





Testing Complex Software

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Developing a Testing and Continuous Integration Strategy for your Team tutorial @ Exascale Computing Project Annual Meeting

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- The requested citation the overall tutorial is: Gregory R. Watson and David M. Rogers, Developing a Testing and Continuous Integration Strategy for your Team tutorial, in Exascale Computing Project Annual Meeting, online, 2022. DOI: 10.6084/m9.figshare.19608927
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial...

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How to build your test suite?

- Two "levels"
 - Automated / scheduled testing
 - May be long running
 - Provide comprehensive coverage
 - Continuous integration
 - · Quick diagnosis of error
- 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/





Why not always use the most stringent testing?

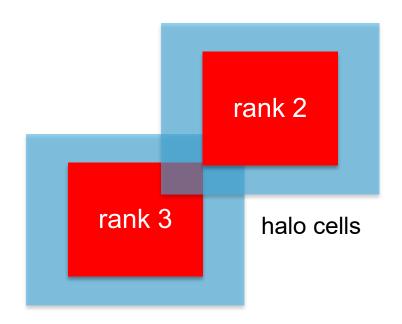
- Effort spent in devising running and maintaining test suite is a tax on team resources
- When the tax is too high...
 - Team cannot meet code-use objectives
- When is the tax is too low...
 - Necessary oversight not provided
 - Defects in code sneak through





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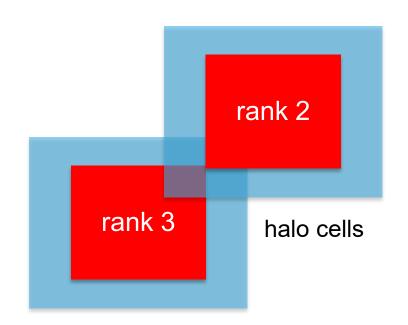






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- Evaluate project needs:
 - Objectives: expected use of the code
 - Lifecycle stage: new or production or refactoring
 - Team: size and degree of heterogeneity
 - Lifetime: one off or ongoing production
 - Complexity: modules and their interactions







Additional Notes: Good Testing Practices

- Verify Code coverage
- Must have consistent policy on dealing with failed tests
 - Issue tracking
 - How quickly does it need to be fixed?
 - Who is responsible for fixing it?
- Someone should be watching the test suite
- When refactoring or adding new features, run a regression suite before check in
 - Add new regression tests or modify existing ones for the new features
- Code review before releasing test suite is useful
 - Another person may spot issues you didn't
 - Incredibly cost-effective





Example 1: Test Development For a New Code

- Development of tests and diagnostics goes handin-hand with code development
 - Compare against simpler analytical or semi-analytical solutions
 - Build granularity into testing
 - Use scaffolding ideas to build confidence
 - Always inject errors to verify that the test is working
 - Non-trivial to devise good tests, but extremely important

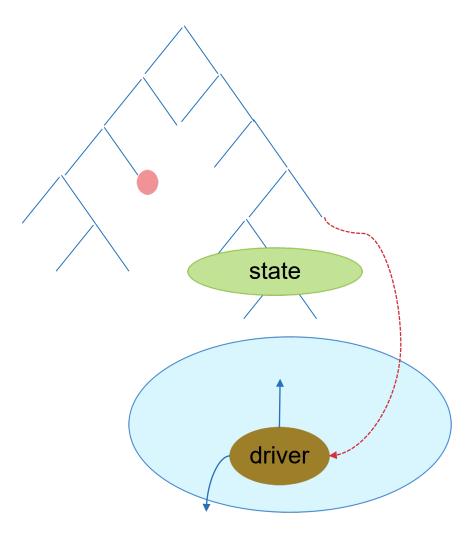




Example 2: Test Development For a Legacy Code

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



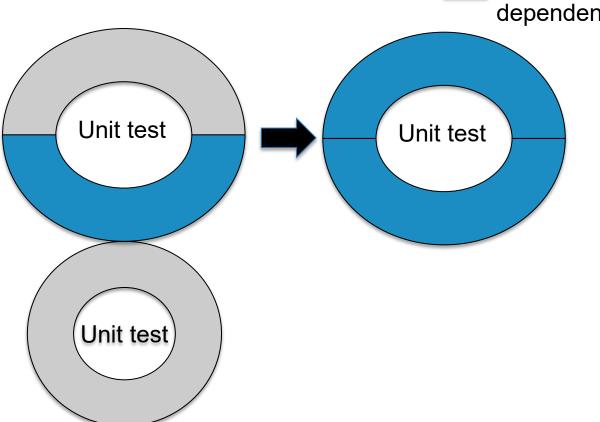




Example 3: Structuring Tests to pinpoint bugs

- Real dependency
- Mocked up dependency

- Bottom-up picture
 - Components can be exercised against known simpler applications
 - Same applies to combination of components
- Build a scaffolding of verification tests to gain confidence

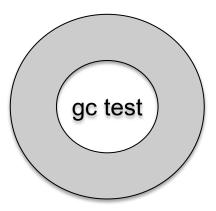


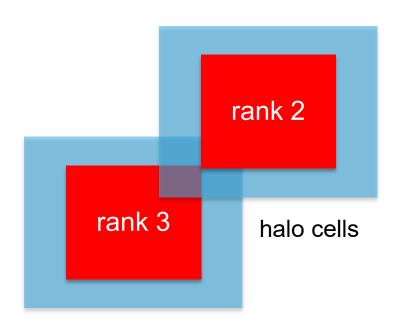




Unit test for Grid halo cell fill

- Verification of guard/ghost/halo cell fill
- Initialize field on interior cells (red)
- Apply guard cell fill
- Check for equivalence with known fill pattern



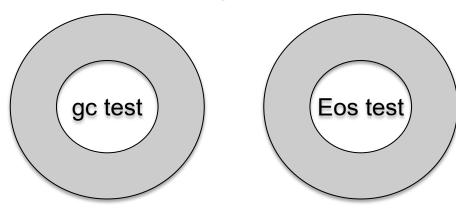


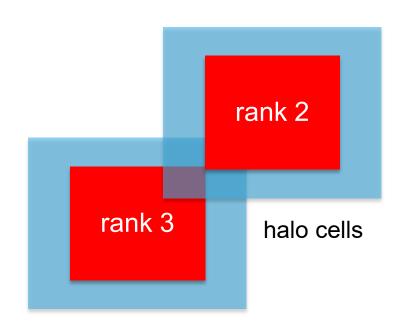




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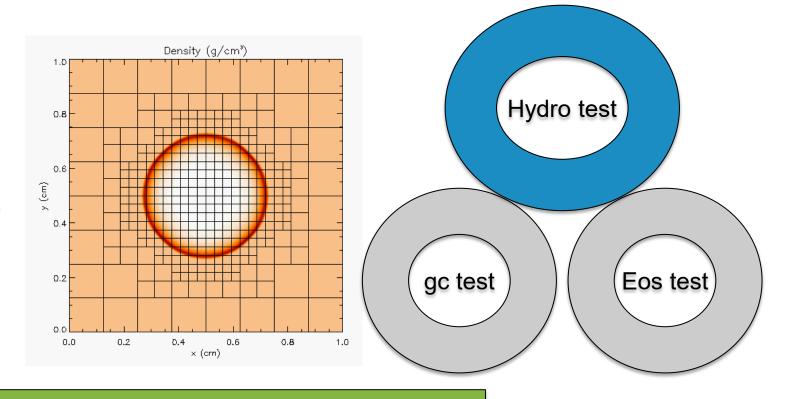
Next, build an EOS Test – is E(V,T) consistent with P(V,T)?





Unit test for Hydrodynamics

- Sedov blast wave
- High pressure at the center
- Shock moves out spherically
- Known analytical solution



Though it exercises mesh, hydro and eos, if mesh and eos are verified first, then this test verifies hydro







For AMR, correct behavior of flux conservation and regridding should also be verified.

Reason about correctness for testing Flux correction and regridding

IF Guardcell fill and EOS unit tests passed

- Run Hydro without AMR
 - If failed fault is in Hydro
- Run Hydro with AMR, but no dynamic refinement
 - If failed fault is in flux correction
- Run Hydro with AMR and dynamic refinement
 - If failed fault is in regridding





Example 4: Coverage Matrix (Interoperabilities)

First line of defense – code coverage tools

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

| | Hydro | EOS | Gravity | Burn | Particles |
|-----------|-------|-----|---------|------|-----------|
| AMR | CL | CL | | CL | CL |
| UG | SV | SV | | | SV |
| Multigrid | WD | WD | WD | WD | |
| FFT | | | PT | | |

- 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!)

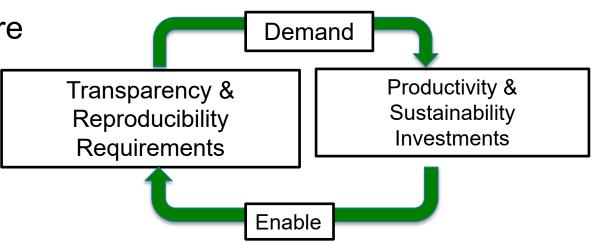




Incentives for Paying Attention to Reproducibility

Common statement: "I would love to do a better job on my software, but I need to..."

- Get this paper submitted
- Complete this project task
- Do something my employer values more



Goal: Change incentives to include valuing of better software, better science

This is a long-term goal, requiring a culture change in (computational) science which in the early stages

Additional 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.











Strategies for Improving Reproducibility

Solid versioning practices are fundamental to reproducibility

Source code, dependencies, copy through to outputs

Build in quality from the start

- Expectation for documentation and level of testing (write in-sync with code).
- Increasing expectations as code becomes more "public"
- Peer review / team productivity tracking meetings

Watch Out for Numerical Artifacts

- Integer overflows, floating point underflows, numerical algorithm stability
- Plan Ahead for Experimental Campaign Progression
 - How do scaling tests & intermediate outputs relate to code features?
 - What in-run correctness checks exist?
 - What if a patch needs to be applied during a campaign?





Testing Strategies for Improving Reproducibility

- Testing, testing, and more testing!
- Add "regression tests"
 - If you fix a bug, add a test to make sure that bug doesn't creep back in
- Add more tests
 - Be creative
 - Think about common cases, then corner cases
 - Think about misuse (unintentional or intentional)
 - Think about synthetic tests with synthetic data
 - Think about low-cost tests that can be "always on" (even if they're not so stringent)
 - Can you detect silent data corruption?
- Physics / Math Based Strategies
 - Conserved quantities, symmetries, synthetic operators
- Design by Contract
 - Input / Output specifications, program invariants

- Test your third-party dependencies
 - Are your tools doing what you think they're doing?
 - What if you're using a new version?
 - How do you decide if it is okay to upgrade to a new version?
- Test your tests!
 - Make sure tests fail when they're supposed to!
- Thoroughly verify the code
 - Does the code do what you intended it to do?
 - On all relevant platforms (compilers, hardware, etc.)
- Test regularly
 - To identify and document where changes to the underlying platform change code behavior/results





Takeaways

- Context: understand testing needs and costs
- Devise tests to enable quick pinpointing of errors through reasoning about their behavior
- test at various granularities bottom-up (UNIT/verification) through top-down (integration/validation)
- Tests at various complexities CI vs. regression
- Maintain a holistic validation strategy: think globally, act locally
-Questions?



