

Employing DevOps in HPC Operational Management

By Aaron Barlow



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Introduction to Speaker & Organization



Aaron Barlow

HPC Software Engineer with over 8 years of industry experience



Oak Ridge Leadership Computing Facility (OLCF)

Provides world-leading high-performance computing (HPC) resources like Frontier to scientists and engineers to solve significant and complex problems in a broad range of scientific fields



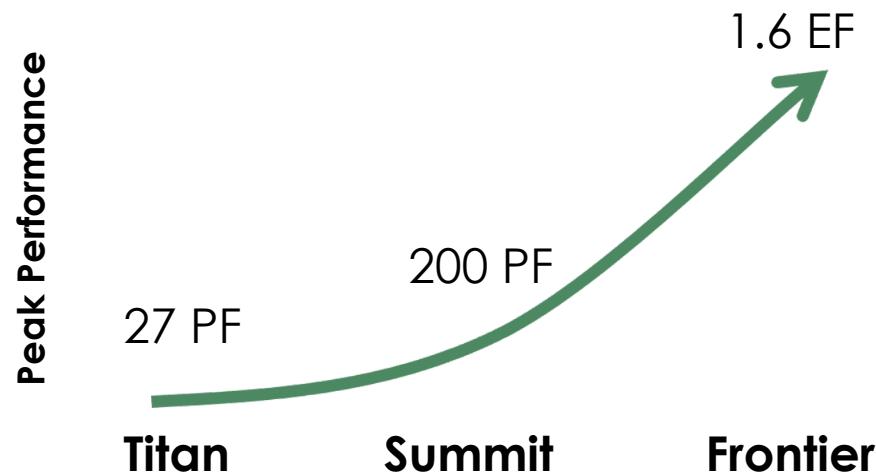
Software Services Development Group (SSD)

Develops and maintains large software applications and services used by the staff and end-users of the OLCF's computational ecosystem

HPC Operational Management

Scale and Complexity

- Our software supports the business of running HPC at our scale and complexity
 - Complexity: thousands of projects and users
 - Scale: Exaflop supercomputer Frontier



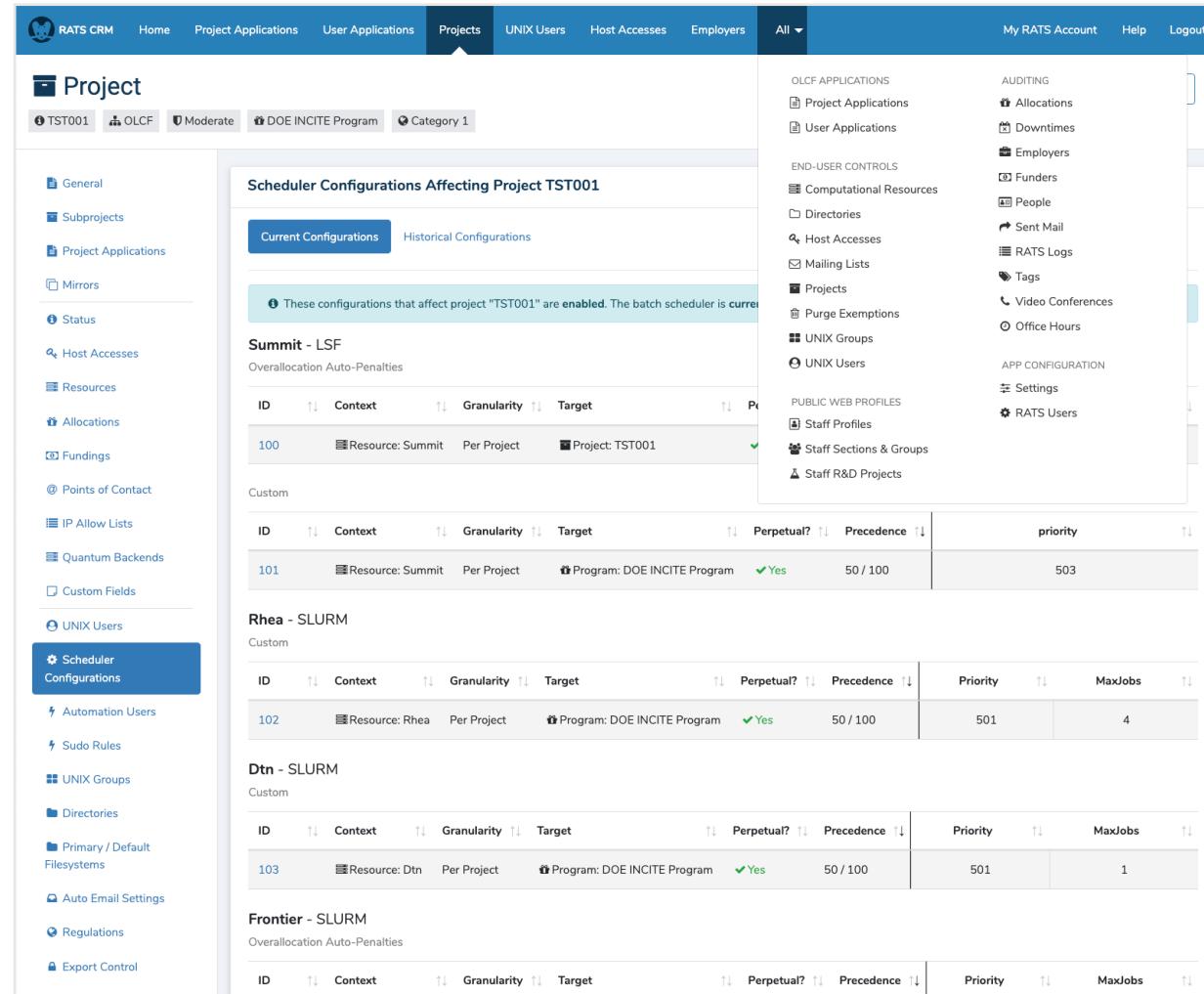
Provided Software Services

- User facing portal applications
- Business analytics systems
- Customer relationship management (CRM) applications
- API driven HPC system integration and management services
- Select auditing capabilities

RATS CRM: HPC Management Application

HPC Operational Management Software

- It directly controls many of the day-to-day operational needs of the center in real-time
- Some core HPC system features RATS CRM manages:
 - Filesystem directories
 - Scheduler configurations
 - HPC allocations
 - User and system access
 - Projects
 - Mailing lists
 - Auto sending select emails to users
- 162 API endpoints to disseminate information to our systems and services



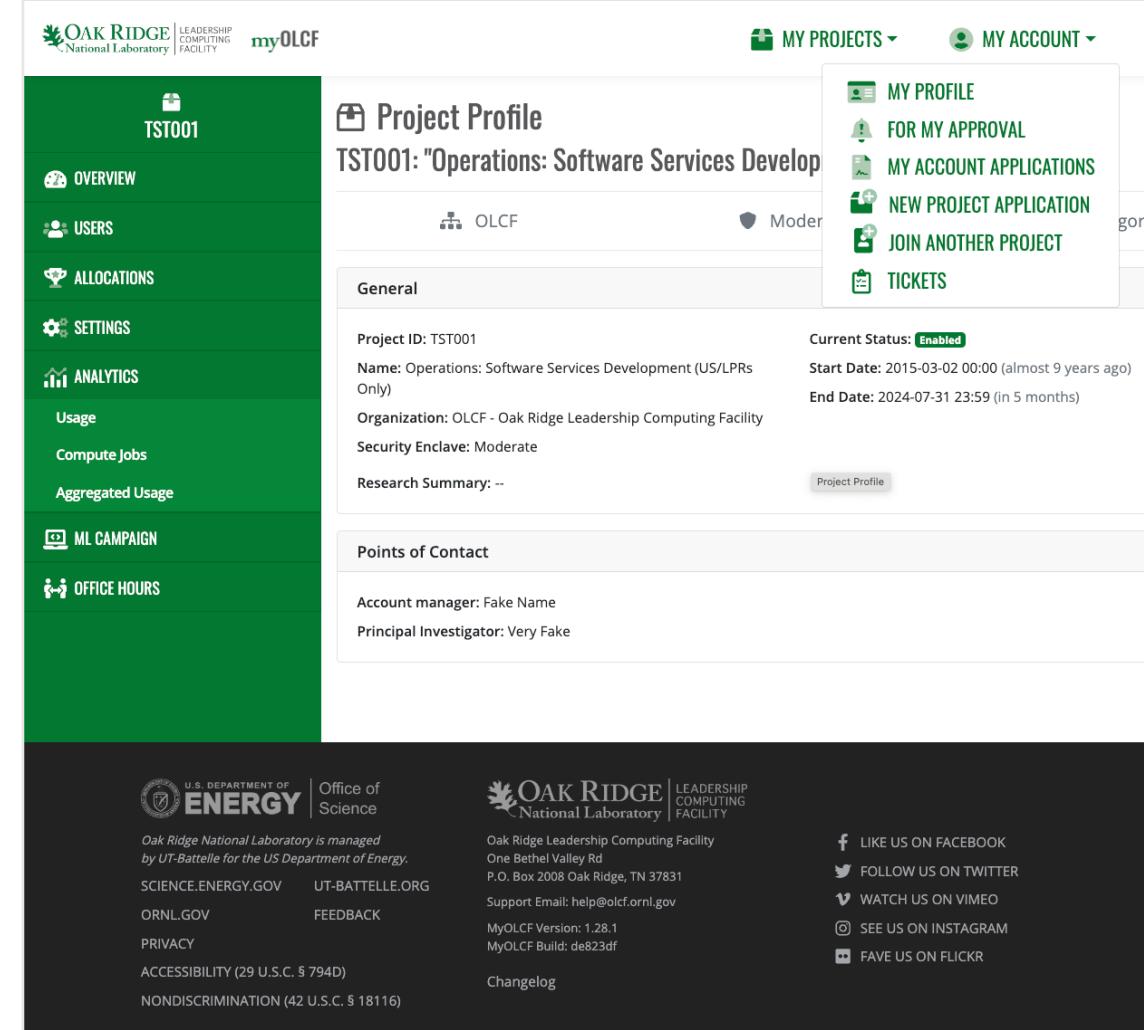
The screenshot shows the RATS CRM interface with the 'Scheduler Configurations' section for Project TST001. The interface is divided into several panels:

- Header:** RATS CRM, Home, Project Applications, User Applications, Projects (selected), UNIX Users, Host Accesses, Employers, All, My RATS Account, Help, Logout.
- Left Sidebar:** General, Subprojects, Project Applications, Mirrors, Status, Host Accesses, Resources, Allocations, Fundings, Points of Contact, IP Allow Lists, Quantum Backends, Custom Fields, UNIX Users, Scheduler Configurations (selected), Automation Users, Sudo Rules, UNIX Groups, Directories, Primary / Default Filesystems, Auto Email Settings, Regulations, Export Control.
- Project Overview:** Project TST001, OLCF, Moderate, DOE INCITE Program, Category 1.
- Scheduler Configurations Affecting Project TST001:**
 - Summit - LSF:** Overall allocation Auto-Penalties. Table shows ID 100, Context Resource: Summit, Granularity Per Project, Target Project: TST001, Perpetual? Yes, Priority 50 / 100, MaxJobs 503.
 - Rhea - SLURM:** Custom. Table shows ID 102, Context Resource: Rhea, Granularity Per Project, Target Program: DOE INCITE Program, Perpetual? Yes, Priority 50 / 100, MaxJobs 4.
 - Dtn - SLURM:** Custom. Table shows ID 103, Context Resource: Dtn, Granularity Per Project, Target Program: DOE INCITE Program, Perpetual? Yes, Priority 50 / 100, MaxJobs 1.
 - Frontier - SLURM:** Overall allocation Auto-Penalties. Table shows ID 104, Context Resource: Frontier, Granularity Per Project, Target Program: DOE INCITE Program, Perpetual? Yes, Priority 50 / 100, MaxJobs 1.
- Right Sidebar:** OLCF APPLICATIONS, END-USER CONTROLS, PUBLIC WEB PROFILES, APP CONFIGURATION.

RATS-CRM with fake data

Public HPC Self-Service Application

- Publicly available application that extends management capabilities and provides insights into available resources for users
 - my.olcf.ornl.gov
- Some key features:
 - Apply for and renew projects and accounts on HPC systems
 - Check the status of their applications
 - Monitor their submitted issues
 - Allocation usage monitoring
 - Compute usage report generation
 - Schedule office hours for help



Project Profile
TST001: "Operations: Software Services Develop

General

Project ID: TST001
Name: Operations: Software Services Development (US/LPRs Only)
Organization: OLCF - Oak Ridge Leadership Computing Facility
Security Enclave: Moderate
Research Summary: --

Current Status: **Enabled**
Start Date: 2015-03-02 00:00 (almost 9 years ago)
End Date: 2024-07-31 23:59 (in 5 months)

Points of Contact

Account manager: Fake Name
Principal Investigator: Very Fake

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SCIENCE.ENERGY.GOV | UT-BATTELLE.ORG
ORNL.GOV | FEEDBACK
PRIVACY
ACCESSIBILITY (29 U.S.C. § 794D)
NONDISCRIMINATION (42 U.S.C. § 18116)
Changelog

OAK RIDGE | LEADERSHIP COMPUTING FACILITY
Oak Ridge Leadership Computing Facility
One Bethel Valley Rd
P.O. Box 2008 Oak Ridge, TN 37831
Support Email: help@olcf.ornl.gov
MyOLCF Version: 1.28.1
MyOLCF Build: de823df

MY PROJECTS **MY ACCOUNT** **LOG OUT**

MY PROFILE
FOR MY APPROVAL
MY ACCOUNT APPLICATIONS
NEW PROJECT APPLICATION
JOIN ANOTHER PROJECT
TICKETS

MyOLCF GUI with fake data

Embracing DevOps and GitOps for HPC Management



Uptime



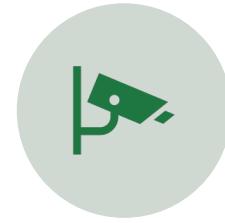
Reliability



Scalable



Quality



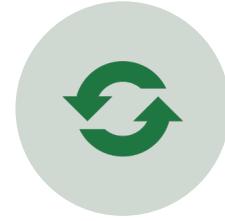
Security



Monitoring



Alerts



Reproducibility

Components of our GitOps



GitLab Pipelines: automate our workflows



Kustomize: configure Kubernetes applications & deployments



Argo CD: providing continuous delivery of deployments



Kubernetes: container management by Kustomize



MinIO: object store for backups and caching



KubeDB and Stash: database deployment and management



SonarQube: identify bugs, vulnerabilities, and code quality issues



HashiCorp Vault: securely store our passwords

GitLab Pipelines: Automating CI/CD Workflows

```
1 Running with gitlab-runner 16.6.1 (f5da3c5a)
2 on gitlab-mini-runner-gitlab-runner-566c78b44-n2grn DKxTSzcr, system ID: r_UeulMNUpYQiW
3 Resolving secrets
4 Preparing the "Kubernetes" executor
5 "ServiceAccount" overwritten with "gitlab-runner-builder"
6 Using Kubernetes namespace: stf040-ci-runner
7 Using Kubernetes executor with image image-registry.openshift-image-registry.svc:5000/stf040-ci-runner/slate-ci:latest ...
8 Using attach strategy to execute scripts...
9 Preparing environment
10 Using FF_USE_POD_ACTIVE_DEADLINE_SECONDS, the Pod activeDeadlineSeconds will be set to the job timeout: 24h0m0s...
11 Waiting for pod stf040-ci-runner/runner-dkxtszcr-project-949-concurrent-0-xhxbe8nn to be running, status is Pending
12 Waiting for pod stf040-ci-runner/runner-dkxtszcr-project-949-concurrent-0-xhxbe8nn to be running, status is Pending
13 ContainersNotReady: "containers with unready status: [build helper]"
14 ContainersNotReady: "containers with unready status: [build helper]"
15 Running on runner-dkxtszcr-project-949-concurrent-0-xhxbe8nn via gitlab-mini-runner-gitlab-runner-566c78b44-n2grn...
16 Getting source from Git repository
17 Fetching changes with git depth set to 1...
18 Initialized empty Git repository in /builds/uadev-team/rats-crm/.git/
19 Created fresh repository.
20 Checking out 8941a555 as detached HEAD (ref is refs/merge-requests/1816/head)...
21 Skipping Git submodules setup
22 Executing "step_script" stage of the job script
23 $ sha256=$(sha256sum Gemfile.lock | awk '{ print $1 }') # collapsed multi-line command
24 $ export BUILD_ARG_BASE_VERSION=${BASE_VERSION}
25 $ export BUILD_ARG_NAMESPACE_UID=${NAMESPACE_UID}
26 $ if [ "${BUILD_DEBUG}" = "true" ] ; then # collapsed multi-line command
27 $ [ -z "${KUBE_NAMESPACE+x}" ] && KUBE_NAMESPACE=$(cat /run/secrets/kubernetes.io/serviceaccount/namespace) # collapsed multi-line command
28 $ oc create imagestream --namespace=${KUBE_NAMESPACE} ${IMG_STREAM} || true
29 Error from server (AlreadyExists): imagestreams.image.openshift.io "rats-crm-ci" already exists
30 $ BUILD_CHART=.build-templates/build-chart" # collapsed multi-line command
31 Cloning into '.build-templates'...
32 Using default SSD group build-chart for rats-crm-ci...
33 Set BuildArg: RUBY_VERSION=3.0.6
34 Set BuildArg: BASE_VERSION=c4bc76ef12003b0a6f00f704270042e481ed0df41c0a40f5a6e16101a86317a3
35 Set BuildArg: NODE_VERSION=16.18.1
36 Set BuildArg: NAMESPACE_UID=16647
37 Set BuildArg: NPM_VERSION=8.19.2
38 ++ helm -n stf040-ci-runner upgrade rats-crm-2159618 .build-templates/build-chart -i --wait --reset-values --set BuildArgs.RUBY_VERSION=3.0.6 --set BuildArgs.NODE_VERSION=16.18.1 --set BuildArgs.NAMESPACE_UID=16647 --set BuildArgs.NAME=rats-crm-ci --set Tag=8941a5552149a46557ffc287de6d2c630e7cd2a7 --set Dockerfile=container/ci/Dockerfile
39 Release "rats-crm-2159618" does not exist. Installing it now.
40 NAME: rats-crm-2159618
41 LAST DEPLOYED: Wed Feb 28 15:59:56 2024
42 NAMESPACE: stf040-ci-runner
43 STATUS: deployed
44 REVISION: 1
45 TEST SUITE: None
46 ++ set +x
```

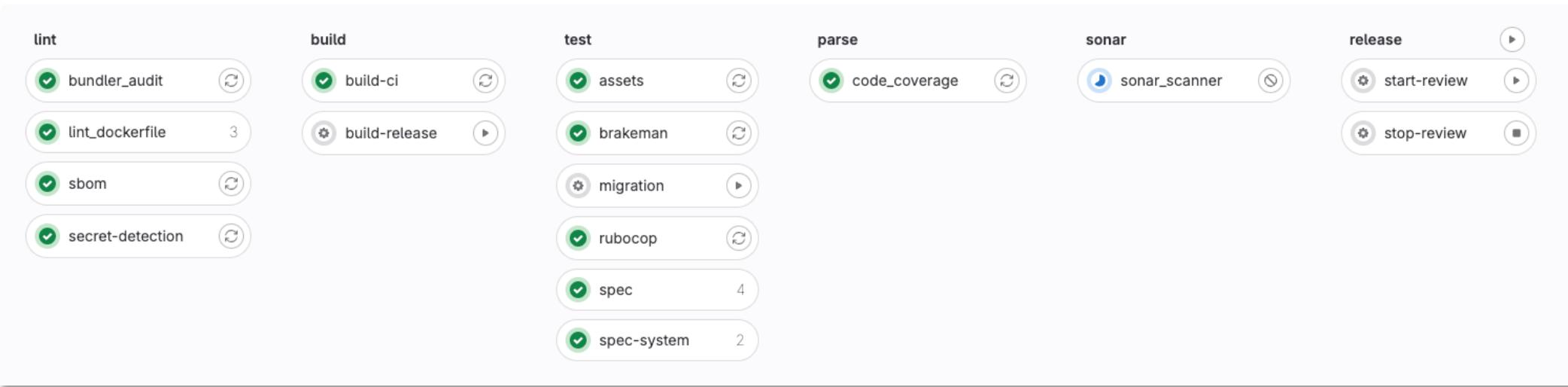
Real RATS-CRM build CI GitLab job

GitLab CI/CD Configuration

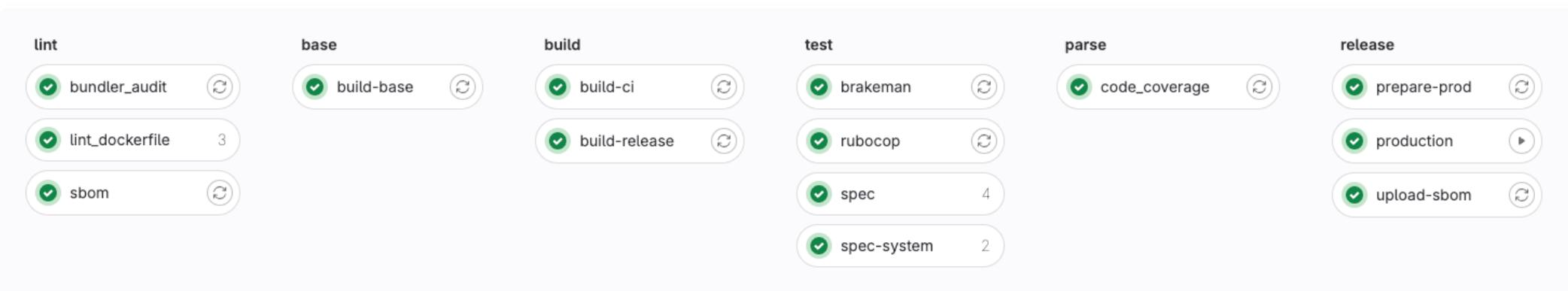
- GitLab jobs are run by GitLab Runners, which run on Kubernetes
- CI/CD workflows are defined in each repository's `gitlab-ci.yml`
- Key GitLab Pipeline features & benefits:
 - Automated and repeatable workflows
 - Efficiency with caching and parallel job execution

GitLab Pipelines: Visualizing CI/CD Workflows

Development Pipeline



Production Pipeline



GitLab Pipeline Example: Code Coverage

Code Coverage Explanation

- GitLab Pipeline `code_coverage` step is defined in `gitlab-ci.yml`
 - `code_coverage` step defines process to generate and capture coverage metric(s)
 - `code_coverage` job generates a report job artifact which is observed by GitLab and made available

Code Coverage Job

```

30 Reading package lists...
31 Building dependency tree...
32 Reading state information...
33 The following additional packages will be installed:
34   xz-utils
35 Suggested packages:
36   seccomp
37 The following NEW packages will be installed:
38   glibc-source libseccomp-dev xz-utils
39 0 upgraded, 3 newly installed, 0 to remove and 0 not upgraded.
40 Need to get 20.9 MB of archives.
41 After this operation, 27.6 MB of additional disk space will be used.
42 Get:1 http://deb.debian.org/debian bookworm/main amd64 xz-utils amd64 5.4.1-0.2 [471
43 Get:2 http://deb.debian.org/debian bookworm/main amd64 glibc-source all 2.36-9+deb12u4 [100
44 Get:3 http://deb.debian.org/debian bookworm/main amd64 libseccomp-dev amd64 2.5.4-1+deb12u4 [100
45 debconf: delaying package configuration, since apt-utils is not installed
46 Fetched 20.9 MB in 0s (88.5 MB/s)
47 Selecting previously unselected package xz-utils.
48 (Reading database ... 15610 files and directories currently installed.)
49 Preparing to unpack .../xz-utils_5.4.1-0.2_amd64.deb ...
50 Unpacking xz-utils (5.4.1-0.2) ...
51 Selecting previously unselected package glibc-source.
52 Preparing to unpack .../glibc-source_2.36-9+deb12u4_all.deb ...
53 Unpacking glibc-source (2.36-9+deb12u4) ...
54 Selecting previously unselected package libseccomp-dev:amd64.
55 Preparing to unpack .../libseccomp-dev_2.5.4-1+b3_amd64.deb ...
56 Unpacking libseccomp-dev:amd64 (2.5.4-1+b3) ...
57 Setting up libseccomp-dev:amd64 (2.5.4-1+b3) ...
58 Setting up glibc-source (2.36-9+deb12u4) ...
59 Setting up xz-utils (5.4.1-0.2) ...
60 update-alternatives: using /usr/bin/xz to provide /usr/bin/lzma (lzma) in auto mode
61 $ curl -sSL https://raw.githubusercontent.com/golangci/golangci-lint/master/install.sh | bash
62 golangci/golangci-lint info checking GitHub for tag 'v1.55.2'
63 golangci/golangci-lint info found version: 1.55.2 for v1.55.2/linux/amd64
64 golangci/golangci-lint info installed /go/bin/golangci-lint
65 $ make test-quality
66 golangci-lint --version
67 golangci-lint run --timeout="2m0s"
68 golangci-lint has version 1.55.2 built with go1.21.3 from e3c2265f on 2023-11-03T12:00:00Z
69 Cleaning up project directory and file based variables
70 Job succeeded

```

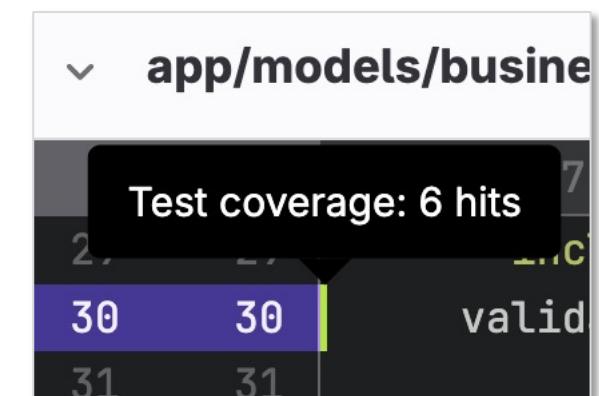
GitLab Test Coverage

A Merge Request's test coverage

 Merge request pipeline #730341552 passed

Merge request pipeline passed for a9d34d7c 1 year ago
 Test coverage 94.60% (0.10%) from 1 job [?](#)

Individual code changes' test coverage



Kubernetes Configuration

- Open-source Kubernetes configuration management
 - We use Kustomize to configure our Kubernetes deployments
- Key Benefits:
 - Define base configurations and use overlay configurations apply patches
 - Uses configuration inheritance to minimize redundant configuration
 - Easy integration with Kubernetes (kubectl)
 - Open-source

```
1  apiVersion: kustomize.config.k8s.io/v1beta1
2  kind: Kustomization
3
4  resources:
5    - deployment-app.yaml
6    - service.yaml
7    - serviceaccount.yaml
8    - stateful-sphinx.yaml
9
10 < configMapGenerator:
11   - name: nginx
12     files:
13       - configs/nginx/nginx.conf
14       - configs/nginx/security.conf
15       - configs/nginx/listen.conf
16   - name: rats-cfgs
17     files:
18       - configs/rats/ldap.yml
19   - name: sphinx-svc
20     files:
21       - configs/rats/thinking_sphinx.service.yml
22   - name: rats-scripts
23     files:
24       - scripts/migrate_index.bash
25       - scripts/prep_server.bash
26
27 < secretGenerator:
28   - name: rats-env
29     files:
30       - configs/rats/database.yml
31       - configs/rats/secrets.yml
32 < configurations:
33   - kustomizeconfig.yaml
34
35 < generatorOptions:
36   - labels:
37     app.kubernetes.io/component: configuration
```

Real Kustomize configuration example

Kustomize vs Helm: Key Differences

Kustomize

1. No Templates
2. Applies changes with patches and overlays

Pros

- Template free
- Configuration simplicity

Cons

- Fewer features

Helm

1. Uses templates
2. Uses values file to adjust settings in template

Pros

- Vast repository of preconfigured deployments
- More popular with 2.5x the stars on GitHub

Cons

- Steep learning curve

Why Migrate to Kustomize?

1. Strong control over Kubernetes ConfigMaps
2. We don't support many deployments
3. Attaches checksum to configurations to ensure configuration change
4. Simplified configuration

Harnessing the Power of GitOps with Argo CD

What is GitOps?

- Git driven operations
- Uses Git to define infrastructure
- Automates deployment and enables infrastructure version control

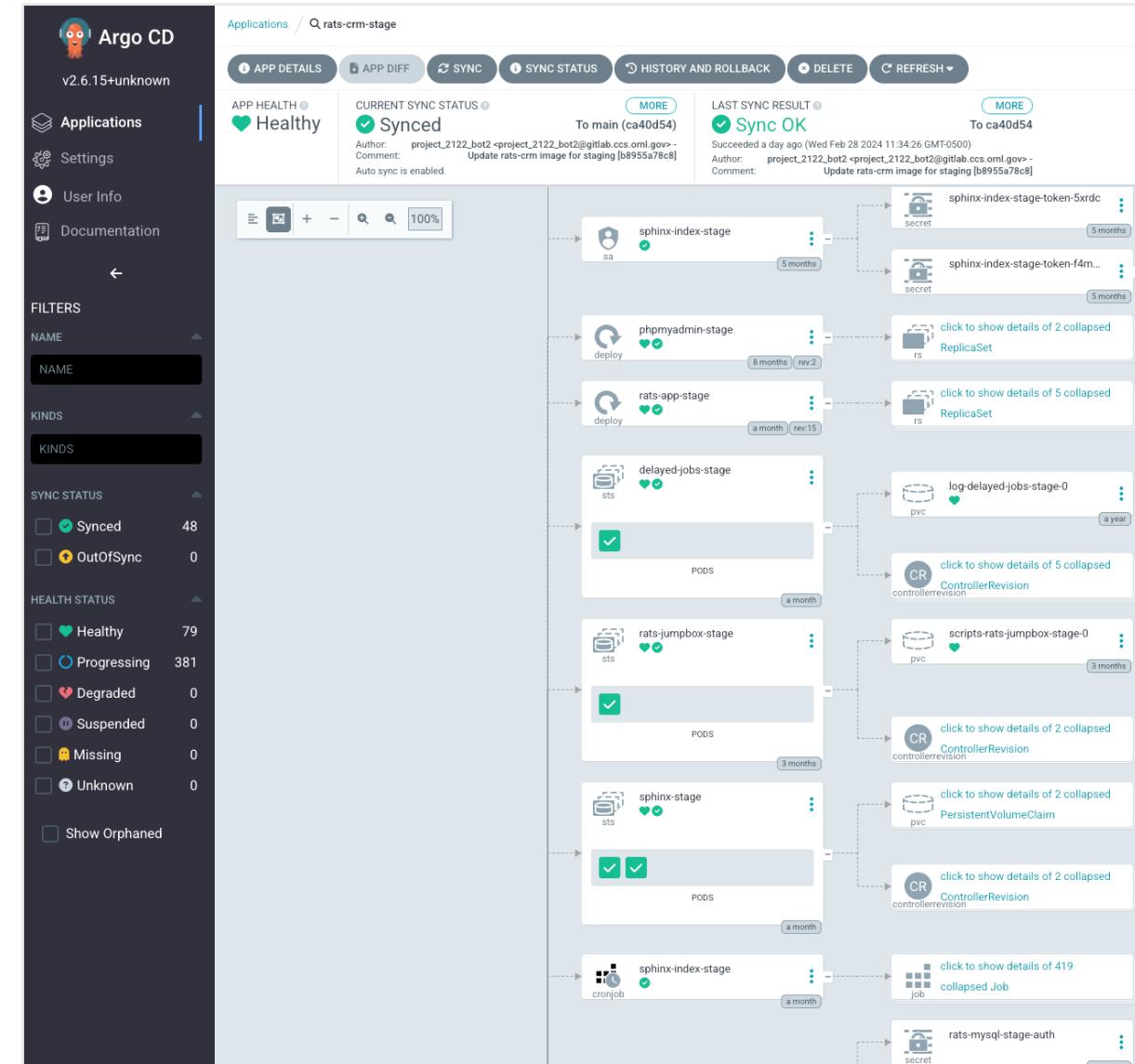
What is Argo CD?

- Our GitOps deployment tool
- It's a declarative continuous deployment for Kubernetes

Argo CD: Automated Kubernetes Deployment

Argo CD Key Features

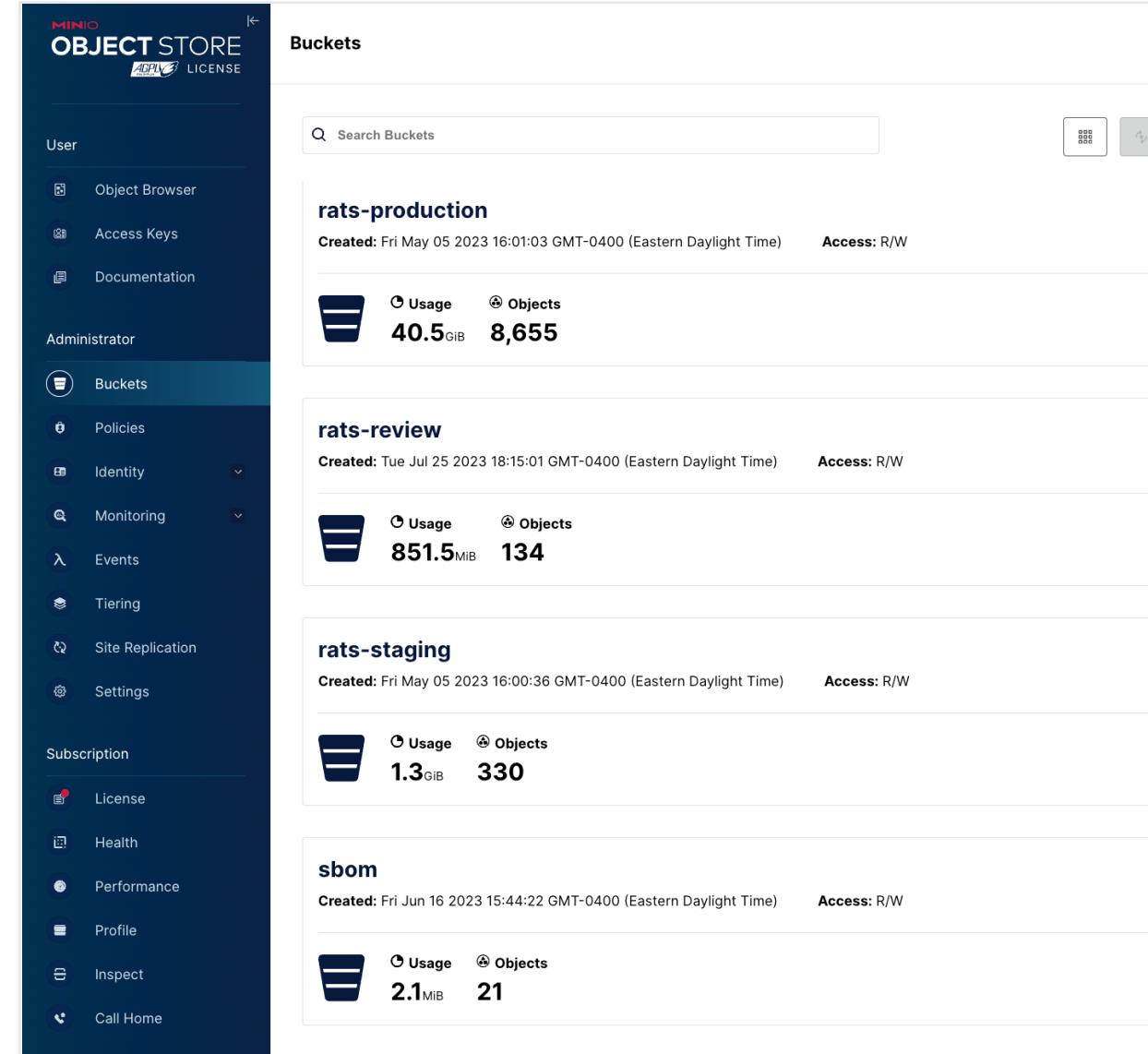
- Automatically syncs our applications to ensure desired state defined in our Kustomize configurations
- Provides a GUI for real-time monitoring and management of applications
- Provides us the ability to rollback and see our changes
- Automatically fixes drift



Argo CD: real partial view of RATS CRM

Cloud-native Object Store

- Offers scalable object storage with high performance and reliability
- We use MinIO for
 - Database backups
 - GitLab Runner cache
 - User-uploaded file storage
 - User-uploaded file backups
 - Internal application backups
 - Tracking Software Bills of Materials (SBOMs) for each release



Buckets

Search Buckets

rats-production
Created: Fri May 05 2023 16:01:03 GMT-0400 (Eastern Daylight Time) Access: R/W

Usage 40.5 GiB Objects 8,655

rats-review
Created: Tue Jul 25 2023 18:15:01 GMT-0400 (Eastern Daylight Time) Access: R/W

Usage 851.5 MiB Objects 134

rats-staging
Created: Fri May 05 2023 16:00:36 GMT-0400 (Eastern Daylight Time) Access: R/W

Usage 1.3 GiB Objects 330

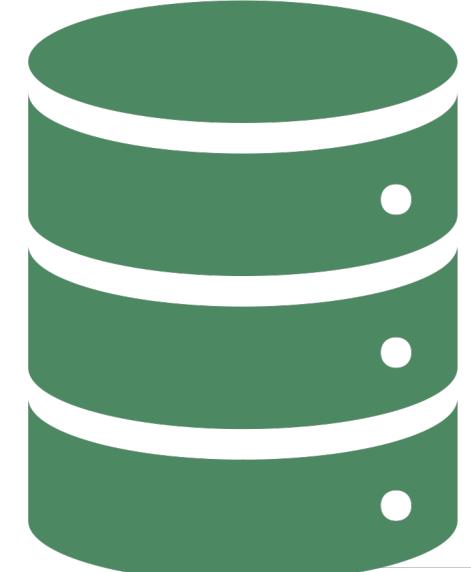
sbom
Created: Fri Jun 16 2023 15:44:22 GMT-0400 (Eastern Daylight Time) Access: R/W

Usage 2.1 MiB Objects 21

Real MinIO instance

KubeDB and Stash: Database Management

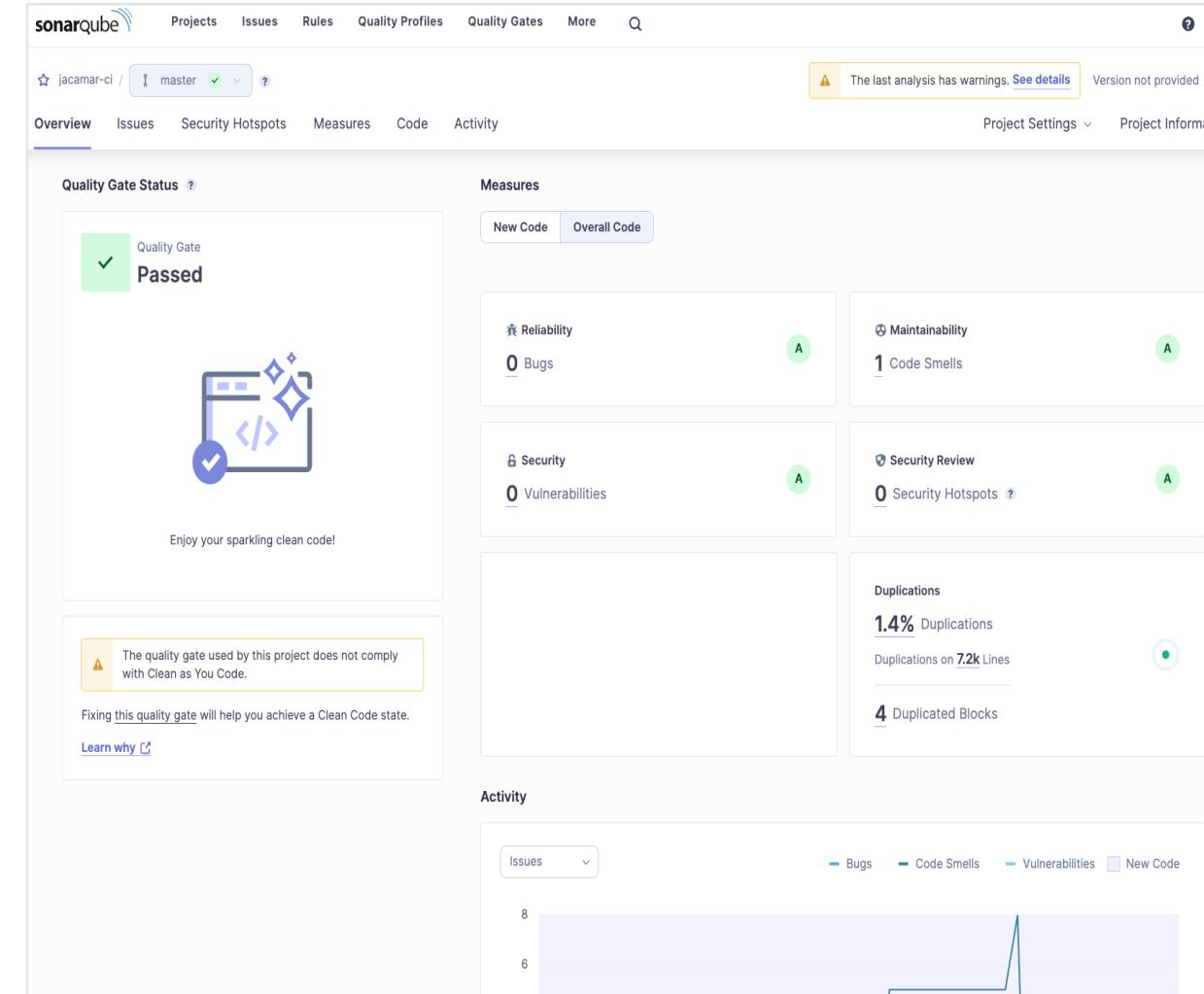
- KubeDB
 - Administrates the complete workflow for deploying and managing our databases on Kubernetes
- Stash
 - Provides us an easy data backup and recovery on Kubernetes
 - We use Stash in our review environment with heavily obfuscated data that we restore to our review deployment's database
- We integrate these services with Kustomize



SonarQube: Application Quality Assurance

Cloud-native Quality Assurance

- Integrated into our development GitLab pipelines
- Provides automated:
 - Code quality (“smells”) based on preset rules
 - Security vulnerability detection
- Provides timeline view of our project’s quality in several domains



View of Jacamar CI on real SonarQube instance

Note: the SonarQube data is from a public repository

HashiCorp Vault: Securing Digital Assets

Cloud-native Secure Secrets Store

- Open-source software for secure secret storage with versioned secrets and access management
- Our secrets are synced to our Kubernetes secrets
- Our software applications can access the secrets as environment variables

Store secrets in Vault

Set roles in Vault

Kubernetes uses service account to authenticate with Vault

Pod requests secrets from Vault based on matching namespace and project (e.g., TST001-prodci → rats-crm)

Secrets are injected and made available to the Kubernetes pod as environment variables

OLCF Acknowledgement

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Questions

