



Continuous Integration



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Better Scientific Software tutorial @ ISC 2022

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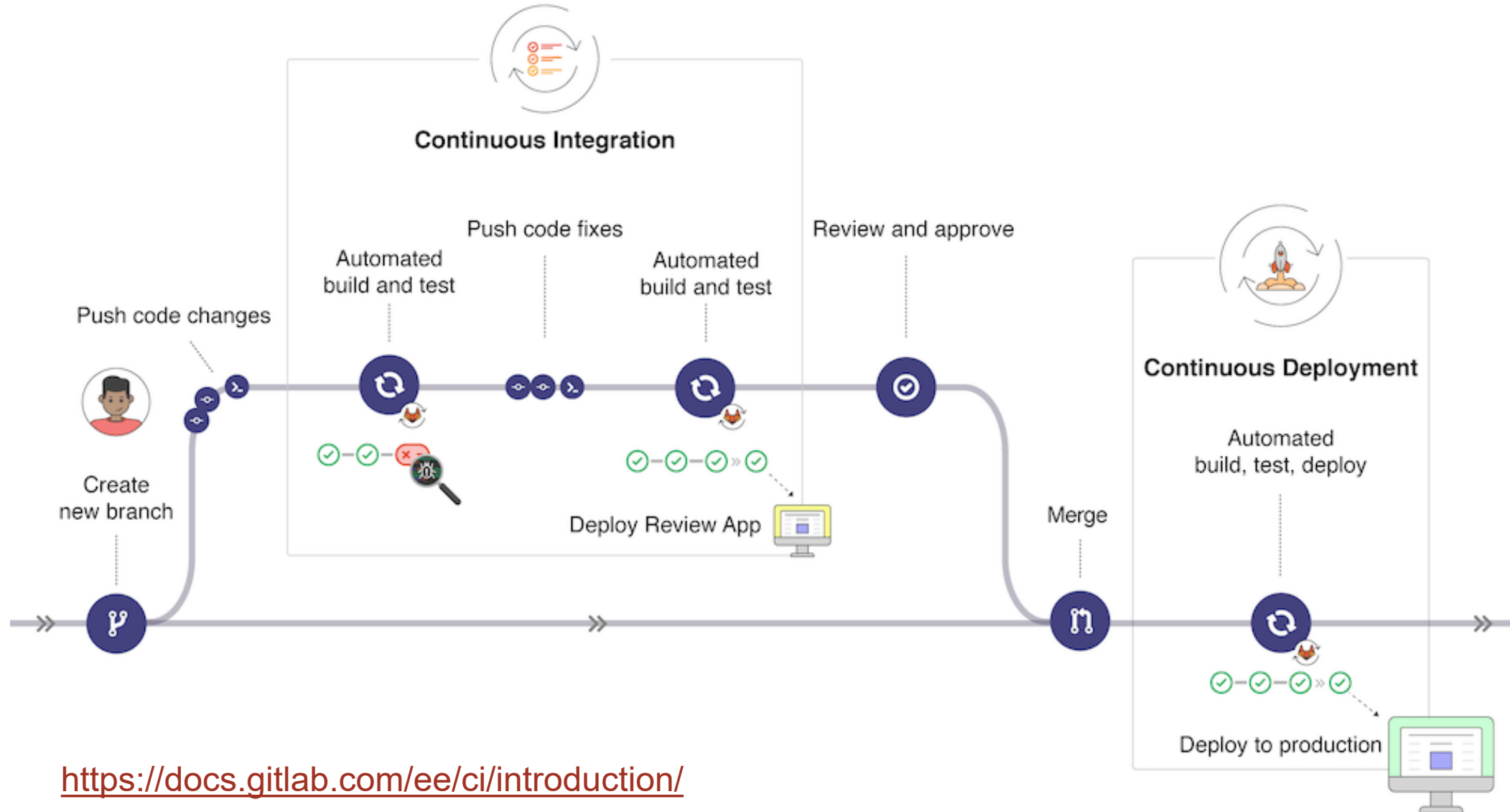
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- **The requested citation the overall tutorial is: Anshu Dubey and Gregory R. Watson, Better Scientific Software Tutorial, in ISC High Performance, 2022, Hamburg Germany. DOI: 10.6084/m9.figshare.19781752**
- Individual modules may be cited as *Speaker,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



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What is Continuous Integration (CI)



<https://docs.gitlab.com/ee/ci/introduction/>

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)
- CI generally implies a lot of automation

Test Driven Development vs. Automated Testing vs. CI

- ***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, 3rd-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	Status	Runtime (sec)
243	rendering	ospray.py	Unacceptable	5.0
273	simulation	batch.py	Unacceptable	38.0
24	databases	chgcarr.py	Succeeded With Skips	11.0
32	databases	exodus.py	Succeeded With Skips	14.0
66	databases	silos.py	Succeeded With Skips	50.0
67	databases	silos_altdriver.py	Succeeded With Skips	87.0
75	databases	xdmf.py	Succeeded With Skips	14.0
109	hybrid	merge_tree.py	Succeeded With Skips	11.0
136	meshtype	emptydomains.py	Succeeded With Skips	7.0
256	rendering	view.py	Succeeded With Skips	17.0
275	simulation	curve.py	Succeeded With Skips	8.0
281	simulation	life.py	Succeeded With Skips	8.0
296	simulation	zerocopy.py	Succeeded With Skips	32.0
0	databases	ANALYZE.py	Succeeded	10.0
1	databases	ANSYS.py	Succeeded	9.0
2	databases	CGNS.py	Succeeded	11.0
3	databases	Cale.py	Succeeded	6.0
4	databases	Chombo.py	Succeeded	7.0
5	databases	EnSight.py	Succeeded	9.0
6	databases	FITS.py	Succeeded	8.0
7	databases	Fluent.py	Succeeded	7.0
8	databases	GDAL.py	Succeeded	20.0
9	databases	NASTRAN.py	Succeeded	15.0


CI Testing Lives embedded in your development work


Add more commits by pushing to the `exodus-patch-1` branch on `exodus/chromium-dashboard`.



✓ All checks have passed [Hide all checks](#)

2 successful checks


✓  **Lighthouse** — Passed. New Lighthouse score would be 100/100. [Details](#)

✓  **continuous-integration/travis-ci/pr** — The Travis CI build passed [Details](#)

✓ **This branch has no conflicts with the base branch**
Merging can be performed automatically.

Merge pull request

You can also [open this in GitHub Desktop](#) or view [command line instructions](#).



Write

Preview

AA B i “ < > 🔗 ⋮ ≡ ≡ ↶ @ 📌

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?)

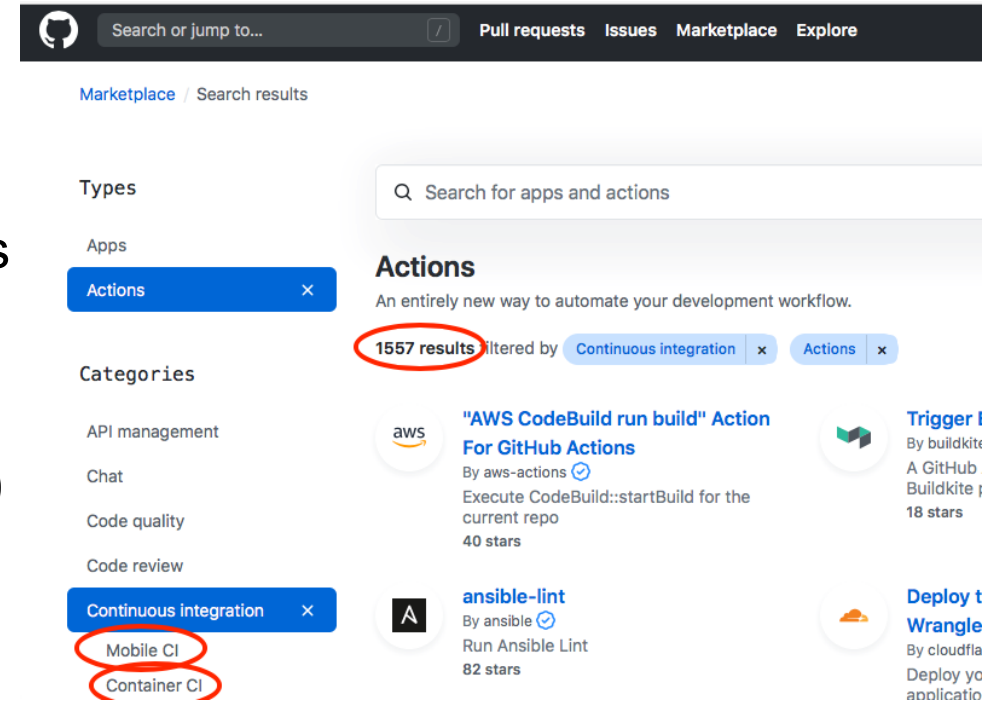
- Free Resources

- 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.

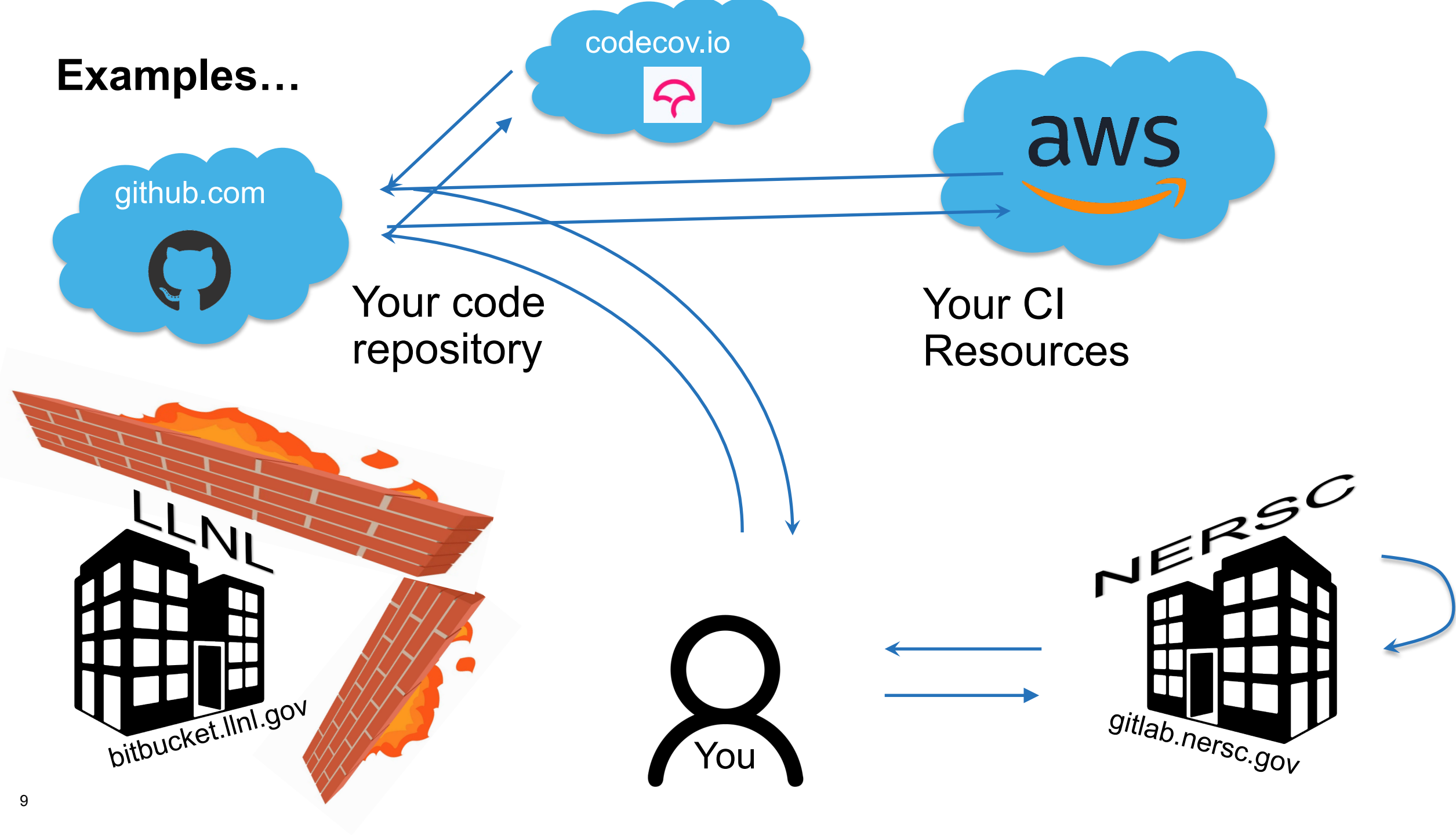
- Site-local Resources

- 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



Examples...



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>.yaml
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

bssw-tutorial / hello-numerical-world Template

<> Code Issues 3 Pull requests 5 Actions

Get started with GitHub Actions

Build, test, and deploy your code. Make code reviews, branch management, and issue triaging work the way you want. Select a workflow template to get started.

Skip this and [set up a workflow yourself](#) →

C/C++ with Make

By GitHub Actions

Build and test a C/C++ project using Make.

Set up this workflow

./configure
make
make check

actions/starter-workflows

Getting started with GitHub Actions:

19 lines (15 sloc) | 359 Bytes

```
1  name: Check Results
2
3  on:
4    push:
5      branches: [ main ]
6    pull_request:
7      branches: [ main ]
8
9  jobs:
10   build:
11
12     runs-on: ubuntu-latest
13
14     steps:
15     - uses: actions/checkout@v2
16     - name: make coverage
17       run: make CXXFLAGS=--coverage LDFLAGS="--coverage -lm" check_all
18     - name: upload coverage
19       run: bash <(curl -s https://codecov.io/bash)
```

github.com

[Code](#)[Issues](#)[Pull requests](#)[Actions](#)[Projects](#)[...](#)

Added workflows.

✓ Check Results #1

✓ build ▾

succeeded 4 minutes ago in 7s

> ✓ Set up job

2s

> ✓ Run actions/checkout@v2

1s

▾ ✓ make coverage


3s

```
1 ▶ Run make CXXFLAGS=--coverage LDFLAGS="--coverage -lm"
  check_all
4 g++ -c --coverage heat.C -o heat.o
5 g++ -c --coverage utils.C -o utils.o
6 g++ -c --coverage args.C -o args.o
7 g++ -c --coverage exact.C -o exact.o
```

codecov.io

[gh](#)[markcmiller86](#)[hello-numerical-world](#)[Docs](#)[Support](#)[Blog](#)[...](#)

fix error threshold

 [markcmiller86](#) 3 hours ago ✓ CI Passed

[26d69cd](#) [main](#) [d24c2f3](#)

51.60%

Files

Coverage

[Double.H](#)

65.63%

[args.C](#)

82.05%

[crankn.C](#)

0.00%

[exact.C](#)

0.00%

[ftcs.C](#)

100.00%

[heat.C](#)

73.81%

[upwind15.C](#)

0.00%

[utils.C](#)

49.35%

Project Totals (8 files)

51.60%

CALE
UTING
ECT

GitHub Actions – results of workflow test runs

Workflows

All workflows

- (TEST) Pyomo Windows Tests ...
- (WIP) Pyomo Windows Test (P...
- (WIP) Pyomo Windows Test (P...
- (WIP) Pyomo Windows Tests (...)
- (WIP) Windows Pip Cmd Pyom...
- GitHub Branch CI
- GitHub CI
- Pyomo Release Distribution Cr...
- Python package
- Ubuntu Pyomo Single Python ...
- Ubuntu Pyomo Workflow (Slim,...

GitHub CI

Showing runs from all workflows named GitHub CI

event:push workflow:"GitHub CI"

461 workflow run results

Event ▾ Status ▾ Branch ▾ Actor ▾

✓ Merge pull request #1902 from jsiirola/fix-unittest-rc GitHub CI #121: Commit 901b487 pushed by blnicho	main	20 hours ago 1h 3m 55s	...
✓ Merge pull request #1901 from mrmundt/remove-six GitHub CI #117: Commit a101b6d pushed by mrmundt	main	2 days ago 1h 3m 12s	...
✓ Merge pull request #1896 from jsiirola/abstract-disa... GitHub CI #112: Commit 1f9dd19 pushed by jsiirola	main	2 days ago 1h 5m 39s	...
✗ Merge pull request #1898 from mrmundt/py-unittest GitHub CI #109: Commit 1beb848 pushed by michaelbynum	main	3 days ago 1h 3m 33s	...
✓ Merge pull request #1893 from jsiirola/config-enum GitHub CI #105: Commit 9aa1186 pushed by jsiirola	main	3 days ago 1h 11m 3s	...

GitHub Pull Request Status Indicators

Filters ▾

🔍

is:pr is:open

🏷️ Labels 26

📌 Milestones 3

New pull request

🔗 17 Open ✓ 1,018 Closed

Author ▾Label ▾Projects ▾Milestones ▾Reviews ▾Assignee ▾Sort ▾

🔗 Allow string args to external fuctions ✖

#1904 opened 19 hours ago by eslickj • Review required

🚫 1💬 1

🔗 Port Cloning ✓

#1899 opened 3 days ago by michaelbynum • Approved

🚫 1💬 3

🔗 Remove pyomo.solvers.tests.core ✓

#1897 opened 3 days ago by mrmundt • Approved

💬 2

🔗 [WIP] Model partition package ●

#1895 opened 4 days ago by rahuljoglekar47 • Review required

💬 1

GitHub Actions – Key Elements of Defining Tests

```
1  name: GitHub CI
2
3  on:
4    push:
5      branches:
6        - main
7    pull_request:
8      branches:
9        - main
10   workflow_dispatch:
11     inputs:
12       git-ref:
13         description: Git Hash (Optional)
14         required: false
15
```

← Name

← Trigger

← Manual trigger with git-ref input

GitHub Actions – Key Elements of Defining Tests

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

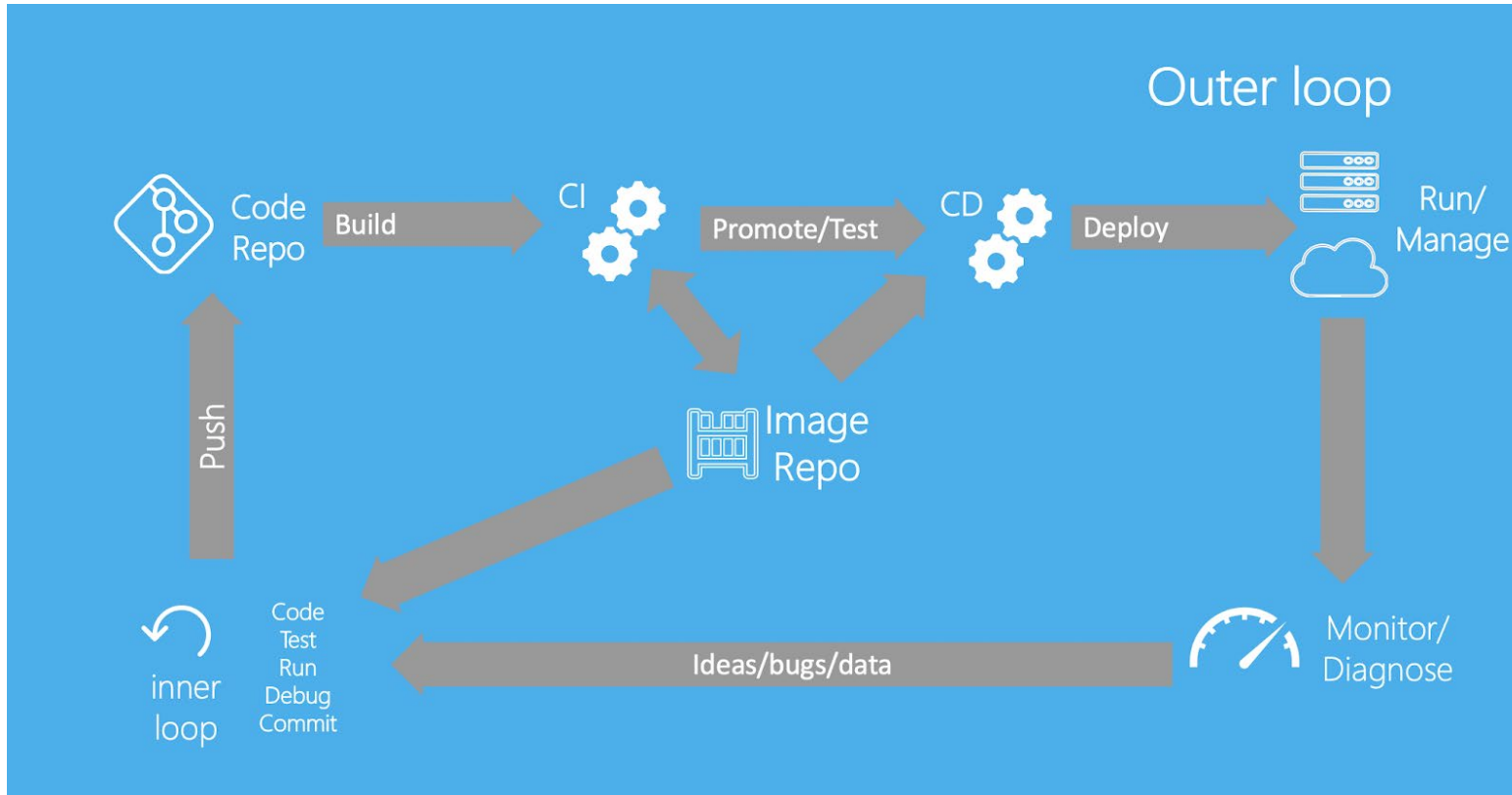
← Job setup

GitHub Actions – Key Elements of Defining Tests

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

← Job steps

Going Further with CI



- 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

<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 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