EXASCALE COMPUTING PROJECT

Motivation and Overview

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Developing a Testing and Continuous Integration Strategy for your Team tutorial @ ECP Annual Meeting, April 2021

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License and Citation

- **The requested citation the overall tutorial is: David E. Bernholdt, Patricia A. Grubel, and James M. Willenbring, Developing a Testing and Continuous Integration Strategy for your Team tutorial, in Exascale Computing Project Annual Meeting, online, 2021. DOI: 10.6084/m9.figshare.14376956**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial…

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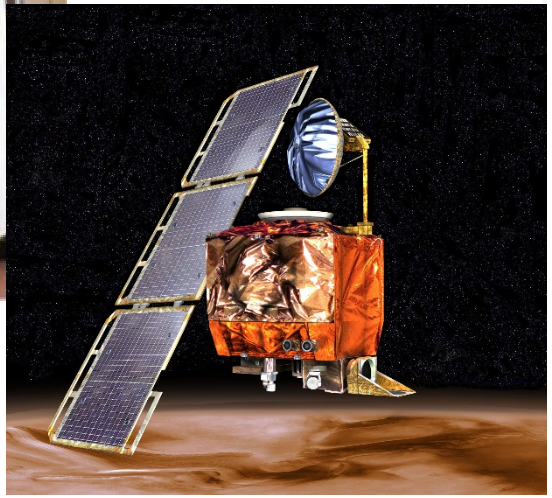
Science through computing is,
at best,
as credible as the software that produces it!

High-Consequence Software-Related Scientific Failures

Therac-25 (1985-1987)

- Computer-controlled radiation therapy system
- **Poor software design, development and testing practices** allowed flaws that let to at least six cases of substantial radiation overdoses, three fatal



Mars Climate Orbiter (1999)

- Incorrect trajectory adjustment caused loss of the orbiter as it was supposed to enter Martian orbit
- Discrepancy in the units used in two different software components
- One component **didn't follow specifications**
- **Inadequate testing** at the interface
- Concerns raised earlier in the mission were ignored because they **weren't properly documented**

Just two of many examples

IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Challenges Developing Scientific Applications Today

Technical

- All parts of the model and software system can be under research
- Requirements change throughout the lifecycle as knowledge grows
- Verification complicated by floating point representation
- Real world is messy, so is the software
- Increasing architectural diversity

Sociological

- Competing priorities and incentives
  - Sponsors often care more about scientific publications than software per se
- Limited resources
- Need for interdisciplinary interactions
  - Many different kinds of expertise to be successful

Best Practices for Scientific Software Development

Baseline

- Invest in extensible code design
- Use version control and automated testing
- **Institute a rigorous verification and validation regime**
- **Define and enforce coding and testing standards**
- Clear and well-defined policies for
  - Auditing and maintenance
  - Distribution and contribution
  - Documentation

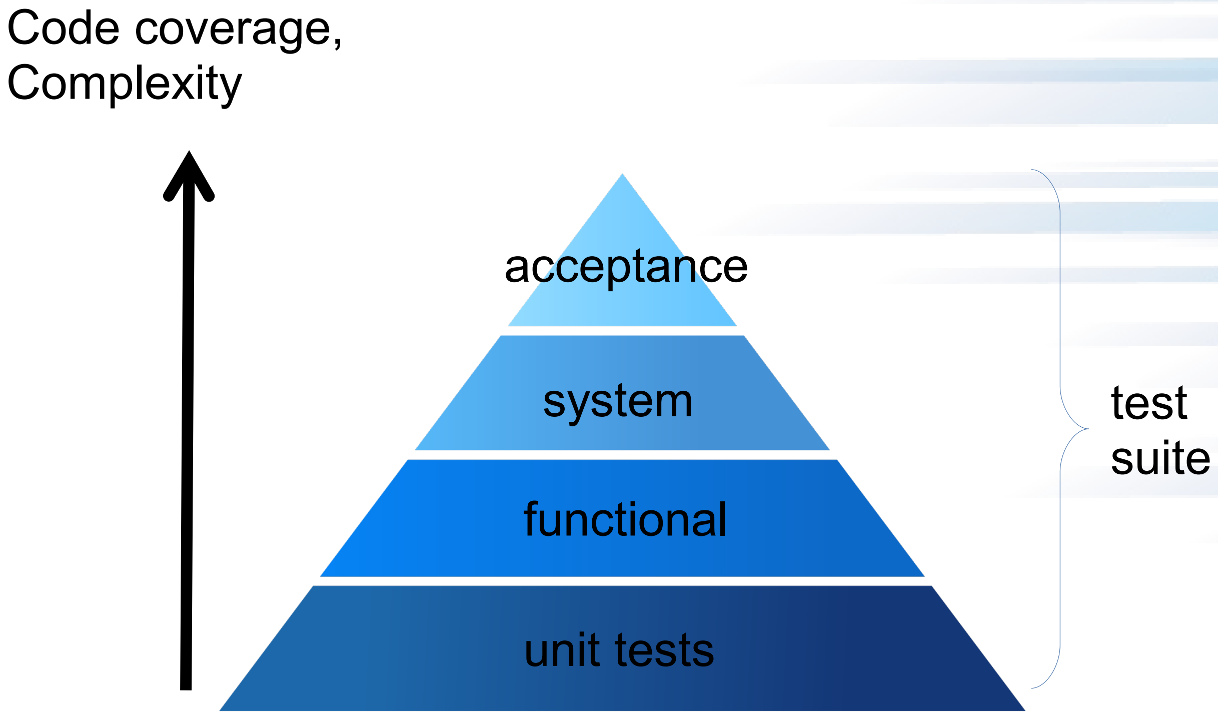
Desirable

- Provenance and reproducibility
- Lifecycle management
- Open development and frequent releases

This tutorial will focus primarily on scientific software as distinct from more generic software engineering best practices

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



(Some) 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
- Implementing tests
  - Introducing testing into legacy code (legacy == untested)
  - Understanding and progressively improving code coverage
- Automating tests
  - Just get started – easy to get lost in all of the options
  - You have to *have* tests to be able to automate them!
- What to run where, and when?
  - Consider what resources are required, and what the tests are used for

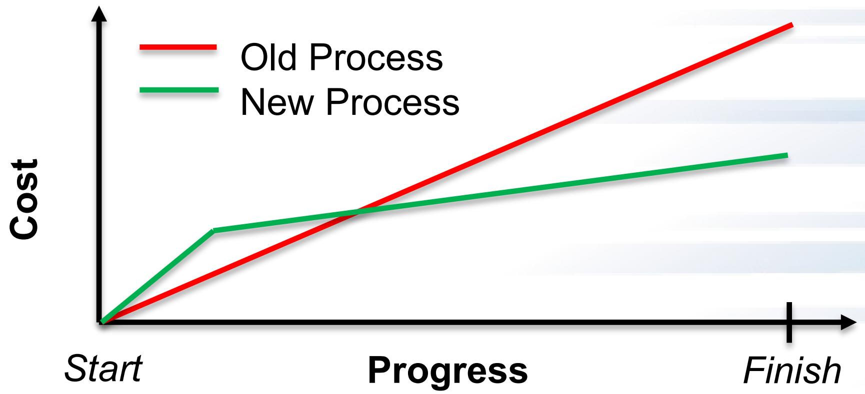
Testing is a very large subject. This is what we have time for today

Continual, Incremental Software Process Improvement

Target: your project should include "just enough" software engineering so that you can meet your short-term and longer-term scientific goals effectively

1. Identify your team's "pain points" in your software development processes
2. Set a goal for something to improve
   – Target processes and behaviors, not just tasks
   – Pick something that you can address in a few months that will give you a noticeable benefit
3. Agree on a plan to address it, identify markers of progress and what is "done"
   – Write them down
4. Work your plan, track your progress
5. When you are done, celebrate…

…then pick a new pain point to address



The new process costs something to implement, but it pays off over time

Productivity and Sustainability Improvement Planning
https://bssw.io/psip

Agenda

Time (EDT)	Module	Topic	Speaker
2:30-2:35pm	00	Introduction	David E. Bernholdt, ORNL
2:35pm-2:40pm	01	Motivation and Overview	Patricia A. Grubel, LANL
2:40pm-3:00pm	02	Software Testing 1	Patricia A. Grubel, LANL
3:00pm-3:25pm	03	Software Testing 2	David E. Bernholdt, ORNL
3:25pm-3:55pm	04	Continuous Integration	James M. Willenbring, SNL
3:55pm-4:00pm	05	Summary	James M. Willenbring, SNL