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Better Scientific Software tutorial @ SC21

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- The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku K. Gupta, and Gregory R. Watson, Better Scientific Software tutorial, in the International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC21), St. Louis, MO, USA and online, 2021. DOI: 10.6084/m9.figshare.16556628
- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software tutorial...

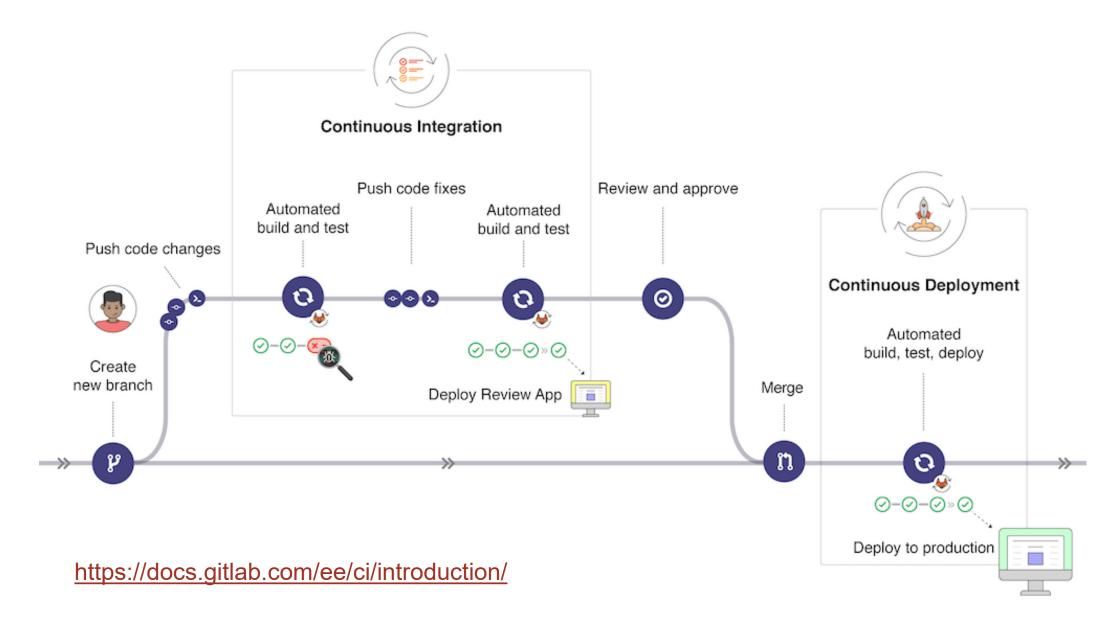
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## What is Continuous Integration (CI)



### **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, merge, test, develop, merge, test, develop, merge, test...YES!

#### Continuous

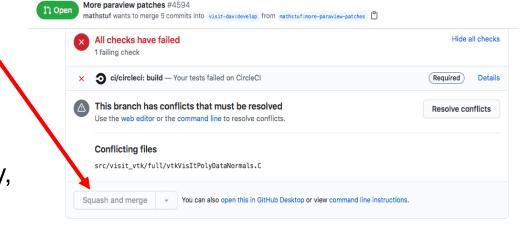
- Changes tested every commit and/or pull-request (like auto-correct)
- CI generally implies a lot of <u>automation</u>





## **Automated Testing vs. CI Testing**

- Automated Testing: Software that automatically performs tests and reliably detects and reports anomalous behaviors/outcomes.
  - Examples: Auto-test, CTest/CDash, nightly testing, `make check'
  - 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)
  - Example: Disabled/enabled "Merge Pull Request" button on GitHub
    - Can also be run post merge
  - Lives "within" your development workflow
  - Potential issues: extreme automation, test granularity, coverage, 3<sup>rd</sup>-party services/resources

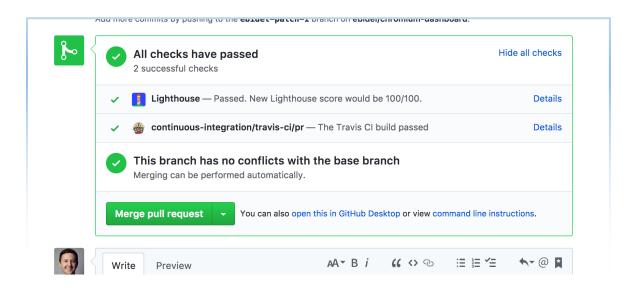


### Examples...

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

#### Results of 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 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: Perf. instrumentation and scheduled testing





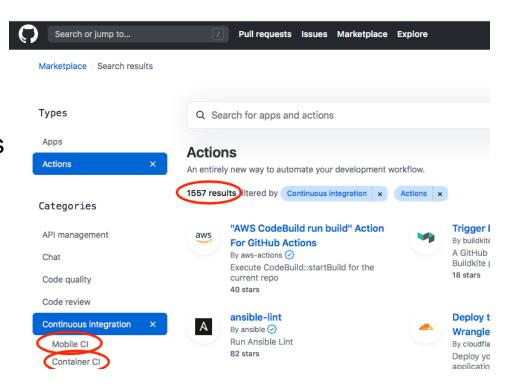
### CI Resources (Where do jobs run?)

#### 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.

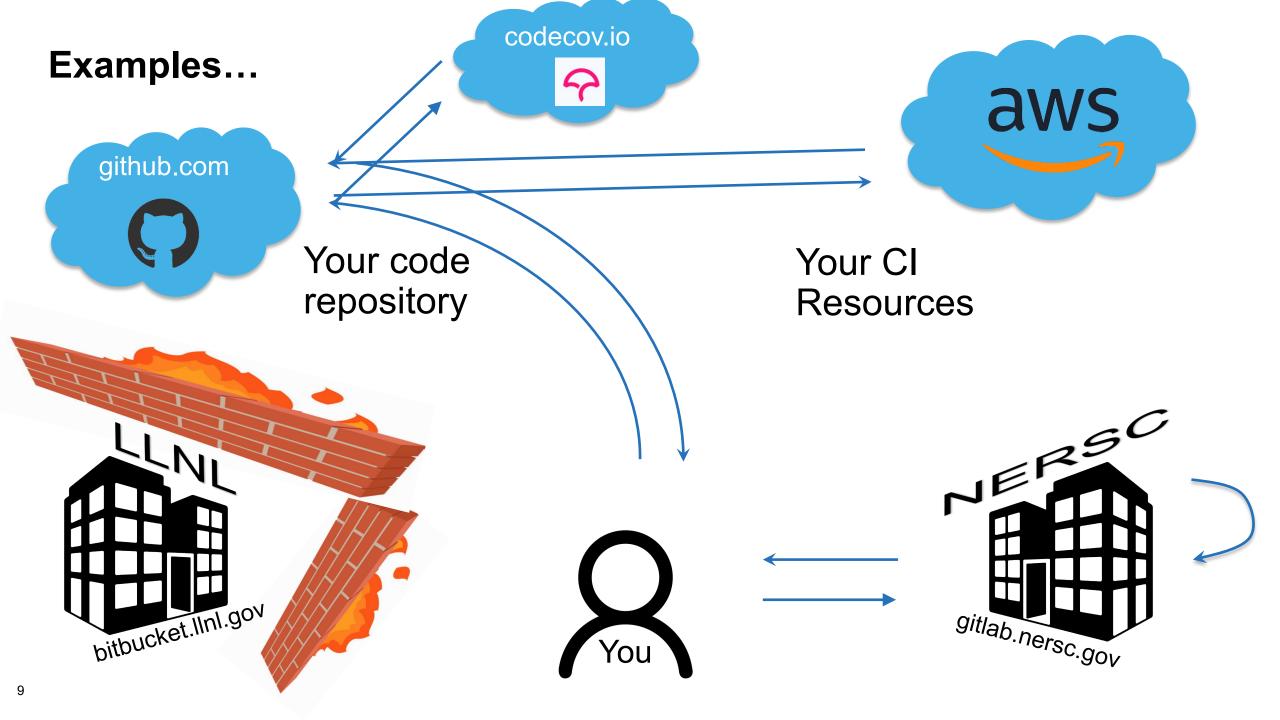
#### Site-local Resources

- Group, department, institution, computing facility
- Examples: Bamboo @ LLNL, Jenkins @ ANL, Travis+CDash @ NERSC, etc.
- 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

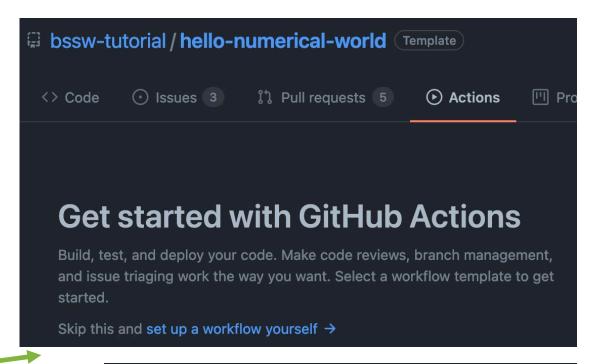


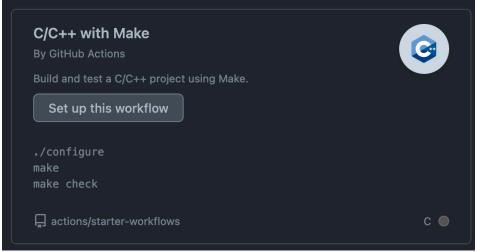


## **Getting started with CI:**

#### **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









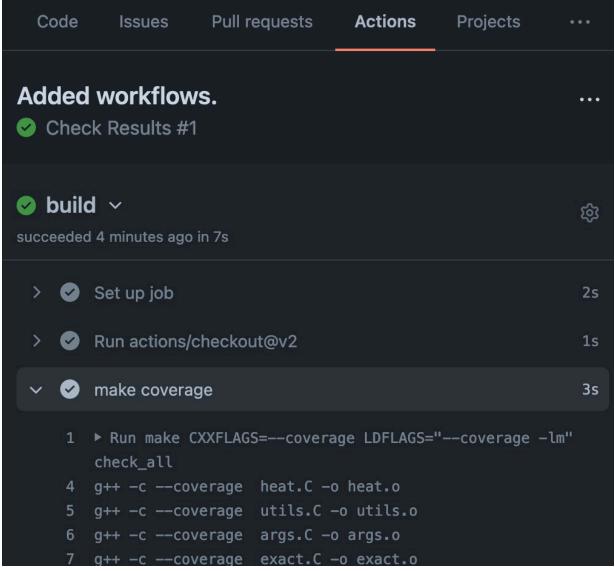
### **Getting started with Github Actions:**

```
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>
```

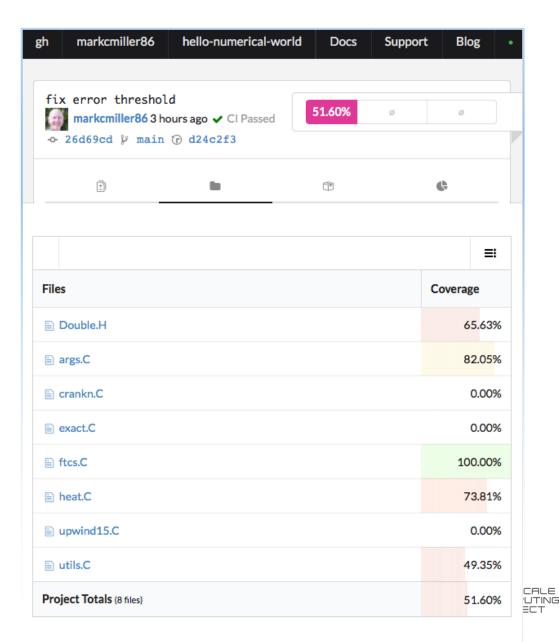




## github.com



#### 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...

인 (WIP) Pyomo Windows Tests (...

인 (WIP) Windows Pip Cmd Pyom...

C GitHub Branch CI

C GitHub CI

Co Pyomo Release Distribution Cr...

₽ Python package

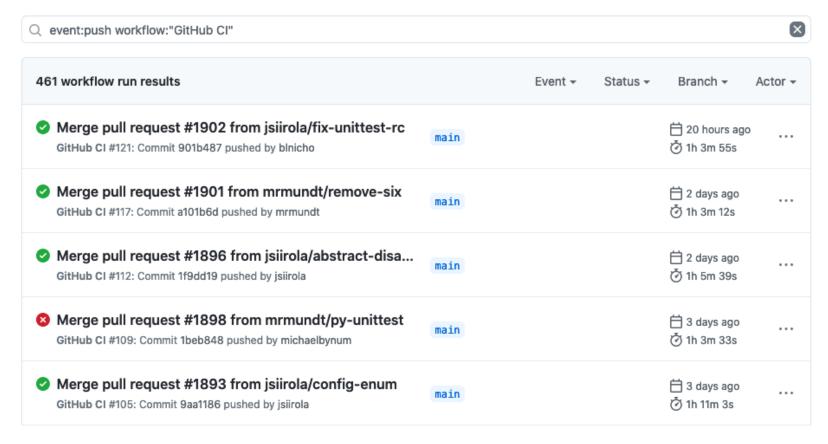
€ Ubuntu Pyomo Single Python ...

Co Ubuntu Pyomo Workflow (Slim,...

n ...... ... ... ...

#### GitHub CI

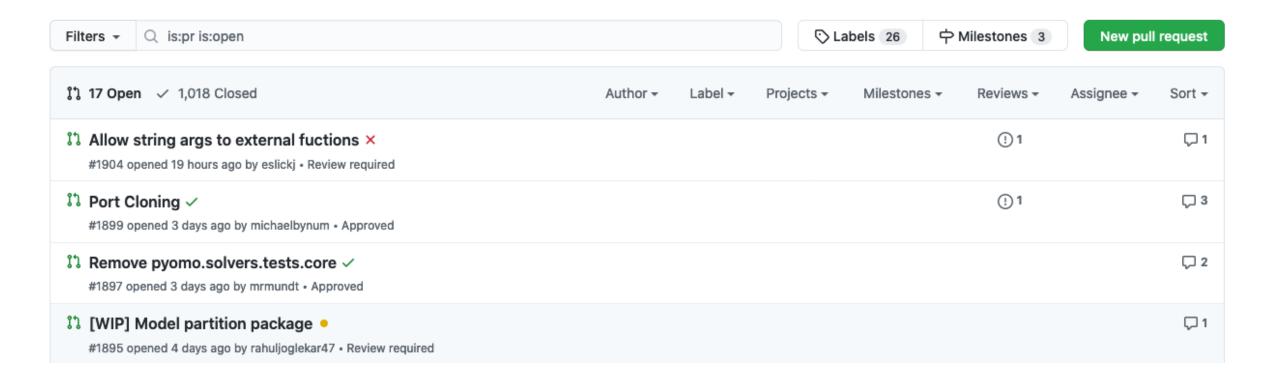
Showing runs from all workflows named GitHub CI







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







## **GitHub Actions – Key Elements of Defining Tests**

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





### **GitHub Actions – Key Elements of Defining Tests**

```
jobs:
35
       build:
36
         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
             other: [""]
45
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
             include:
51
             - os: ubuntu-18.04
               TARGET: linux
53
               PYENV: pip
54
55
             - os: macos-latest
56
57
               TARGET: osx
58
               PYENV: pip
```







### **GitHub Actions – Key Elements of Defining Tests**

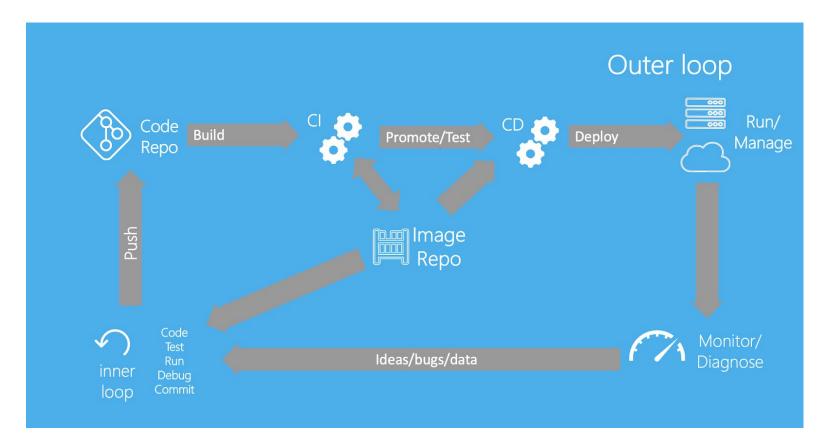
```
111
         steps:
         - name: Checkout Pyomo source
112
113
           uses: actions/checkout@v2
114
         - name: Configure job parameters
115
116
           run: |
117
             JOB="${{matrix.TARGET}}/${{matrix.python}}${{matrix.other}}"
             echo "GHA_JOBNAME=$JOB" | sed '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**



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

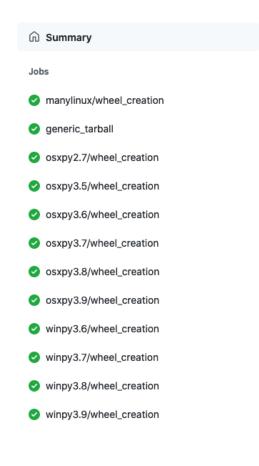
- Mirror inner and outer test loops
- High-level build systems
  - cmake
  - spack (spack.readthedocs.io)
  - containers? (e.g. in e4s-project)
- Enable caching
  - uses: actions/cache@v2 (github)
  - cache: (gitlab)
- Automate Releases

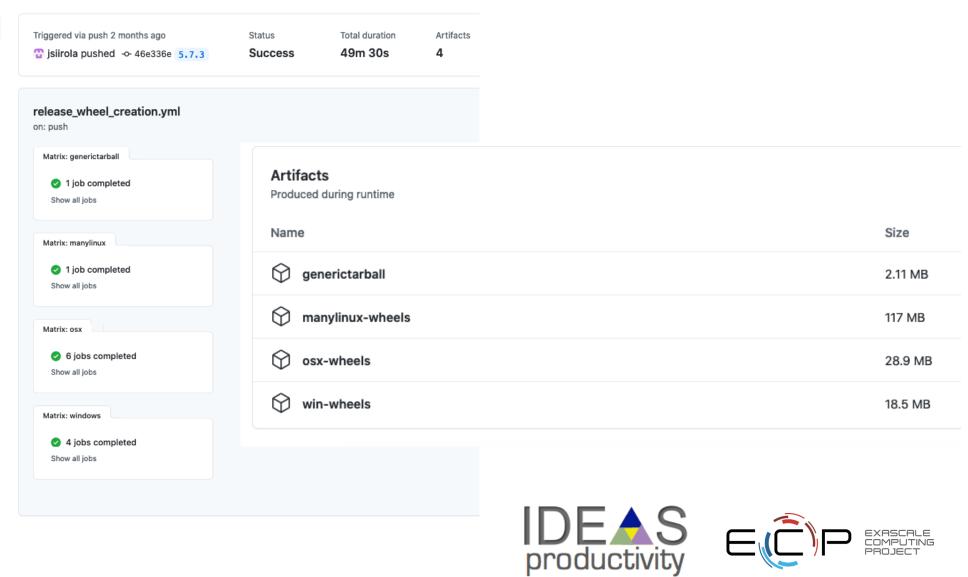




### **GitHub Actions - Release Automation**

✓ Merge pull request #1807 from Pyomo/finalize-release Pyomo Release Distribution Creation #9





### **Summary**

- The purpose of Continuous Integration Testing is to identify problems early
  - Catch things that would "break the build" or adversely impact other developers
  - Need to provide sufficient confidence, but run quickly balance varies by project
- CI testing should complement (not replace) more extensive automated "nightly" testing
  - Use scheduled testing for more and more detailed tests, more configurations and platforms, performance testing, etc.
- 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
  - Make sure your testing expands to cover new code



