Software Testing and Verification

Anshu Dubey (she/her)
Argonne National Laboratory

Software Productivity and Sustainability track @ Argonne Training Program on Extreme-Scale Computing summer school

Contributors: Anshu Dubey (ANL), Patricia Grubel (LANL), Rinku Gupta (ANL), Alicia Klinvex (SNL), Mark C. Miller (LLNL), Jared O’Neal (ANL), David M. Rogers (ORNL), Gregory R. Watson (ORNL)
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• The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Todd Gamblin, Jared O’Neal, and Boyana R. Norris, Software Productivity and Sustainability track, in Argonne Training Program on Extreme-Scale Computing, St. Charles, Illinois, 2022. DOI: 10.6084/m9.figshare.20416215.

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

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Motivation – Testing Practices

• Supercomputer Cycles are Scarce Resources
  – Goal = capture QA details during science runs

• Many people need to have confidence in your results:
  – You
  – Your project lead or boss
  – Your sponsor
  – Your reviewers or referees
  – Your readers

• Testing helps build credibility without repeating runs.
What about Verification and Validation?

- Scientific computing and software engineering use different definitions

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

• 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 test\(^1\) 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

\(^1\)In numerical methods there are times when a single test may not suffice
Testing within the software development lifecycle
Developing Tests

We verify correct behavior

How?
Developing Tests

We verify correct behavior

How?

We think of ways in which we can tell whether the code is doing what it is supposed to do
Developing Tests

We verify correct behavior.

How?

1. Compare against a known analytical solution.
2. Compare against a manufactured solution.

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Developing Tests

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How?

Compare against a known analytical solution

Compare against a manufactured solution

Right there are all the ingredients for building tests

All that is needed is automating directly or indirectly

We think of ways in which we can tell whether the code is doing what it is supposed to do
Developing Tests

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How?

We think of ways in which we can tell whether the code is doing what it is supposed to do

Visualize and inspect output

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Compare against a manufactured solution

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Develop diagnostics (indirect ways of verification)

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Right there are all the ingredients for building tests

All that is needed is automating directly or indirectly

Including these through automation is equally important

Comparison utility
Conserved quantities
Error bars
Statistical analysis
Test Development For a New Code

For every new functionality being added, think about its verification

Simple functions: relation between input and output => unit test

If it has limited dependencies, manufacturing input for known output will give you a self test

Other functions: build scaffolding

If manufacturing input is too difficult, again apply scaffolding
Test Development For a New Code

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Example – Shock Hydrodynamics with Adaptive Mesh Refinement

Components needed

• Mesh
• Hydrodynamics solver
• Equation of state
• Parallelization

Strategy for development
Think of an application with analytical solution
Example – Shock Hydrodynamics with Adaptive Mesh Refinement

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Strategy for development
Think of an application with analytical solution

- Sedov blast wave
- High pressure at the center
- Shock moves out in a circle
- Analytical solution for how far the shock has travelled
Step 1 – Equation of State

• Initialize density and internal energy with known values
• Compute pressure and temperature using EOS
• Next use density and computed pressure as input and compute internal energy and temperature using EOS
• Compare computed values against initialized values
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- Initialize density and internal energy with known values
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- Next use density and computed pressure as input and compute internal energy and temperature using EOS
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We have a unit test
Step 2 – Mesh

- Start with uniform grid
- Domain decomposition for parallelization
  - Halo fill operation
- Initialize the interior (red) with a known function
- Apply halo fill
- Compute values for the halo using the known function
- Compare against filled values
Step 2 – Mesh

• Start with uniform grid
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Step 3 – Hydrodynamics

• Apply initial conditions to the mesh
  – zeroes everywhere except at the center

• Write code for the analytical expression of the distance traveled by the shock

• Do time integration

• At time $T$ compare evolved solution against analytical solution

If both mesh and EOS unit test pass, then any failure is in Hydrodynamics

This is the idea behind scaffolding
Step 4: AMR

• The same halo fill unit test for mesh also works for AMR

• Additional functionalities to test are:
  – Fine-coarse boundary resolution
  – Regridding

• Steps in testing
  – Run Sedov with UG
  – Run Sedov with AMR, but no dynamic refinement
    • If failed fault is in flux correction
  – Run Sedov with AMR and dynamic refinement
    • If failed fault is in regridding
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We have continued to build scaffolding and are able to pinpoint cause of error
Test Development For a Legacy Code

There may not be existing tests

- Isolate a small area of the code
- Dump a useful state snapshot
- Build a test driver
  - Start with only the files in the area
  - Link in dependencies
    - Copy if any customizations needed
- Read in the state snapshot
- Restart from the saved state
- Verify correctness
  - Always inject errors to verify that the test is working
How to build your test suite?

- Two “levels”
  - Automated / scheduled testing
    - May be long running
    - Provide comprehensive coverage
  - Continuous integration
    - Quick diagnosis of error
How to build your test suite?

• A mix of different granularities works well
  – Unit tests for isolating component or sub-component level faults
  – Integration tests with simple to complex configuration and system level
  – Restart tests

• Rules of thumb
  – Simple
  – Enable quick pin-pointing

Useful resources https://ideas productivity.org/resources/howtos/
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
  - Codecov.io in CI module

- Hosted servers (e.g. coveralls, codecov)

- graphical visualization of results

- push results to server through continuous integration server
Building Test-suite

First line of defense – code coverage tools

- Code coverage tools necessary but not sufficient
- Do not give any information about interoperability

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<th>EOS</th>
<th>Gravity</th>
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- Map your tests and examples – what do they do?
- Follow the order
  - All unit tests – including full module tests (e.g. CL)
  - Tests sensitive to perturbations (e.g. SV)
  - Most stringent tests for solvers (e.g. WD, PT)
  - Least complex test to cover remaining spots (Aha!)
Good Rules of Thumb

• Test your tests!
  – Make sure tests fail when they’re supposed to!

• Add “regression tests”
  – Ensure that bugs aren’t creeping in

• Test regularly
  – Critical when teams are adding code regularly
  – To identify and document where changes to the underlying platform change code behavior/results

• Automate regular testing
  – Inculcate the discipline of monitoring the outcome of regular testing

• Exercise third-party dependencies

• Physics/math based strategies
  – Conserved quantities, symmetries, synthetic operators
  – Eliminate complete dependence on bitwise reproducibility
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.
Resources

