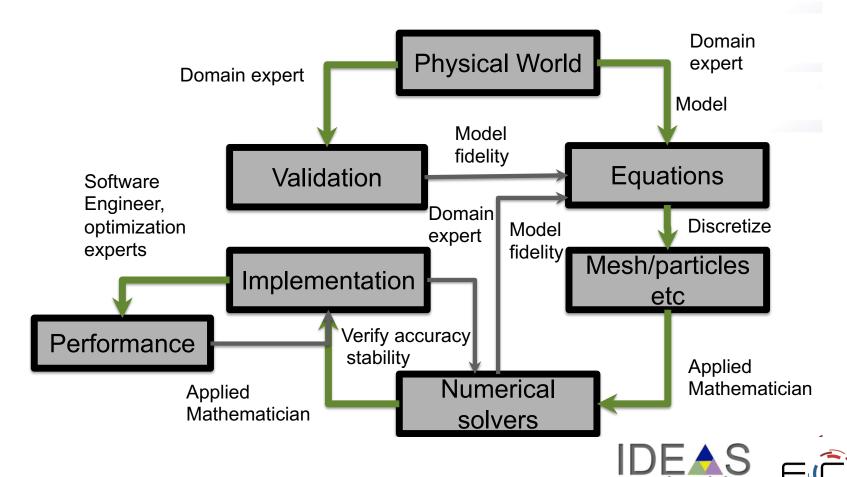
	Scientific computing	Software engineering
Verification	Confirms the mathematical accuracy and stability of a numerical solution in addition to specifications.	Confirms that the software conforms to its specifications (i.e. requirements.)
Validation	Confirms the physical accuracy of a given model by comparing against experimental data.	Confirms that the software actually meets the customer's needs.

- Validation in scientific computing requires a comparison to the experimental data, whereas in software engineering it is based on customer needs
- Also, for a real problem, there is typically no way to check for correct output given some inputs. Validation is still required however, so an indirect method must be used.





# Testing within the software development lifecycle



# Testing within the software development lifecycle

- When should functional tests be provided?
- Ideally before the code is written
  - Also known as test driven development (TDD)
  - Tests then become the specification for the program
- This approach also ensures that thought is given to what it means for the program to be correct, rather than just what the program should do
- Requires:
  - Care in writing tests
  - Frequent running of tests (see our Continuous Integration module)
  - Wide adoption by development team





# Steps for test driven development

- Write a single test¹ describing an aspect of the program
- Run the test, which should fail because the feature does not exist
- Write just enough code to make the test pass
- Refactor the code
- Repeat, creating new tests as new functionality is added

<sup>&</sup>lt;sup>1</sup>In numerical methods there are times when a single test may not suffice





# **Challenges of Testing Complex Software Systems**

#### Designing tests

- Complex software tends to have an extensive network of interdependencies
- For complex scientific software it may be hard to construct a priori tests for some cases
- Exploratory software implies the outcome is not known or when the model is valid
- Validation from domain experts feeds back into the design

#### Implementing tests

- Introducing testing into legacy code (legacy == untested)
- Original verification has been lost in the mists of time.
- Assumptions, conditions, interactions unknown: "Bad code or necessary evil?"
- Understanding and progressively improving code coverage





# **More Challenges of Testing Complex Software Systems**

- Automating tests
  - Just get started easy to get lost in all the options
  - You must have tests to be able to automate them!
  - Automation does not just mean running every test you have
- What to run where, and when?
  - Consider what resources are required, and what the tests are used for





#### How do we determine what tests are needed?

#### **Code coverage tools**

- Expose parts of the code that aren't being tested
  - gcov standard utility with the GNU compiler collection suite (we will use it in the next few slides)
  - Compile/link with –coverage & turn off optimization
  - Counts the number of times each statement is executed
  - Necessary for testing, but not sufficient
- gcov also works for C and Fortran
  - Other tools exist for other languages
  - JCov for Java
  - Coverage.py for python
  - Devel::Cover for perl
  - profile for MATLAB

- Lcov
  - a graphical front-end for gcov
  - available at http://ltp.sourceforge.net/coverage /lcov.php
  - Codecov.io in CI module
- Hosted servers (e.g. coveralls, codecov)
- graphical visualization of results
- push results to server through continuous integration server





# **Summary**

- A testing strategy is essential for producing reliable trustworthy software
  - Invest the time needed to thoroughly test your software at all levels
  - Use automation whenever possible
- Different challenges are associated with exploratory, legacy, and composable codes
  - Adapt your strategy to fit your situation.
  - Eventually you will want to be able to verify all components in a code release.
- Don't get distracted by all the technologies out there focus on exercising your code.
  - Scaffolding projects can help with mechanics.





# **Going Further**

- C, C++, Fortran
  - Running and Reporting Tests: ctest / cdash / pFUnit / FlashTest
  - Code Coverage: gcov / Icov (C, C++, Fortran)
  - Static Analysis: clang-tidy (only C, C++)
- Python
  - Running and Reporting Tests: pytest / unittest / nose
  - Code Coverage: pytest-cov
  - Static Source Code Analysis: pylint / flake8





### **Hands On Activities**

- Simple Python and C++ examples
- Checking code coverage example
- Test driven development example

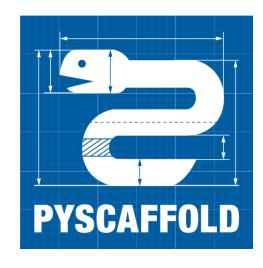




## **Python Example**

```
$ pip install pyscaffold
$ pip install tox
$ putup autoQCT
$ cd autoQCT # tests in tests/ subdir.
$ tox
```

```
default run-test: commands[0] | pytest
platform darwin -- Python 3.9.0, pytest-6.2.2, py-1.10.0, pluggy-0.13.1 -- plugins: cov-2.11.1
collected 2 items
tests/test_skeleton.py::test_fib_PASSED
                                     [50%]
tests/test skeleton.py::test main PASSED
                                       [100%]
----- coverage: platform darwin, python 3.9.0-final-0 ------
              Stmts Miss Branch BrPart Cover Missing
Name
src/autoqct/ init .py
                             0 100%
src/autogct/skeleton.py
                  32
                              0 97% 135
TOTAL
               38
                             98%
default: commands succeeded
congratulations:)
```



pyscaffold.org



## **CMake Example**

```
$ cat >CMakeLists.txt <<.
cmake_minimum_required(VERSION 3.8)
project( blank )
set(CMAKE_CXX_STANDARD 11)
set(CMAKE_CXX_STANDARD_REQUIRED ON)
include(blt/SetupBLT.cmake)
.
$ git clone https://github.com/LLNL/blt/
$ mkdir build && cd build
$ cmake ..
$ make -j</pre>
```

IlnI-blt.readthedocs.io



# Checking Code Coverage Example <a href="https://github.com/bssw-tutorial/hello-numerical-world">https://github.com/bssw-tutorial/hello-numerical-world</a>

- Example of heat equation
  - Add -coverage as shown below to Makefile
  - Run ./heat runame="ftcs results"
  - Run gcov heat.C
  - Examine heat.C.gcov

```
HDR = Double.H
SRC = heat.C utils.C args.C exact.C ftcs.C upwind15.C crankn.C
OBJ = S(SRC:.C=.o)
GCOV = (SRC: C=.C.gcov) (SRC: C=.gcda) (SRC: C=.gcno) (HDR: COV)
H=.H.gcov)
EXE = heat
# Implicit rule for object files
%.o: %.C
        $(CXX) -c -coverage $(CXXFLAGS) $(CPPFLAGS) $< -o $@</pre>
# Linking the final heat app
heat: $(OBJ)
        $(CXX) -coverage -o heat $(OBJ) $(LDFLAGS) -lm
```

- A dash indicates non-executable line
- A number indicated the times the line was called
- ##### indicates line wasn't exercised

```
143:static bool
        144:update_solution()
        145:
        146:
                if (!strcmp(alg, "ftcs"))
        147:
                    return update_solution_ftcs(Nx, curr, last, alpha, dx, dt, bc0, bc1);
        148:
                else if (!strcmp(alg, "upwind15"))
#####:
        149:
                    return update solution upwind15(Nx, curr, last, alpha, dx, dt, bc0, bc1);
#####:
                else if (!strcmp(alg, "crankn"))
####:
                    return update_solution_crankn(Nx, curr, last, cn_Amat, bc0, bc1);
####:
                return false;
        153:}
        154:
        155:static Double
        156:update_output_files(int ti)
 500:
                Double change;
 500:
        160:
                if (ti>0 && save)
                    compute exact_solution(Nx, exact, dx, ic, alpha, ti*dt, bc0, bc1);
#####:
#####:
                    if (savi && ti%savi==0)
#####:
                        write array(ti, Nx, dx, exact);
####:
```



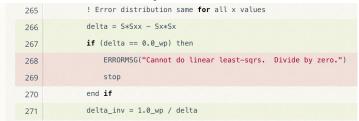


# Graphical View of Gcov Output and Tutorials for Code Coverage

### **Coverage Summary**



## Line-by-line details



Online tutorial - <a href="https://github.com/amklinv/morpheus">https://github.com/amklinv/morpheus</a>
Other example - <a href="https://github.com/jrdoneal/infrastructure">https://github.com/jrdoneal/infrastructure</a>





## **Test Driven Development Example**

https://github.com/bssw-tutorial/hello-numerical-world/tree/main/tdd-

```
$ wc *.C
     125
             494
                    4161 args.C # parse arguments
                     5667 heat.C # main() — stores all vars
     220
             718
                    3888 utils.C # l2_norm, write, copy, init
     151
             498
                     820 ftcs.C # standard, centered stencil
             119
                     833 upwind15.C # alternate integration schemes
             123
                    2134 crankn<sub>•</sub>C
             344
                                     # comparison solution
             190
                     1299 exact<sub>•</sub>C
```

- Lots of setup code prepares problem for kernel calls
- Isolated, swappable kernel calls
  - Imagine adding kernels to larger, multi-physics application.
- How do we add new kernels using test driven development?





#### Build and run the code

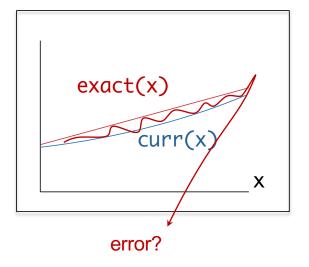
```
$ cd tdd-example
$ cmake.
$ make
$ ./heat alg=ftcs outi=0 maxt=-5e-8 ic="rand(0,0.2,2)"
    runame="heat_results"
    alpha=0.2
    lenx=1
    dx = 0.1
    dt = 0.004
    maxt=-5e-08
    bc0=0
    bc1=1
    ic="rand(0,0.2,2)"
    alg="ftcs"
Stopped after 001490 iterations for threshold 2.46636e-15
```





#### Add a new kernel

- Need to add test first
- What to test?
  - ensure arguments are correct, bad cases detected, etc.
  - steady-state (should be straight line)
    - external script can test file write() as well
  - solution time-dependence vs. reference
    - $(d/dx)^2 \sin(ax) = -a^2 \sin(ax)$
  - test multiple precisions
    - combinatorial problems listing tests in for() or matrix...

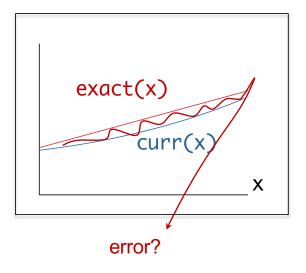






# check.sh will check for steady state

```
$ sh check.sh ./heat ftcs
runame="check_ftcs"
    alpha=0.2
    lenx=1
    dx=0.1
    dt=0.004
    maxt=-5e-08
    bc0=0
    bc1=1
    ...
Stopped after 001490 iterations for threshold 2.46636e-15
Error = 0
```



steady-state test (should be straight line)





#### Create our tests before we write the code

```
$ mkdir tests
$ cp check.sh tests/check.sh
$ cd tests
```

- Create CMakeLists.txt
- Add test for new kernel
- Optionally add test for existing kernel

```
enable_testing()

add_test(NAME ftcs COMMAND check.sh $<TARGET_FILE:heat> ftcs)
add_test(NAME upwind15 COMMAND check.sh $<TARGET_FILE:heat> upwind15)
```

https://cmake.org/cmake/help/latest/command/add\_test.html





#### Re-run cmake to enable tests

```
$ cd ...
$ cmake -DBUILD_TESTS=ON .
$ cd tests
```

#### Run tests

```
$ ctest
Test project /home/tutorial/hello-numerical-world/tests
   Start 1: ftcs
1/2 Test #1: ftcs ..... Passed
                                                     0.23 sec
   Start 2: upwind15
2/2 Test #2: upwind15 ...............***Failed
                                                     0.01 sec
50% tests passed, 1 tests failed out of 2
Total Test time (real) = 0.25 sec
The following tests FAILED:
Errors while running CTest
```

#### Add new kernel to make test succeed

```
$ cd ..
```

- Edit heat
- Add prototype

```
68
69 extern bool
70 update_solution_upwind15(int n,
71 Double *curr, Double const *last,
72 Double alpha, Double dx, Double dt,
73 Double bc_0, Double bc_1);
```

Modify assertion

```
91 assert(strncmp(alg, "ftcs", 4)==0 || strncmp(alg, "upwind15", 8)==0);
```

Call kernel

```
if (!strcmp(alg, "ftcs"))
return update_solution_ftcs(Nx, curr, last, alpha, dx, dt, bc0, bc1);
else if (!strcmp(alg, "upwind15"))
return update_solution_upwind15(Nx, curr, last, alpha, dx, dt, bc0, bc1);

productivity
```

#### Add new kernel to build

#### CMakeLists.txt

#### Re-build executable

```
$ make
-- Configuring done
-- Generating done
-- Build files have been written to: /home/tutorial/hello-numerical-world
Scanning dependencies of target heat
[ 14%] Building CXX object CMakeFiles/heat.dir/heat.C.o
[ 28%] Building CXX object CMakeFiles/heat.dir/upwind15.C.o
[ 42%] Linking CXX executable heat
[100%] Built target heat
```



#### Re-run tests

- Succeeded!
- This is all there is to start to use test driven development





# **Going Further**

- Add another kernel
  - crankn.C
  - Note: requires an extra initialization step!
- Reproduce these testing strategies on another repository
  - https://github.com/frobnitzem/simple-heateq (same problem, different design)
- Brainstorm some simple tests you could add to your own project
  - checks you've run manually
  - difficult-to-setup and reproduce cases that could be automated
- Add some "blank tests" to your project
  - reduces the barrier to increased testing
  - What would make reporting on your build / run status better/simpler/more accessible?

#### Resources

- Oberkampf, W., & Roy, C. (2010). Verification and Validation in Scientific Computing. Cambridge: Cambridge University Press. doi:10.1017/CBO9780511760396
- Michael Feathers. 2004. Working Effectively with Legacy Code. Prentice Hall PTR, USA. ISBN: 9780131177055



