

Popper 2.0: A Container-Native Workflow Execution Engine For Testing Complex Applications and Reproducing Scientific Explorations

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Abstract—Software containers allow users to “bring their own environment” to shared computing platforms, reducing the friction between system administrators and their users. In recent years, multiple container runtimes have arisen, each addressing distinct needs (e.g. Singularity, Podman, rkt, among others), and an ongoing effort from the Linux Foundation (Open Container Initiative) is standardizing the specification of Linux container runtimes. While containers solve a big part of the “dependency hell” problem, there are scenarios where multi-container workflows are not fully addressed by existing runtimes or workflow engines. Current alternatives require a full scheduler (e.g. Kubernetes), a scientific workflow engine (e.g. Pegasus), or are constrained in the type of logic that users can express (e.g. Docker-compose). Ideally, users should be able to express workflows with the same user-friendliness and portability of `Dockerfiles` (write once, run anywhere). In this article, we introduce “Popper 2.0” a container-native workflow execution engine that allows users to express complex workflows similarly to how they do it in other scientific workflow languages, but with the advantage of running in container runtimes, bringing portability and ease of use to HPC scenarios. Popper 2.0 cleanly separates the three main concerns that are common in HPC scenarios: experimentation logic, environment preparation, and system configuration. To exemplify the suitability of the tool, we present three different case studies where we take examples from Machine Learning and HPC experiments and turn them into Popper workflows.

I. INTRODUCTION

Although Software (Linux) containers are a relatively old technology [1], it was not until recently, with the rise of Docker, that they entered mainstream territory [2]. Since then, this technology has transformed the way applications get deployed in shared infrastructures, with 25% of companies using this form of software deployment [3] (popularly termed as “cloud-native software development”), and a market size projected to be close to 5B by 2023 [4]. Docker has been the *de facto* container runtime, with other container runtimes such as Singularity [5], Charliecloud [6] and Podman¹ having emerged. The Linux Foundation bootstrapped the Open Container Initiative (OCI) [7] and is close to releasing version 1.0 of a container image and runtime specifications.

While containers solve a big part of the “dependency hell” problem [8], there are scenarios where a single container image is not suitable for implementing workflows associated to complex application testing or validating scientific explorations [9]. For example, a workflow might involve executing two

```
version: 1
steps:
- id: build
  uses: ./workflows/containerized/actions/normalmodes
  runs: ./workflows/containerized/scripts/build.sh
  env:
    PEVSL_MAKEFILE_IN: ./workflows/containerized/makeconf/pevsl_mkl.in
    NORMALMODES_MAKEFILE_IN: ./workflows/containerized/makeconf/NormalModes_mkl.in
    NUM_BUILD_JOBS: 1
- id: test
  uses: ./workflows/containerized/actions/normalmodes
  runs: ./workflows/containerized/scripts/test.sh
- id: run
  uses: ./workflows/containerized/actions/normalmodes
  runs: ./workflows/containerized/scripts/run.sh
  env:
    MPI_NUM_PROCESSES: 1
    INPUT_DIR: submodules/NormalModes/demos/
- id: validate
  uses: popperized/bin/sh@master
  runs: ./workflows/containerized/scripts/validate.sh
- id: generate vtk
  uses: docker://popperized/octave:4.4
  args: ./workflows/containerized/scripts/visualCmain.m
```

Figure 1: An end-to-end example of a workflow. On the left we have the `.yaml` file that defines the workflow. On the right, a pictorial representation of it.

steps, both of them requiring conflicting versions of a language runtime (e.g. Python 2.7 and Python 3.6). In this scenario, users could resort to solving such conflicts with the use of package managers, but this defeats the purpose of containers, which is to *not* have to do this sort of thing inside a container. More generally, the more complex a container image definition gets (a more complex `Dockerfile`), the more “monolithic” it gets, and thus the less maintainable and reusable it is. On the other hand, if an experimentation pipeline can be broken down into finer granular units, we end up having pieces of logic that are easier to maintain and reuse.

Through this paper, we propose a protocol in which a complex workflow is decomposed into several steps and each step executes in a separate container. This protocol is implemented through the tool called Popper, which follows a container-native strategy for building reproducible workflows easily. The tool is described in detail in section II. In section III, we present three case studies of how popper can be used to quickly reproduce complex workflows in different environments. From the point

¹<https://github.com/containers/libpod>

of view of UX design, this opens the possibility for devising languages to express multi-container workflows such as the one implemented in application testing and scientific study evaluations.

II. POPPER 2.0

In the remaining of this section we briefly expand on choosing YAML as the workflow specification language, as well as the design and implementation of the workflow execution engine (Popper 2.0); in particular, we dive into the container engine and the resource manager API layer.

A. Architecture

Here we describe the architecture or the dfd of popper

B. YAML as the workflow definition language

Here we show how yml serves better than other config languages

C. Workflow execution engine

Here we describe components of the workflow execution engine

- 1) **Command line interface (PopperCLI):** Here we talk about the features that PopperCLI provides.
- 2) **Workflow runner:** Here we talk about the work of the Workflow Runner
- 3) **Internal representation of the workflow:** Here we talk about how is the workflow interpreted internally
- 4) **Resource managers:** Here we talk about the functions of the resource manager
- 5) **Container runtimes:** Here we talk about the container runtimes.

III. CASE STUDY

A. Background

- 1) **Docker:** Here we talk about docker
- 2) **Singularity:** here we talk about singularity
- 3) **SLURM:** Here we talk about slurm
- 4) **Kubernetes:** Here we talk about Kubernetes
- 5) **CI Services:** Here we talk about some CI services

B. Execution Scenarios

Here we describe the 3 different execution scenarios

- 1) **Single-Node local workflow execution:** Single node workflow execution in the local machine for development purposes

- 2) **Workflow execution in the Cloud using Kubernetes:** Escalating the workflow execution to a GPU enabled cluster in the cloud for production grade execution
- 3) **Exascale workflow execution in SLURM clusters:** Planetscale workflow execution is super computing environments

IV. RESULTS

A. System Resource Usage

B. Overheads

V. RELATED WORK

Here we talk about other workflow execution solutions and how popper differentiates to them.

- 1) **Generic workflow execution engines:**
- 2) **Container native workflow execution engines:**
- 3) **Cloud native workflow execution engines:**
- 4) **Workflow definition languages:**

VI. CONCLUSION

A. Benefits

B. Challenges

C. Learning Curve

VII. FUTURE WORK

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