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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...

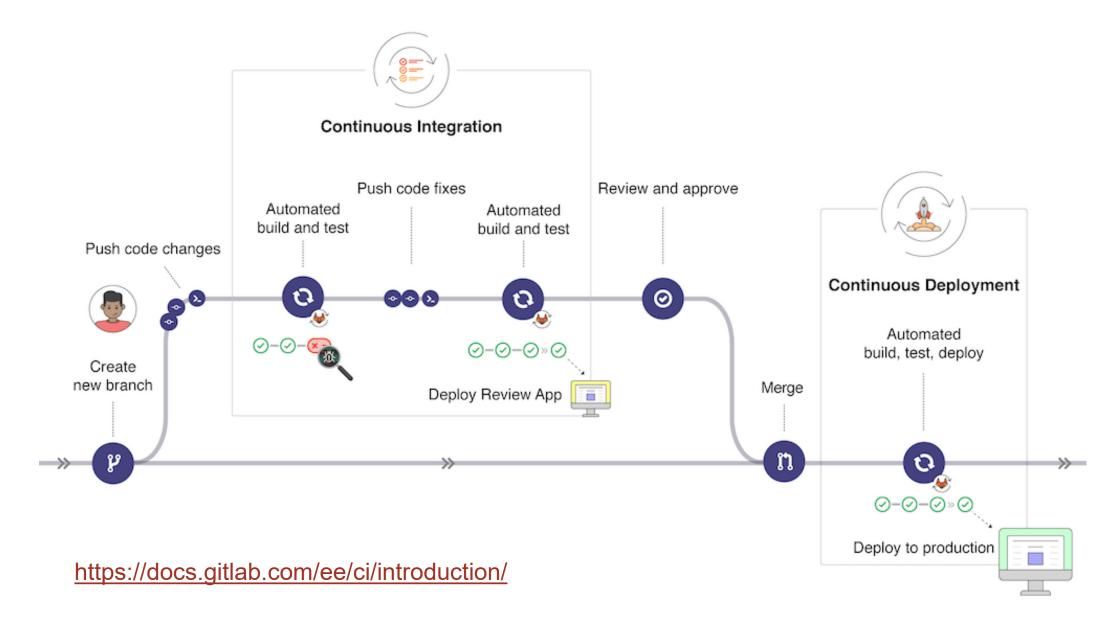
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What is Continuous Integration (CI)



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...NO!
- Develop, test, merge, develop, test, merge, develop, test, merge...YES!

Continuous

- Changes tested every commit and/or pull-request (like auto-correct)
- CI generally implies a lot of <u>automation</u>





Test/Doc Driven Development vs. Automated Testing vs. Cl

- **Test/Documentation Driven Development:** A development methodology where documentation and/or functional tests are written before the code
 - These are strategies for organizing the development cycle to manage complexity
 - For TDD, initial CI will show failing tests, and code commits will trigger re-testing
 - For both, developers must simultaneously update tests/documentation with code
- 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, 3rd-party services/resources





Examples...

- Flash test
- Buildtest

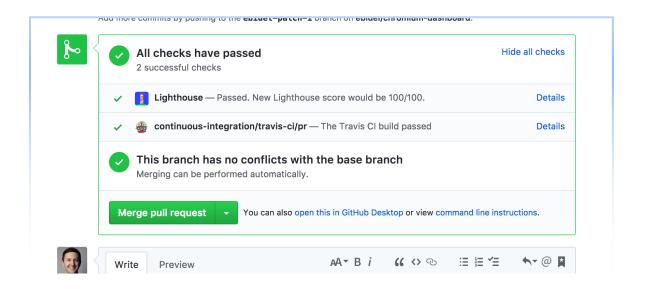
- Nightly
- Fluid-numerics



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

Results of Visit 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** Runtime (sec) 5.0 rendering ospray.py **Jnacceptable** simulation atch.py 11.0 databases hgcar.py ucceeded With Sk databases exodus.py 14.0 databases lo.py ilo_altdriver.py databases databases dmf.py hybrid nerge_tree.py 11.0 meshtype mptydomains.py 256 renderina simulation curve.py simulation fe.py simulation erocopy.py ucceeded With Skip databases NALYZE.py 10.0 ıcceeded NSYS.py 9.0 databases 11.0 CGNS.py databases cceeded 6.0 databases Cale.py ucceeded databases Chombo.py 7.0 ucceeded 9.0 databases nSight.py cceeded 8.0 databases ITS.pv cceeded 7.0 luent.pv ucceeded 20.0 databases

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 3rd 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





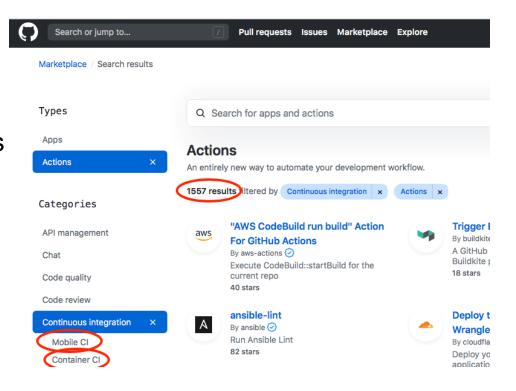
CI Resources (Where do jobs run?)

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.

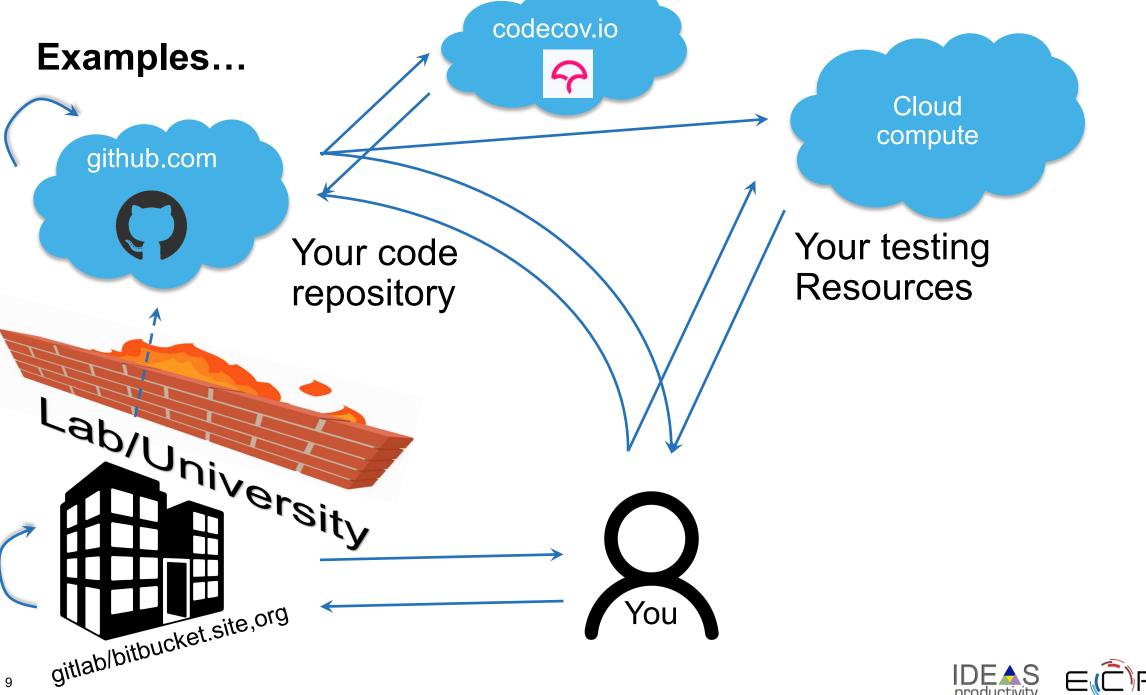
Site-local Resources

- 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

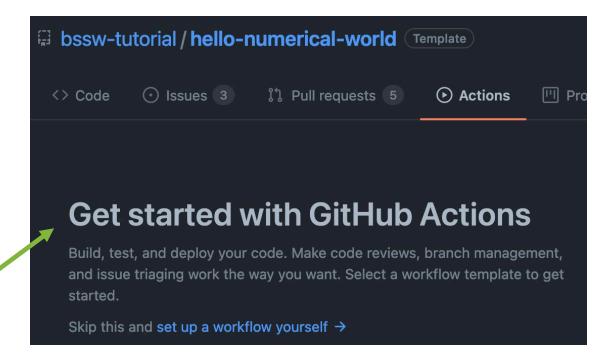


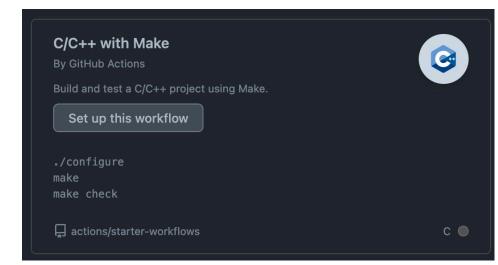


Getting started with CI:

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





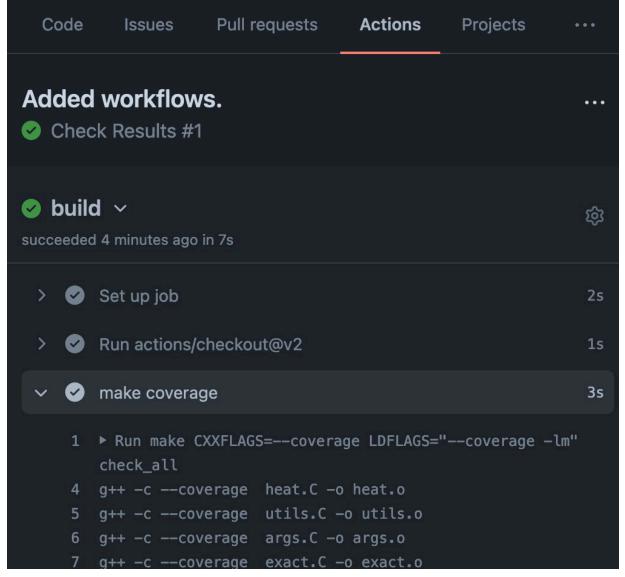
Getting started with GitHub Actions:

```
19 lines (15 sloc) | 359 Bytes
      name: Check Results
      on:
        push:
          branches: [ main ]
        pull_request:
          branches: [ main ]
      jobs:
        build:
 12
          runs-on: ubuntu-latest
 13
          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>
```

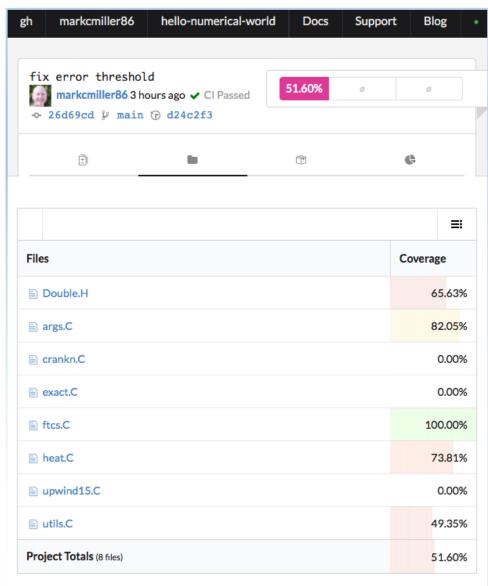




github.com



codecov.io



GitHub Actions – results of workflow test runs

Workflows

All workflows

ੳ (TEST) Pyomo Windows Tests ...

인 (WIP) Pyomo Windows Test (P...

€ (WIP) Pyomo Windows Test (P...

₽ (WIP) Pyomo Windows Tests (...

인 (WIP) Windows Pip Cmd Pyom...

Cn GitHub Branch CI

C GitHub CI

₽ Pyomo Release Distribution Cr...

₽ Python package

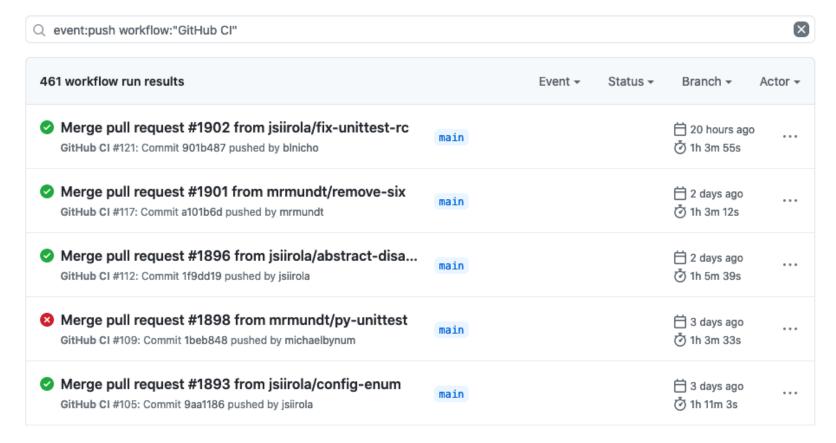
€ Ubuntu Pyomo Single Python ...

Co Ubuntu Pyomo Workflow (Slim,...

n

GitHub CI

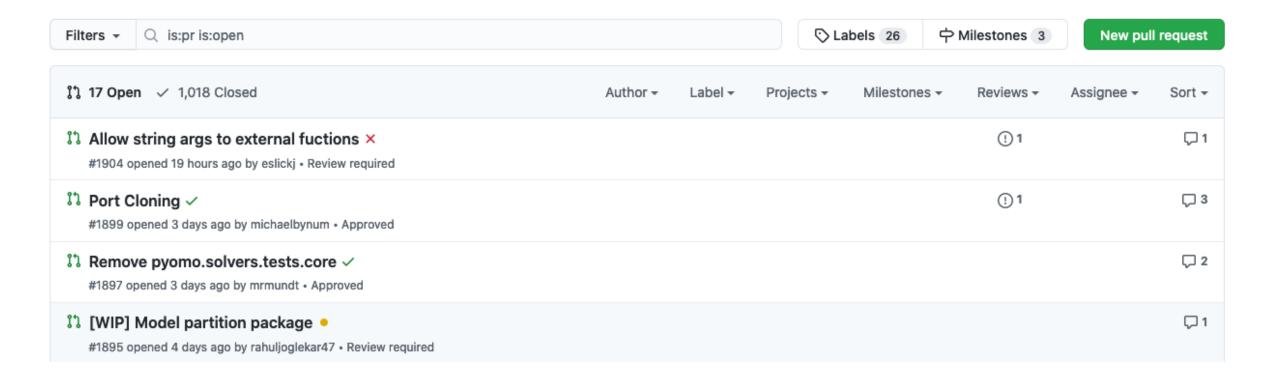
Showing runs from all workflows named GitHub CI







GitHub Pull Request Status Indicators







GitHub Actions – Key Elements of Defining Tests

```
name: GitHub CI
                                      Name
                                      Trigger
    on:
      push:
       branches:
 5
         main
 6
      pull_request:
       branches:
         - main
 9
                                      Manual trigger with git-ref input
      workflow_dispatch:
10
11
        inputs:
         git-ref:
12
           description: Git Hash (Optional)
13
14
           required: false
15
```





GitHub Actions – Key Elements of Defining Tests

```
jobs:
35
36
       build:
        name: ${{ matrix.TARGET }}/${{ matrix.python }}${{ matrix.other }}
37
        runs-on: ${{ matrix.os }}
38
        timeout-minutes: 90
39
40
        strategy:
           fail-fast: false
41
42
           matrix:
             os: [ubuntu-18.04, macos-latest, windows-latest]
43
             python: [3.6, 3.7, 3.8, 3.9, pypy3]
44
45
             other: [""]
46
             category: ["nightly"]
             # Ubuntu-18.04 should be replaced with ubuntu-latest once PyNumero
47
             # build error is resolved:
48
             # https://github.com/Pyomo/pyomo/issues/1710
49
50
51
             include:
52
             - os: ubuntu-18.04
               TARGET: linux
53
54
               PYENV: pip
55
             - os: macos-latest
56
57
               TARGET: osx
               PYENV: pip
58
```



Job setup



GitHub Actions – Key Elements of Defining Tests

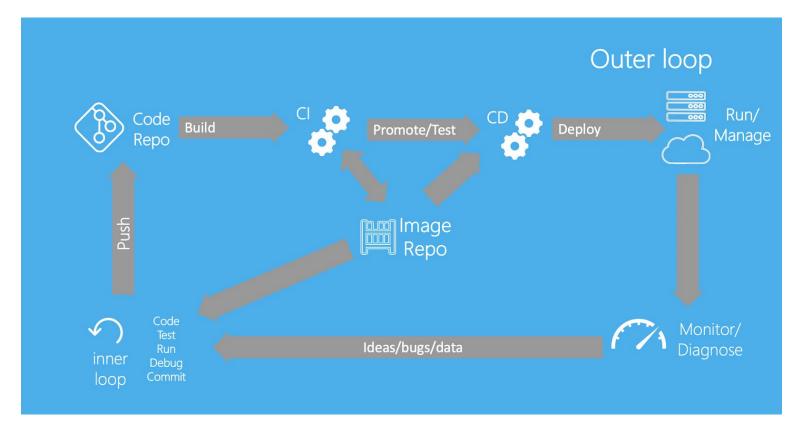
```
111
         steps:
         - name: Checkout Pyomo source
112
           uses: actions/checkout@v2
113
114
         - name: Configure job parameters
115
116
           run: |
117
             JOB="${{matrix.TARGET}}/${{matrix.python}}${{matrix.other}}"
             echo "GHA_JOBNAME=$JOB" | sed 's|/|_|g' >> $GITHUB_ENV
118
             if test -z "${{matrix.other}}"; then
119
                 echo "GHA JOBGROUP=${{matrix.TARGET}}" >> $GITHUB ENV
120
121
             else
122
                 echo "GHA_JOBGROUP=other" >> $GITHUB_ENV
123
             fi
             # Note: pandas 1.0.3 causes gams 29.1.0 import to fail in python 3.8
124
             PYTHON_PACKAGES="${PYTHON_REQUIRED_PKGS}"
125
126
             if test -z "${{matrix.slim}}"; then
127
                 PYTHON_PACKAGES="$PYTHON_PACKAGES ${PYTHON_BASE_PKGS}"
             fi
128
             if [[ ${{matrix.python}} != pypy* && ! "${{matrix.slim}}" ]]; then
129
                 # NumPy and derivatives either don't build under pypy, or if
130
                 # they do, the builds take forever.
131
                 PYTHON PACKAGES="$PYTHON PACKAGES ${PYTHON NUMPY PKGS}"
132
133
             fi
             PYTHON_PACKAGES="$PYTHON_PACKAGES ${{matrix.PACKAGES}}"
134
             echo "PYTHON_PACKAGES=$PYTHON_PACKAGES" \
135
                 | tr '\n' ' | sed 's/ \+/ /g' >> $GITHUB ENV
136
```



Job steps



Going Further with CI



- Mirror inner and outer test loops
 - containers help here (apt-get deps)
 - see, e.g. E4S minimal spack
- High-level build systems
 - cmake
 - spack (spack.readthedocs.io)
- Enable caching
 - uses: actions/cache@v2 (github)
 - cache: (gitlab)
- Automate Releases

https://docs.docker.com/ci-cd/best-practices/





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 alongside 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



