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Better Scientific Software Tutorial RF SciDAC 2020 Workshop



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- The requested citation the overall tutorial is: David E. Bernholdt, Better Scientific Software tutorial, in RF SciDAC 2020 Workshop, Knoxville, Tennessee. DOI: <u>10.6084/m9.figshare.11918397</u>
- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software Tutorial...

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### The Short & Sweet of Continuous Integration

### A master branch that always works

- DVCS workflow isolate master from integration environment
- Extend workflow to address difficulties of integrating
  - Minimize likelihood of merge conflict
  - Detect bugs immediately
  - Make debugging process quick and easy

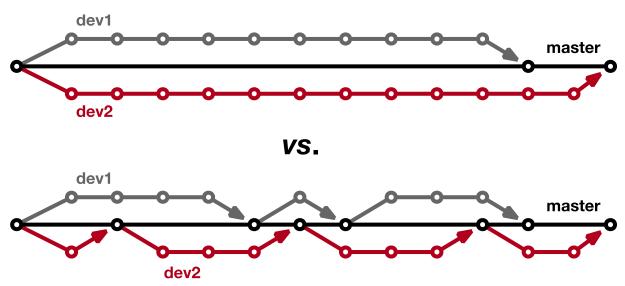




### **Work Decomposition**

### Commit and integrate often

- Limit divergence between feature and master branches
- Decreased probability of conflict
- Conflict resolution is simpler and less risky







### **Error Detection**

Test at integration to identify failures immediately

- Control quality of code
- Isolate failure to few commits
- No context switching for programmer

We want a system that

- triggers automated builds/tests on target environments when code changes and
- ideally tests on proposed merge product without finalizing merge.





### **Test Servers**

### Servers that

- automate the execution of a test suite or a subset of a test suite,
- allow for running tests on different environments,
- host an interface for viewing results, and
- allows for configuring when the tests are run.

### Examples

- CTest/CDash
- Jenkins
- Travis CI and GitLab CI





### **Cloud-based Test Servers**

- Linked to VCS hosts
  - GitHub & Travis CI
  - GitLab CI
  - BitBucket Pipelines
- Automated builds/tests triggered via pushes and pull requests
- Builds/tests can be run on cloud systems
- Test results are reported in repository's web interface
- Can trigger code coverage analysis & documentation build





## **Continuous integration (CI) Summary**

- Has existed for some time and interest is growing
- HPC community working to adapt CI for HPC machines
- Setup, maintenance, and monitoring required
- Prerequisites
  - A reasonably-automated build system
  - An automated test system with significant test coverage & useful feedback
  - Builds/tests must finish in reasonable about of time
  - Ability to bundle subset of tests



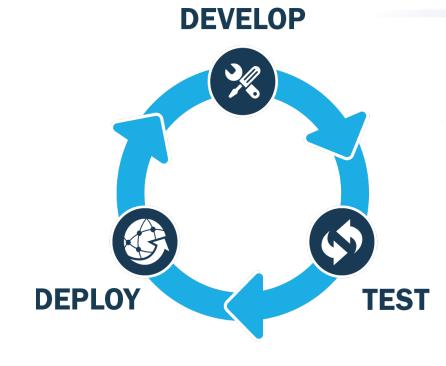


## ECP Project: WBS 2.4.4 Software Deployment at Facilities - Software Integration

The Software Integration effort was established to bridge the ECP ST software development effort with the Exascale hardware and software environments deployed at the Facilities.

 Continuous Integration (CI) - Provide the ability to continuously test AD/ST software on facility hardware resources with software environments established at the Facility.

Key for software development teams targeting systems being deployed agile feedback loop is key for development







## CI Solution for Large-Scale HPC Facilities

Need: HPC centers need new security features within Continuous Integration systems to serve thousands of users with unique hardware and security requirements.

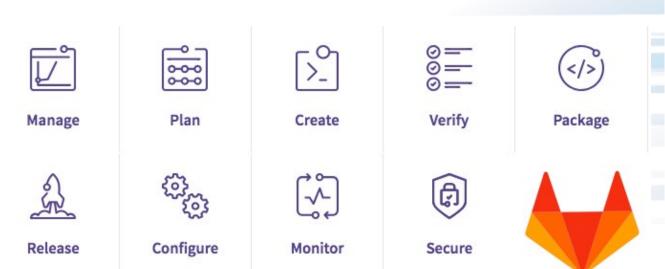
Response: Using GitLab as a basis, extend security, permissions, and auditing features while improving intra-Lab and inter-Lab accessibility to CI pipelines.





### **GitLab**

- GitLab is a single platform for the entire DevOps lifecycle
  - Plan, create, verify, and release
- Core functionality (free)
  - Version control, collaboration, CI/CD, and documentation tools
- Open source and capable of self management
  - MIT License
- Additional tiers of functionality are only available via license
  - https://about.gitlab.com/pricing/selfmanaged/feature-comparison/



Source: https://docs.gitlab.com/ee/

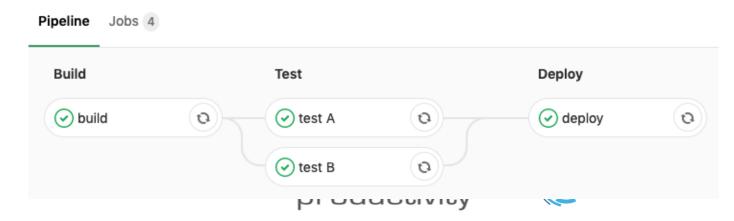






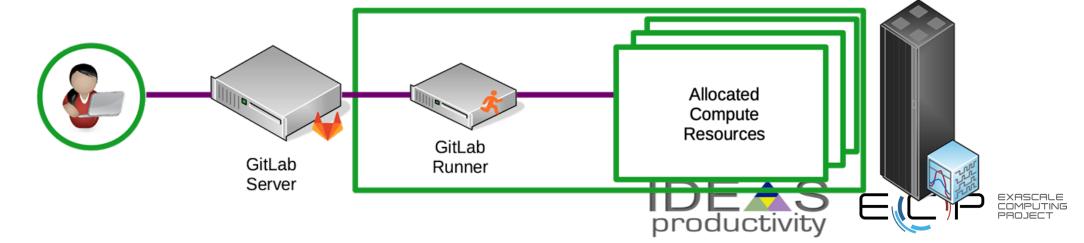
### GitLab CI/CD

- GitLab offers robust support for CI/CD (Continues Delivery)
- Primarily controlled via a '.gitlab-ci.yml' file defined in your project repository
  - Defines the jobs that will be run, their structure, and what will trigger their potential execution
  - https://docs.gitlab.com/ee/ci/yaml/
- Terms:
  - Jobs: Core elements of CI, where commands are defined for execution
  - Stages: Defined order for job execution within a pipeline
  - Pipelines: Collection of jobs
- Pipelines can be triggered through a number of mechanisms, including: commits, manually, api, scheduling, merge requests, upstream projects, and more...



### GitLab Runner

- "GitLab Runner is the open source project that is used to run your CI/CD jobs and send the results back to GitLab"
- Using GitLab CI/CD requires management of a runner:
  - Application supports the execution and reporting of CI jobs on target systems
  - Installed on target test resources and registered to a GitLab instance
  - Responsible for the execution of scripts whose creation is dictated by both the user's CI file as well as administrative configuration



### **Our Vision**

Delivering a secure, easy-to-use CI solution to support Software

Product testing against E6 HPC environments.





## **Security Challenges and Use Cases**

- All GitLab CI jobs run as the single gitlab-runner user
- Achieving any level of isolation between CI jobs requires either:
  - 1) Targeting specific runners such as Docker or Virtual machines
  - 2) Having each user/team manage their own runner
  - Neither of these are ideal
- Use cases we aim to support
  - Runner data isolation
  - Account specific resources
  - Sensitive data sets
  - Administrator management



## **Enhanced GitLab Functionality**

- Developing and supporting enhancements to GitLab applications to ensure targeted HPC testing resources can be available to code teams
  - Integrating facility feedback to improve technical aspects and support logistical challenges.
- Runner capable of setuid, enforcing local permissions
  - Jobs are executed under a users local account
- Batch executor added to interface with Cobalt, LSF, and Slurm
  - A runner side configuration that dictates how a CI job will be executed.
- Federated cross site continuous integration
  - Previously auth endpoints only used at login, now they have been expanded and integrated into the CI process as well.
- Existing GitLab functionality will continue to be supported
  - For instance continued upstream development efforts and improved to GitLab's core CI/CD capabilities
     can be used for





## What is the GitLab Runner Doing?

- The GitLab runner polls the server to identify available CI jobs
  - Will only begin executing a job once it has been scheduled by the server
- Job local to runner result in generated Bash scripts based upon the contents of the .gitlab-ci.yml
  - Works similar to upstream GitLab (<a href="https://docs.gitlab.com/runner/shells/index.html">https://docs.gitlab.com/runner/shells/index.html</a>)
  - Scripts are executed by piping them into a non-interactive Bash login shell.
- Every step in a CI job is executed by a valid local user account
  - This is a key change with setuid enabled runner
- Each user is provided with a clean login shell
  - Ensures runner environment does not compromise subsequent jobs
  - Users experience an environment similar to what they would see on a login node
  - Depending on <u>your</u> environment this may affect the results of your CI





### **Federation**



- Goal of allowing cross site CI in a secure manner while still empowering site admins with the tools to ensure policy is enforced.
  - Site Identify Providers are used and also linked to specific runners
  - Valid site credentials must be present before a job could be run at any specific site.
- Enhanced identity model that establishes a connection between a site runner, auth provider, and the user's session.
- Gitlab Omniauth as a first class citizen:
  - "...Users can choose to sign in using any of the configured mechanisms."
  - I.e. LDAP and standard Gitlab login can still function, but many providers can be added
- Ongoing communication directly with GitLab to upstream enhancements.

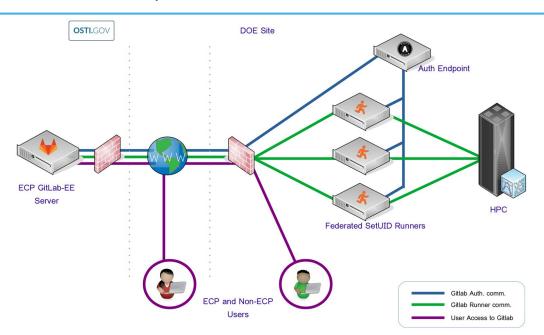




## **Deployment Models**

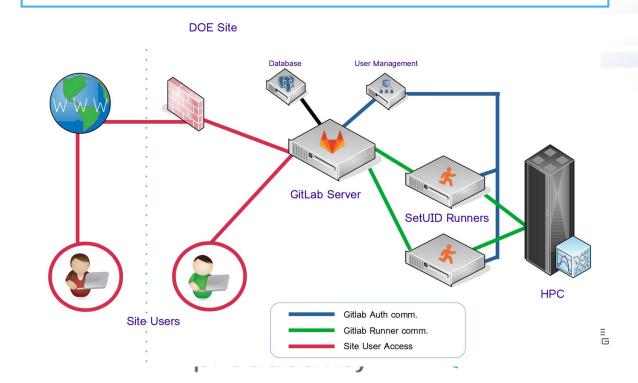
### Federated - Centralized (OSTI) Sever

- Single, centrally managed Gitlab Server instance provided and administered by the OSTI team.
- Federated runners at sites
- Multi-site run capabilities



#### Site - Local Site Server

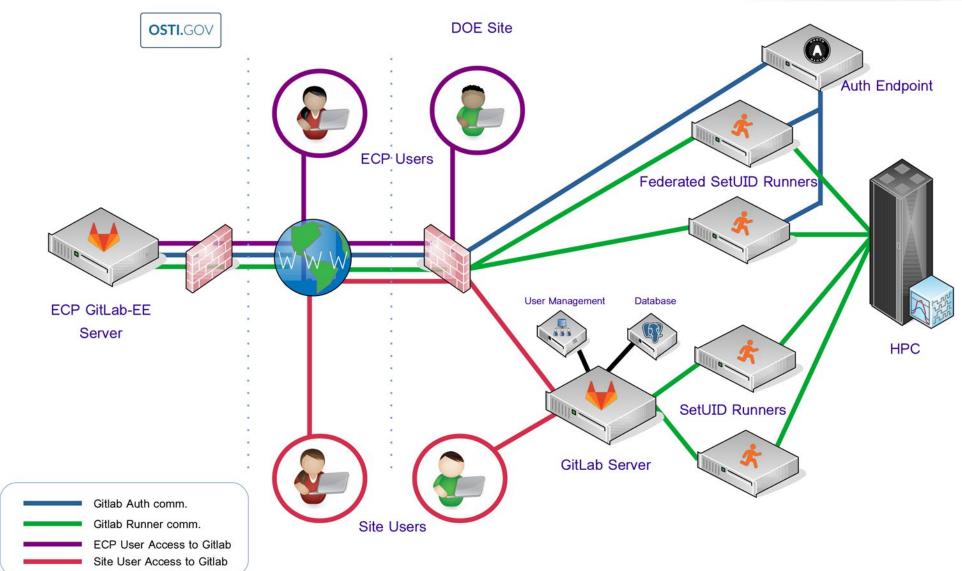
- Separate and isolated Gitlab Server provided and administered by the site's Operations team.
- Local systems/resources capacity



## **Deployment Models - Contd.**

# Federated with Site Local - Hybrid

- Most likely to be the typical deployment model for DOE facilities
- Federated capabilities
- Control over Site deployment









## **CI Testing Tier - HPC Resources**

	Tier 0	<ul><li>What AD/ST projects do now</li><li>Existing CI</li></ul>	May include GitHub/Travis, existing internal systems, cron jobs, etc
CI Cross-Site Targeting	Tier 1	<ul> <li>Base ECP CI - Build and Run resources</li> <li>Possible 2 build and 2 run nodes</li> <li>Build and Smoke tests</li> <li>Run multiple builds on resource</li> <li>Unit / Integration tests</li> <li>Cross-site CI target</li> </ul>	<ul> <li>What is ratio of build to test resources?</li> <li>Work with AD and ST teams to support their needs</li> <li>Possible to allocate from other HPC resources with separate scheduling policy</li> </ul>
CI Cross-Site Facilitating	Tier 2	<ul> <li>Facility test resource (~10 + nodes)</li> <li>In security enclave – site dependent</li> <li>Larger scale tests</li> <li>Facility approval for projects</li> </ul>	<ul> <li>Facility managed and may want to approve projects</li> <li>Possible production security constraints</li> </ul>
	Tier 3	<ul><li>Production machines</li><li>Need allocation</li><li>Production job rules</li><li>Scale tests</li></ul>	<ul> <li>Facility managed and may want to approve projects</li> <li>Production security constraints</li> </ul>





# **CI Testing Tier - HPC Resources**

			TO S
	Tier 0	<ul><li>What AD/ST projects do now</li><li>Existing CI</li><li>Regression tests (no CI)</li></ul>	<ul> <li>May include GitHub/ Travis - internet</li> <li>cron job based regression on misc. hardware</li> </ul>
CI Cross-Site Targeting	Tier 1	<ul> <li>Base ECP CI - Build and Run resources</li> <li>Possible 2 build and 2 run nodes</li> <li>Build and Smoke tests</li> <li>Run multiple builds on resource</li> <li>Unit / Integration tests</li> <li>Cross-site CI target</li> </ul>	<ul> <li>What is ratio of build to test resources?</li> <li>Work with AD and ST teams to support their needs</li> <li>Possible to allocate from other HPC resources with separate scheduling policy</li> </ul>
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### **CI Readiness**

#### Site readiness for OSTI hosted CI with federated runners

	Local CI	MOU	Auth Endpoint	Federated(OSTI) CI
ORNL	Available	In-process	In-process: 2/2020	
NERSC	Available	In-process	Complete	In-process
ANL	Available	In-process	In-process: 2/2020	
LANL	Available	In-process	In-process	
LLNL	Available	In-process	In-process	
SNL	Available	In-process	In-process	
NMC		In-process	In-process: 1/2020	Complete





## What's available and Where?

#### ANL

- Local Gitlab CE Server with ECP enhanced runners
- Integration with lota(test) and Theta HPC systems

#### ORNL

- Local Gitlab EE Server with ECP enhanced runners
- Integration with Ascent(test) HPC system

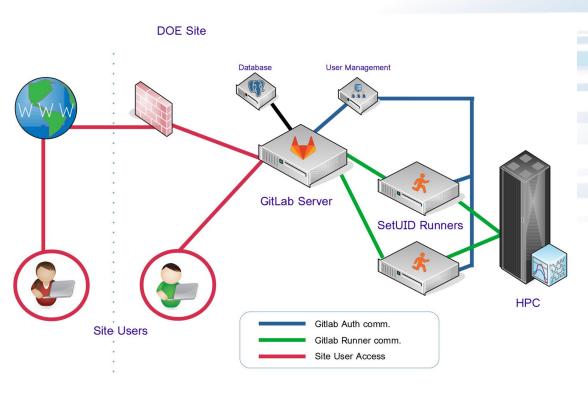
#### **NERSC**

- Local Gitlab EE Server with ECP enhanced runners
- Integration with Cori HPC system

#### Other

- Local Gitlab CE Server with ECP enhanced runners
- Integration with P9, x86, and ARM systems

#### **Local Preview Environments**







### **Documentation**

- Need to address ongoing requests for organized documentation
- https://ecp-ci.gitlab.io
  - Using GitLab Pages
  - Ongoing effort to provide value up to date information
- Goal is not to replace upstream documentation but highlight HPC focused enhancements and best-practices.
- Site specific information organized using Confluence
  - https://confluence.exascaleproject.org/display/HI
     SD/Getting+Started+with+CI

#### Welcome to ECP CI Documentation

#### The DOE Exascale Computing Project's (ECP) mission:

Develop exascale-ready applications and solutions that address currently intractable problems of strategic importance and national interest.



Create and deploy an expanded and vertically integrated software stack on DOE HPC pre-exascale and exascale systems.

Deliver US HPC vendor technology advances and deploy ECP products to DOE HPC pre-exascale and exascale systems.

Deliver exascale simulation and data science innovations and solutions to national problems that enhance US economic competitiveness, improve our quality of life, and strengthen our national security.

The ECP Software Ecosystem is critical to reach exascale computing capabilities. A Continuous Integration (CI) testing capability was identified as a critical need to allow application and software technology projects to test across HPC architectures and software environments.

#### Contents

- Introduction
  - Enhancements
  - CI Use Models
  - Local Model
  - Federated Model
- Customers
  - Quick Start
  - Continues Integration
  - Server
  - Migrating CI
- Example Projects







## CI Integration and AD/ST Project Teams

- Effort includes the on-boarding of ECP AD/ST and E6 software projects onto the ECP/E6 CI infrastructure.
  - Derives capability from the CI Optimization effort and the CI Test Resources effort. It is focused on supporting software teams and helping them port and utilize the ECP CI infrastructure.
- Goals:
  - Helping individual teams on-board and teams
  - Developing documentation and training
  - Support development of tools to support CI teams
  - Identify limitations of CI infrastructure / resources and areas of potential growth
- Ready to support more projects at sites in a preview environment
  - We want to help teams to get running locally at the sites
  - Assist in transition to the OSTI model down the road, if desired





## **Agenda**

Time	Module	Topic	Speaker
1:00pm-1:05pm	00	Introduction	David E. Bernholdt, ORNL
1:05pm-1:30pm	01	Overview of Best Practices in HPC Software Development	David E. Bernholdt, ORNL
1:30pm-2:00pm	02	Agile Methodologies and Useful GitHub Tools	David E. Bernholdt, ORNL
2:00pm-2:30pm	03	Improving Reproducibility through Better Software Practices	David E. Bernholdt, ORNL
2:30pm-2:45pm		Q&A	All
2:45pm-3:30pm		Break	
3:30pm-4:15pm	04	Software Design and Testing	David E. Bernholdt, ORNL
4:14pm-4:45pm	05	Continuous Integration	David E. Bernholdt, ORNL
4:45pm-5:00pm		Q&A	All





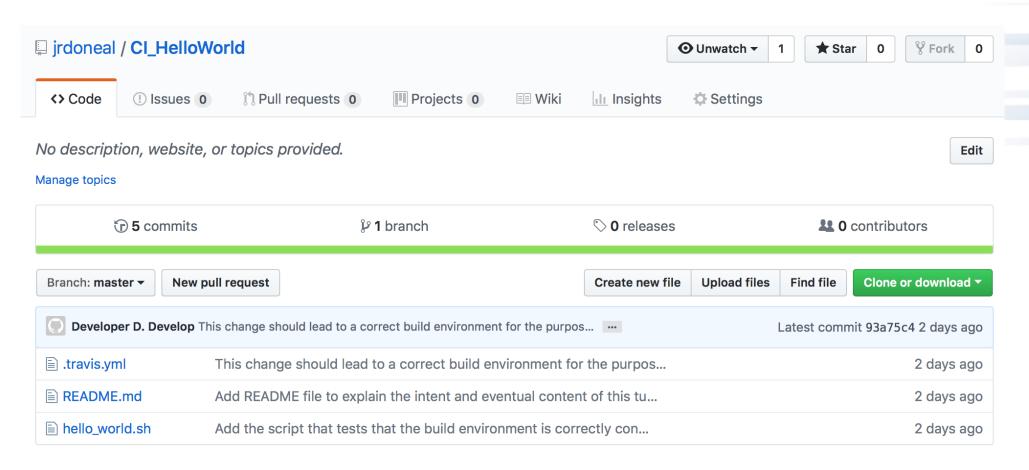
# Simplest CI example https://github.com/jrdoneal/Cl HelloWorld https://travis-ci.org/jrdoneal/CI HelloWorld CI example w/ multiple platforms and specific compiler versions **BACKUP:** https://github.com/jrdoneal/CI Multiplatform CI HELLO WORLD Code coverage, testing and CI tutorial (C++) https://github.com/amklinv/morpheus Code coverage, testing, and CI example (Fortran, C++) https://github.com/jrdoneal/infrastructure





### **GitHub Repository Page**

#### https://github.com/jrdoneal/CI HelloWorld







### **Travis CI Configuration File**

#### .travis.yml

```
env:
- TRAVIS CI ENV="Hello, World"
#before_install:
#- Put commands here to prepare for executing builds/installs
#- Examples would be using apt-get to install dependencies not
# included in the Travis CI build environment by default.
#install:
#- Put build commands here
#- In each phase, you can execute multiple commands
#- Travis CI stops if any single command fails in this phase
before script:
- echo $TRAVIS_CI_ENV
script:
- $TRAVIS_BUILD_DIR/hello_world.sh
#- Travis CI will run each command in this phase even if a previous command
# terminated in failure
after success:
- echo "You should see that Hello, World was printed by before script"
after failure:
- echo "Hello, World should not have been printed by before script"
```



### **The Script Phase**

#### hello\_world.sh

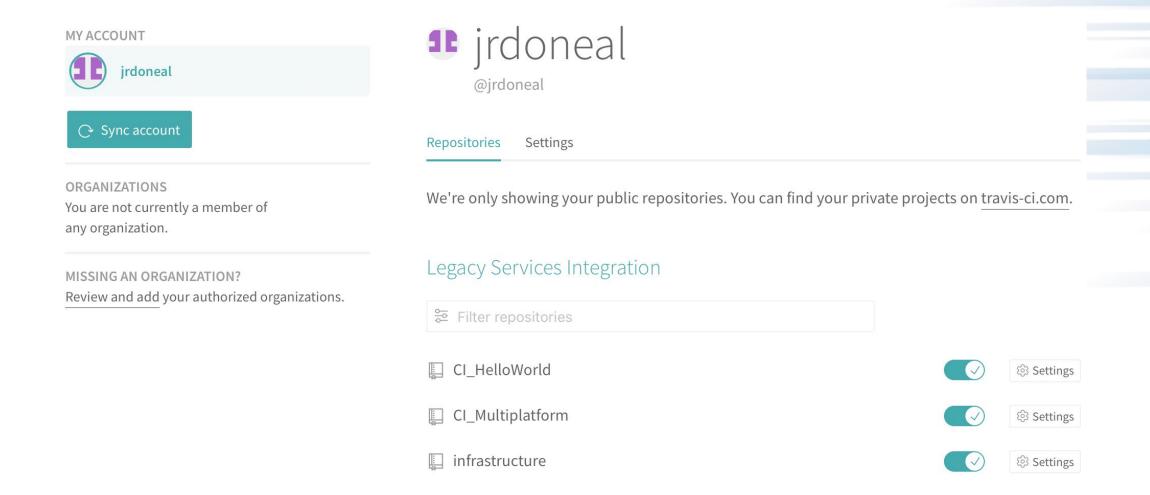
#### #!/bin/bash

```
if [ -z "${TRAVIS_CI_ENV}" ]; then
  echo "Please set the TRAVIS_CI_ENV environment variable"
  exit 1
elif [ "${TRAVIS_CI_ENV}" != "Hello, World" ]; then
  echo "TRAVIS_CI_ENV value is ill-suited for this tutorial"
  exit 2
fi
```





## **Connecting GitHub & Travis CI**



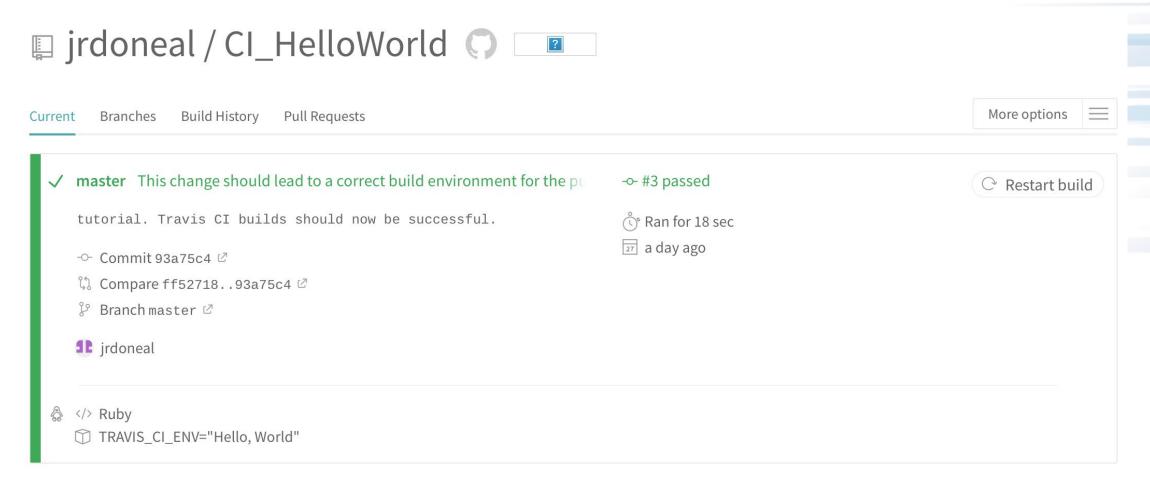






### Repository in Travis CI

https://travis-ci.org/jrdoneal/Cl HelloWorld

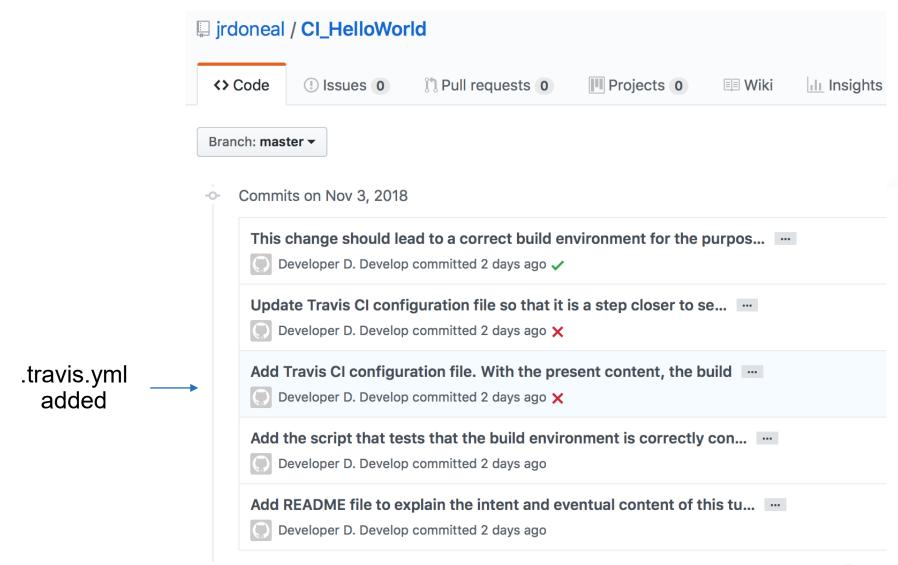








### **Commit History**

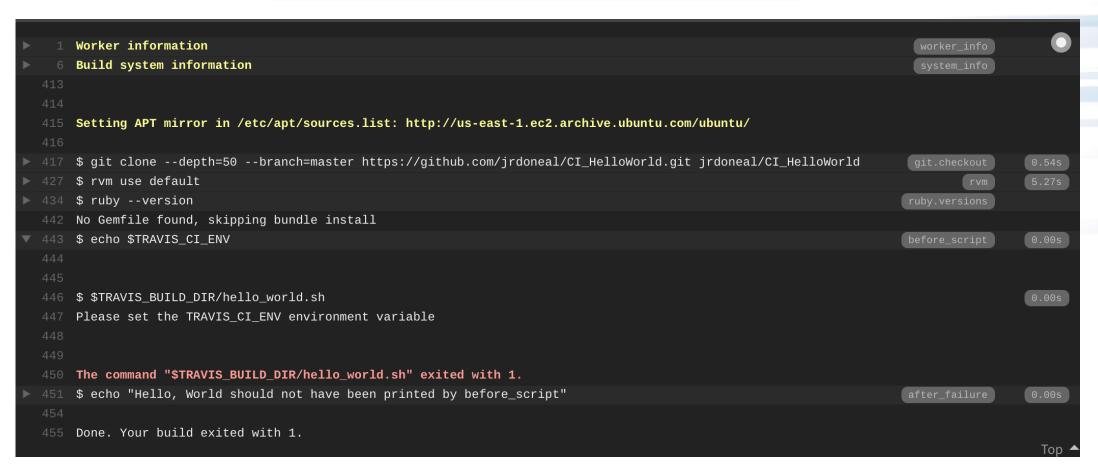






### **Travis CI Build History**

Add Travis CI configuration file. With the present content, the build Developer D. Develop committed 2 days ago X





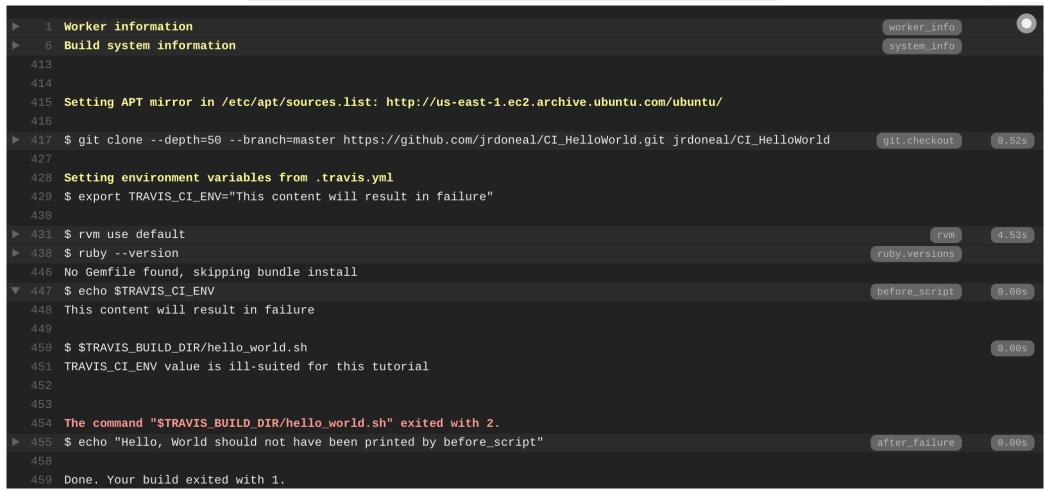




### **Travis CI Build History**

Update Travis CI configuration file so that it is a step closer to se...

Developer D. Develop committed 2 days ago X







### **Travis CI Build History**

This change should lead to a correct build environment for the purpos...

Developer D. Develop committed 2 days ago

