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Better Scientific Software tutorial @ ISC 2022

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- The requested citation the overall tutorial is: Anshu Dubey and Gregory R. Watson, Better Scientific Software Tutorial, in ISC High Performance, 2022, Hamburg Germany. DOI: 10.6084/m9.figshare.19781752
- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software tutorial, ISC, 2022 ...

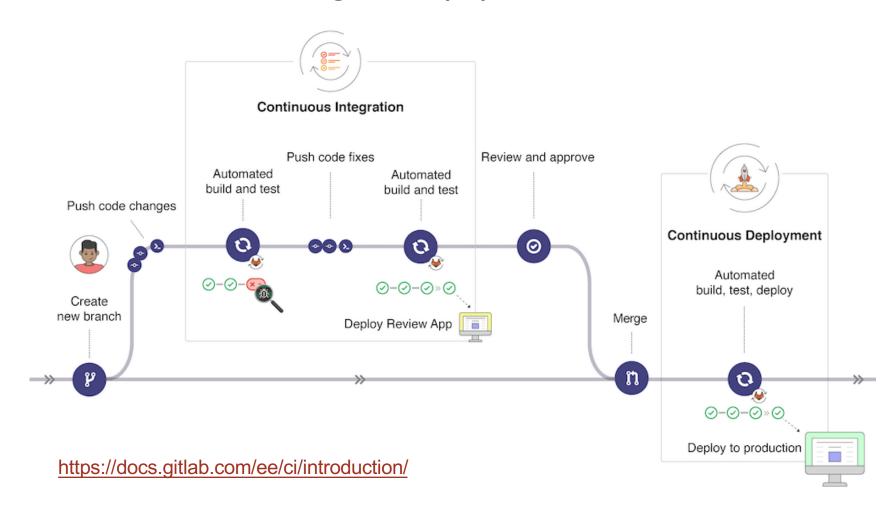
#### **Acknowledgements**

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## What is Continuous Integration (CI)



### **CI Components**

- Testing
  - Focused, critical functionality (infrastructure), fast, independent, orthogonal, complete, ...
  - Existing test suites often require re-design/refactoring for CI
- Integration
  - Changes across key branches merged & tested to ensure the "whole" still works
    - Integration can take place at multiple levels
      - Individual project
      - Spack
      - E4S
  - Develop, develop, develop, merge, merge, merge, test, test, test...NO!
  - Develop, test, merge, develop, test, merge, develop, test, merge...YES!
- Continuous
  - Changes tested every commit and/or pull-request (like auto-correct)
- Cl generally implies a lot of <u>automation</u>





### Test Driven Development vs. Automated Testing vs. Cl

- Test Driven Development: A development methodology where functional test are written before the code
  - Works well with CI as tests are written and committed and are automatically run (failing)
  - Code that implements the functionality being tested retriggers the tests automatically
- Automated Testing: Software that automatically performs tests on a regular basis and reliably detects and reports anomalous behaviors/outcomes.
  - Examples: Auto-test, CTest/CDash, nightly testing, etc.
  - May live "next to" your development workflow
  - Potential issues: change attribution, timeliness of results, multiple branches of development
- Continuous Integration (CI): automated testing performed at high frequency and fine granularity
  - Aimed at preventing code changes from breaking key branches of development (e.g. main)
  - Lives "within" your development workflow
  - Potential issues: extreme automation, test granularity, coverage, 3<sup>rd</sup>-party services/resources



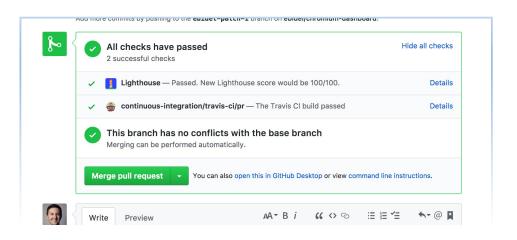


### Examples...

# **Automated Nightly Testing Dashboard Lives "next to" your development work**

#### Results of Vislt Regression Test (pascal,trunk,serial) Test suite run started at 2020:07:09:22:49:46. (Click on table header to sort) Index Category **Test File** 243 rendering 5.0 spray.py 273 simulation 38.0 24 databases 32 databases 11.0 14.0 66 databases 50.0 67 databases silo altdriver.py 75 databases xdmf.py 14.0 109 hybrid 11.0 nerge\_tree.py 136 meshtype 7.0 256 rendering 275 simulation 17.0 281 simulation life.py 8.0 296 simulation 0 databases ANALYZE.py 10.0 databases ANSYS.py 9.0 databases CGNS.py 11.0 databases 7.0 databases 9.0 databases databases FITS.py 8.0 databases 7.0 databases 20.0 GDAL.py

# CI Testing Lives embedded in your development work







### What can make CI difficult

#### **Common situations**

- Just getting started
  - Many technologies/choices; often in the "cloud"
  - Solution: start small, simple, build up
- Developing suitable tests
  - Many project's existing tests not suitable for CI
  - CI testing is a balance of thoroughness and responsiveness
  - Solution: Simplify/refactor and/or sub-setting test suite
- Ensuring sufficient coverage
  - Some changes to code never get tested CI can provide a false sense of security
  - Solution: tools to measure it, enforce always increasing

#### **Advanced situations**

- Defining failure for many configurations / inconsistent failures
  - Bit-for-bit (exact) match vs. fuzzy match
  - Solution: absolute/relative tolerances → AI/ML
- Numerous 3<sup>rd</sup> party libraries (TPLs)
  - Compiling takes too long
  - Solution: cache pre-built TPLs, containers
- Performance testing
  - Avoid time-, space-, scaling-performance degradation
  - Solution: Performance instrumentation and scheduled testing





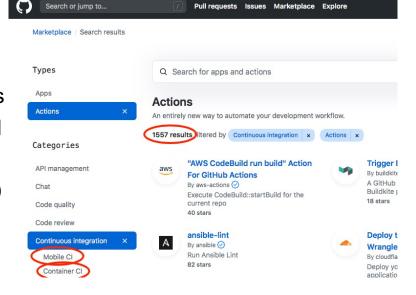
### CI Resources (Where do jobs run?)

#### Free Resources

- GitHub, BitBucket, GitLab, etc. provide shared runners
- AWS, Azure Pipelines have free tiers that can be used
- All launch a VM (Linux variants, Windows and OSX)
  - Constrained in time/size, hardware (e.g. GPU type/count)
  - Not a complete solution for many HPC/scientific codes, but a useful starting point.

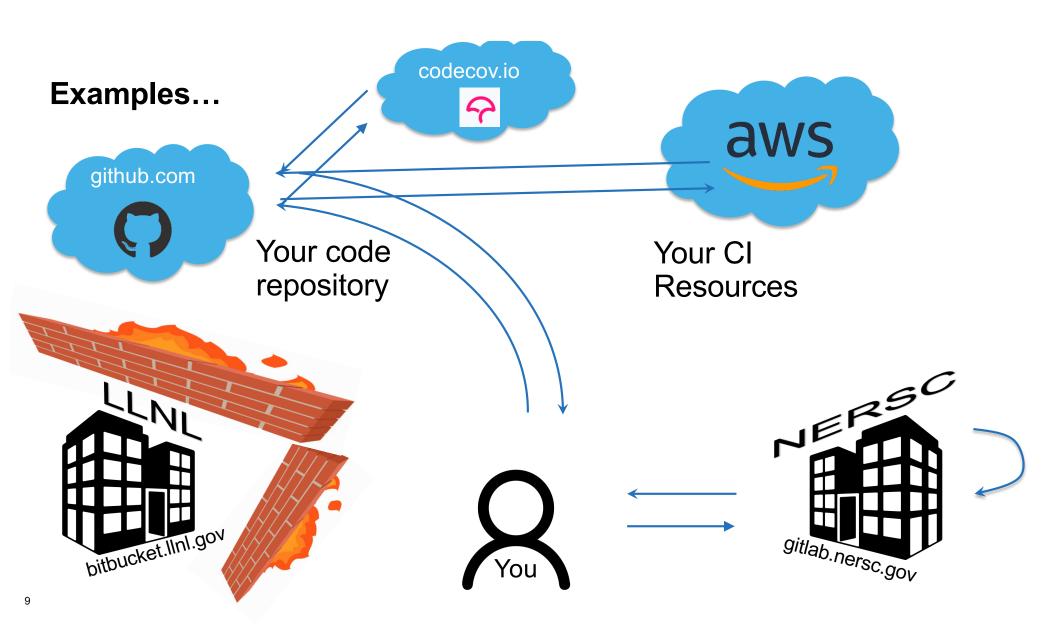
#### Site-local Resources

- Group, department, institution, computing facility
- Examples: CADES @ ORNL, Bamboo @ LLNL, Jenkins @ ANL, Travis+CDash @ NERSC
- ECP Program: GitLab-CI @ ANL, LANL, LLNL, NERSC, ORNL, SNL
- Create your own by setting up resources/services









### **Getting started with CI**

- What configuration is most important?
  - Examples: gcc, icc, xlc? MPI-2 or MPI-3? Python 2, 3 or 2 & 3?
- What functionality is most important?
  - Examples: vanilla numerical kernels? OpenMP kernels? GPU kernels? All of these?
- Good candidates...
  - A "hello world" example for your project
  - At a minimum, even just building the code can be a place to start!
  - Once you've got the basics working, its easy to build up from there

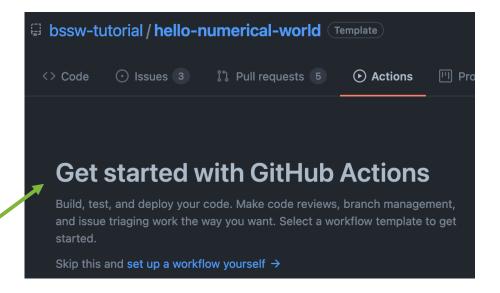


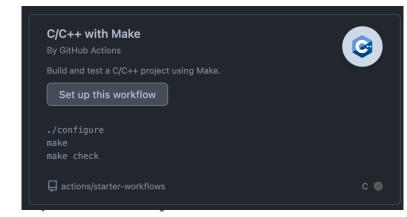


## **Getting started with CI:**

#### **Setting up CI**

Service	Interface	
GitHub Actions	Repo YAML file	.github/workflows/ <test_name>.yml</test_name>
GitLab	Web page configurator + repo YAML file [& repo scripts]	/.gitlab-ci.yml in root of repo
Bamboo	Web page configurator + repo scripts	
Travis	repo YAML file [& repo scripts]	/.travis.yml in root of repo





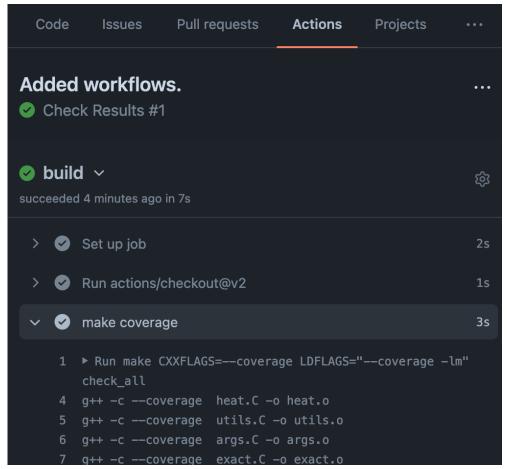
### **Getting started with GitHub Actions:**

```
19 lines (15 sloc)
                     359 Bytes
      name: Check Results
      on:
        push:
          branches: [ main ]
        pull_request:
          branches: [ main ]
      jobs:
        build:
          runs-on: ubuntu-latest
          steps:
         - uses: actions/checkout@v2
         - name: make coverage
            run: make CXXFLAGS=--coverage LDFLAGS="--coverage -lm" check_all
          - name: upload coverage
            run: bash <(curl -s https://codecov.io/bash)</pre>
```

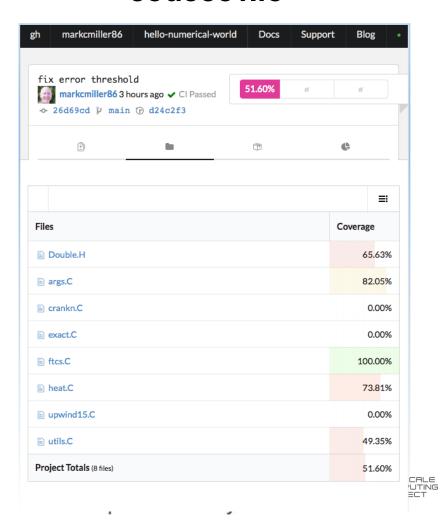




### github.com



### codecov.io



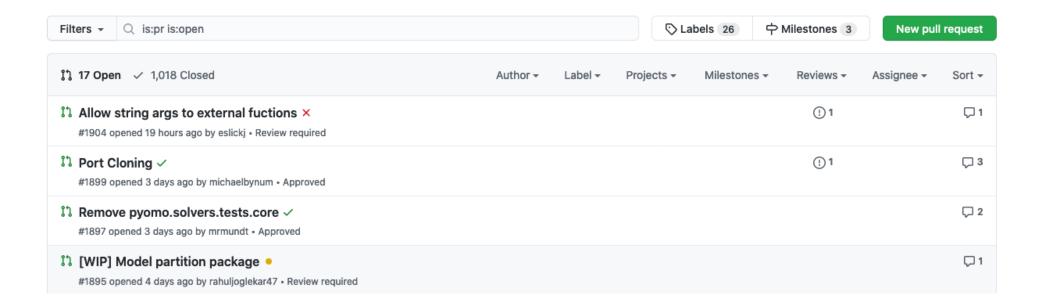
#### GitHub Actions – results of workflow test runs

#### Workflows GitHub CI Showing runs from all workflows named GitHub CI All workflows $\times$ Q event:push workflow:"GitHub CI" ପ୍ର (TEST) Pyomo Windows Tests ... 및 (WIP) Pyomo Windows Test (P... 461 workflow run results Event -Status -Branch -Actor ≠ € (WIP) Pyomo Windows Test (P... Merge pull request #1902 from jsiirola/fix-unittest-rc 20 hours ago main 인 (WIP) Pyomo Windows Tests (... GitHub CI #121: Commit 901b487 pushed by blnicho (7) 1h 3m 55s 인 (WIP) Windows Pip Cmd Pyom... Merge pull request #1901 from mrmundt/remove-six 2 days ago main GitHub CI #117: Commit a101b6d pushed by mrmundt ( 1h 3m 12s € GitHub Branch CI C GitHub CI Merge pull request #1896 from jsiirola/abstract-disa... 2 days ago main GitHub CI #112: Commit 1f9dd19 pushed by jsiirola (i) 1h 5m 39s Pyomo Release Distribution Cr... Merge pull request #1898 from mrmundt/py-unittest Python package 3 days ago main GitHub CI #109: Commit 1beb848 pushed by michaelbynum 1h 3m 33s C Ubuntu Pyomo Single Python ... Merge pull request #1893 from jsiirola/config-enum 🗎 3 days ago 인 Ubuntu Pyomo Workflow (Slim,... ... main GitHub CI #105: Commit 9aa1186 pushed by jsiirola (3) 1h 11m 3s





### **GitHub Pull Request Status Indicators**







### **Summary**

- The purpose of CI is to identify problems early
  - Prevent code that would "break the build" or adversely impact other developers being introduced
  - Need to provide sufficient confidence, but run quickly balance varies by project
- CI should complement (not replace) more extensive automated testing
  - Use scheduled testing for more and more detailed tests, more configurations and platforms, performance testing, etc.
- CI for TDD is a natural fit
  - Writing tests before the code works well with CI
- Many options for where to execute CI tests
  - Free services are a good (easy) place to start
  - But may not be sufficient in the long run (especially large HPC/scientific codes)
- · Start simple to get automation working, then build out what you need
  - Focus initially on key software configurations and aspects of the code to be tested
  - Make sure your testing expands to cover new code, use TDD



