Predictive continuous testing to mitigate software collapse in scientific software

Samuel Grayson
University of Illinois Urbana-Champaign
Urbana, IL
0000-0001-5411-356X

Daniel S. Katz
University of Illinois Urbana-Champaign
Urbana, IL
0000-0001-5934-7525

Reed Milewicz
Sandia National Laboratories
Albuquerque, NM
rmilewi@sandia.gov

Darko Marinov
University of Illinois Urbana-Champaign
Urbana, IL
0000-0001-5023-3492

***Abstract*—Software tends to break or "collapse" over time, even if it is unchanged, due to non-obvious changes in the computational environment. Collapse in computational experiments undermines long-term credibility and hinders day-to-day operations. We propose to create the first public dataset of automatically executable scientific experiments. We explain how that data can be used to identify best practices, make continuous testing feasible, and repair broken programs, in order to increase the reproducibility of computational experiments.**

***Index Terms*—reproducibility; software reliability; continuous testing**

I. Introduction

Software tends to break over time, even if it is unchanged, due to non-obvious changes in the computational environment. This phenomenon is called "software collapse" [1], because software with an unstable foundation is analogous to a building with unstable foundation. Software collapse is not a significant problem in some domains; it is acceptable if Google returns slightly different results one day to the next. But in the scientific domain, software collapse could manifest as irreproducible or unreliable experiment[1], which not only undermine long-term credibility of science but also hinder its day-to-day operations.

1. **Undermines long-term credibility**: Computational experiments are widely used many scientific disciplines. More than 90% of scientists surveyed across all fields use research software and 50% develop software for their research experiments [4]. If computational experiments are allowed to collapse, scientists cannot independently verify or build on each others' results. This undermines two fundamental norms of science identified by Merton, organized skepticism and communalism [5], that make science self-correcting. In recent years, this has manifested itself as the ongoing reproducibility crisis[ˆrep-vs-rec] in computational science [6], which damages the long-term credibility of science [7].
2. **Hinders day-to-day operations**: Consider scientists tasked with securing their nations' nuclear stockpile. They might create a simulation that tests if a physical part is going to properly preform a critical function for nuclear storage. The physical part might last several decades, but the software often collapses much faster than that. As our understanding of material science improves, they might want to reassess if the simulation still predicts the part preforms its function properly given our improved understanding. If the simulation experienced software collapse, this will likely need to be fixed, despite the software not changing. Fixing the software may be difficult or impossible, especially if the original developer is retired.

Unfortunately, software collapse appears to be widespread in the computational science domain. Zhao et al. studied software collapse computational of experiments deposited in the myExperiment registry [8]. They found that 80% of the experiments in their selection did not work, for a variety of causes: change of third-party resources, unavailable example data, insufficient execution environment, and insufficient metadata; of these, change of third-party resources caused the most failures, such as when a step in an experiment referenced data from another server through the internet which was no longer available.

The problem of irreproducibility in scientific computing is not solely technical: the cultural norms around preserving scientific software and attitudes of funding agencies play

[1]In this article, we use Claerbout's terminology to define reproducibility [2]: one can execute the computational experiment in a different computational environment to get an approximately equivalent result. Reproducibility is called "replicability" by some authors; see Plesser [3] for a discussion of terminology. *Reliable* computational experiment, on the other hand, we define here as whether the computational experiment terminates successfully in a different computational environment. Reproducibility implies reliability, but not the other way around.

significant roles in the decision to invest in software sustainability and reproducibility. Our work examines technical solutions which should be part of a holistic effort to address policy, economic, and social factors that drive software collapse in science. Such a solution could be proactive or reactive: a *proactive solution* would control and preserve the environment or application in order to to ensure reproducibility as software ages, whereas a *reactive solution* would wait until reproducibility fails and try to fix that or alert human developers. The following are examples of state-of-the-art proactive tools:

- **Snapshotting the environment**: Container images (e.g., Docker), VM images, CDE [9], and Sumatra [10] attempt to snapshot the entire computational environment. Then, one can ship the entire filesystem to another user so they can reproduce the execution. However, this approach is heavyweight with filesystem snapshots as large as 50 Gb, as it needs to record a large chunk of the filesystem. Finally, these are difficult to modify and audit.
- **Specify environment in scripts**: `Dockerfile`s and shell scripts let the user specify instructions to construct the computational environment enclosing software. However, these instructions are UNIX commands, which can be non-deterministic themselves[2], e.g. `pip install`. Henkel et al. find 25% of Dockerfiles in their already limited sample still fail to build [11].

- **Specify environment in package managers:** Package managers such as Pip, Conda, Nix, Guix, Spack, etc. allow users to specify the computational environment to run their experiment, like a restricted form of scripting. However, the most common of these (Pip, Conda, and Nix) allow users to specify packages *without* pinning a specific version and require extra steps (often not taken!) to lock the versions. Even if the versions are uniquely pinned, data is often not distributed as a package but pulled from ephemeral resources on the internet,

[SAG: Cite work on reproducing Jupyter/IPython notebooks]

The most straightforward way to improve reproducibility is through proactive solutions[3], but none of these solutions can mitigate non-determinism due to network resources, pseudorandomness, and parallel program order. Zhao et al. showed that first of these, networked resources, is the most common cause of software collapse as well [8], so irreproducibility due to the network cannot be ignored. Therefore, important computational experiments should be protected from collapse by proactive *and* reactive solutions. Here are reactive solutions:

- **Continuous testing:** Automated systems can run the computational experiment periodically to assess if the experiment is both not crashing and still producing the same results. Continuous testing is robust to more sources of non-determinism, including networked resources, pseudorandomness, and parallel program order.[4] Traditional continuous testing is usually a part of continuous testing and continuous deployment (CI/CD). The continuous testing we are proposing here differs from traditional continuous testing in CI/CD because the former is triggered periodically while the latter it is triggered when the code is changed. The traditional continuous testing mitigates software regression, which is due to *internal changes*, but periodic continuous testing mitigates software collapse, which is due to *external changes*. The major drawback is increased computational cost. However, one can always trade off computational resources with latency of finding bugs by reducing the period. In addition to this, if one could predict which workflows were more likely to break, one could also prioritize testing on that basis, an optimization we term *predictive continuous testing*. [SAG: revise]

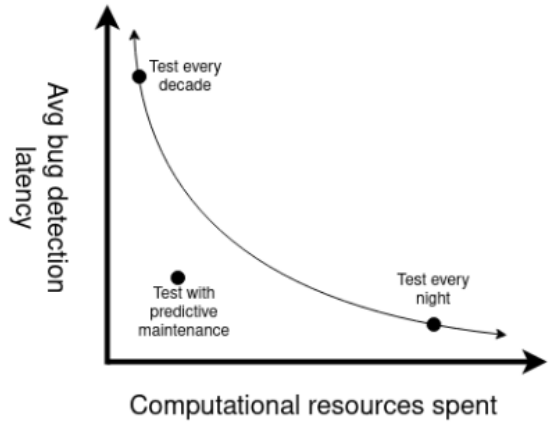

Figure 1: Predicting the rate of software collapse can reduce the resource utilization and increase efficacy of continuous testing.

- **Automatic program repair:** Automatic program repair seeks to encode solutions for common sources of errors. This has been done successfully in other domains [11][5].

[2]Although many people believe Docker gives them reproducibility [11], Docker itself never claims that `Dockerfile`s are reproducible; The term "reproducible" and "reproducibility" only occur three times in Docker's documentation at the time of this writing, and none of them are referring to reproducing the same result from running a `Dockerfile` twice. One occurrence references to ability to reproduce an environment on another machine by pulling the same container image, not by running the `Dockerfile` twice. Distributing the container image is described in the previous bullet.

[3]SAG: citations

[4]Non-determinism in the pseudorandom number generator and program schedule can be injected by the environment.

[5]SAG: cite automatic program repair

Hinsen suggests that most code should build on reliable, well-tested libraries can provide some degree of resistance to collapse [1]. In practice, many experiments fall into collapse despite their best effort to build on reliable foundations. If that level of reliability is insufficient, one can add continuous testing to help get more reliability.

[SAG: Explain why we need dataset (to improve reproducibility through continuous testing, automatic program repair, and identify best practices).]

This paper will build a dataset of software collapse of computational experiments and answer the following research questions:

- **RQ measure rate of software collapse:** What are typical rates of software collapse over time? This number is not well-known, since the last experiment to measure it was Zhao et al., and we have new reproducibility technology (NextFlow over Taverna).
- **RQ categorize causes of software collapse:** When software collapses, what is the immediate technical cause that collapse? Zhao et al. studies these at a high-level, and we plan to replicate those categories as well as delve into more subcategories. For example, when a third-party resource is unavailable, we will assess whether that resource is *data* or a *dependencies*.
- **RQ predict rate of software collapse:** Can we predict the rate of decay for a project based on its history (if available) and code? A predictive model is important for the next research question. The model should operate from a "cold start", where we know nothing about the computational experiments historical results, but also able to learn from historical executions if they are present.
- **RQ optimize continuous testing:** Can we improve the efficiency of continuous testing by predicting the rate of decay? This could be useful for intuitions, such as national labs, wanting to ensure their computational experiments remain valid while using resources efficiently.
- **RQ identify best practices:** What are the best practices that improve reproducibility? This lets us make recommendations that are empirically backed.
- **RQ attempt automatic repair:** In what fraction of the cases does automatic repair work? Automatic repair could let one run old workflows off-the-shelf with no modification.

II. Methods (Collecting data)

We plan to collect data on software collapse of computational experiments by automatically running computational experiments from public registries. These registries include:

- nf-core: *TODO: describe each of these (one sentence).*
- Dockstore
- Snakemake Catalog
- WorkflowHub
- myExperiment
- PegasusHub
- Globus Flows
- Sandia's internal repository

We cannot take one computational experiment and simulate it one, five, and ten years into the future. Instead, we will look for historical versions of an experiment from one, five, or ten years ago and simulate it today. All of the registries above store historical versions of the workflow. We make a *time symmetry* assumption: historical rates of change will be similar to the future rate of change. It is likely that some will still work and some sill fail, due to software collapse.

We will run the following pseudo-code to collect the data. Then we we will analyze it as described in the next section. Finally, we plan to publish the raw data we collect for other researchers.

```
for registry in registries:
    for experiment in registry:
        for version in experiment:
            for i in range(num_repetitions):
                execution = execute(version)
                data.append((
                    execution.date,   execution.output,
                    execution.logs,   execuiton.res_usage,
                    version.date,     version.code,
                    experiment.name,  registry.name,
                ))
```

III. Analysis

- **RQ measure rate of collapse:** We plan to replicate the experiment described by Zhao et al. [8], which assesses if the computational experiments are reproducible in our environment. To this, we add "reproducible results" as a new "level" of success, beyond merely not crashing (i.e. reliability). We will also study how the proportion of broken experiments changes with time. Note that a failure could indicate collapse, or it could indicate that the experiment never worked in the first place, possibly due to incomplete metadata. We can model this using a Bayesian framework that permits either possibility (never working or collapse) as an unobserved random variable.
- **RQ categorize causes of software collapse:** We will examine some of those workflows which not reliable or reproducible and classify their causes. While we would like to classify all of the workflows, this may not be practical. Instead we will analyze a random sample.
- **RQ predict rate of collapse:** We will develop predictive models based on the history of failures, staleness, properties of the code in the version, and other determinants to predict the probability that a given experiment will fail. We will use information

theory criteria to quantify the difference from our predicted distribution to the actual distribution.

- **RQ improve continuous testing:** We can improve resource utilization of continuous testing by using our dataset to predict the rate of collapse of various computational experiments. Testing experiments prone to failure more often than reliable ones could save computational resources while maintaining approximately the same degree of reliability in all experiments.
- **RQ identify best practices:** We can also use this data to identify practices that improve the reproducibility and longevity of computational experiments. We plan to examine choice of workflow manager, cyclomatic complexity, significant lines of code, choice of reproducibility tools (docker, `requirements.txt` with pinned packages, singularity), and other factors.
- **RQ5 attempt automatic repair:** Once we know what kinds of failure are possible, we can also investigate automatic repair. Our dataset will contain the output logs for each failure. Therefore, we can apply similar techniques to Shipwright [11], such as using a language model to categorize many failures into a few clusters.

A. Threats to Validity

There are a number of threats to the validity of our work and planned results.

1. Our time symmetry assumption may not hold. With contemporary efforts on reproducibility, future rates of change may be markedly less than past rates of change. While our computed rates of change will be underestimates, those underestimates can still be useful as bounds. Our method will also be useful, unchanged, for future studies.
2. It is possible that our sample is not representative of the real world of computational experiments. However, we are casting the widest net we can by systematically pulling many experiments from several registries. Still, there is a selection bias in which workflows end up in registries. The model has some factors based on the population and some based on the actual history of the experiment. Its initial guess when there is no history would be biased by our selection, but in the long run it would learn the characteristics of the actual experiment.

IV. Conclusion

Software collapse is an important yet understudied problem. We don't know the rate of software collapse in contemporary computational experiments. In order to do any research in this area, we need to build standard, communal datasets on software collapse.

The dataset would indicate how various reactive solutions compare, allowing us to identify the best practices that correlate with reproducibility. However, no proactive solution is perfect, so we also look at the reactive solution of continuous testing. The dataset would also allow us to optimize continuous testing such that it is feasible. Finally, when the continuous testing finds a failure, the automatic repair we plan to prototype would help fix that failure.

A. Future Work

There is a plethora of exciting future work to be done on this topic and with this dataset. Many studies of reproducibility such as Collberg and Proebsting [6], Zhao et al. [8], Henkel et al. [11] require a dataset of computational experiments with metadata that supports automatic execution. However, each had to construct their own datasets. This dataset mined from 6 community standard experimental registries could serve as a starting point for future research on reproducibility. Notably, our dataset will contain a distributin of the CPU time, RAM, and disk space needed to run the experiment, so researchers can make informed requests to batch schedulers (rather than guessing a constant runtime distribution for running unknown code).

One specific future work is the automatic scaling down of experiments. Some computational experiments are difficult to independently reproduce because they require HPC systems. If one could scale down the computational experiment automatically while perserving as much fidelity as posisble, anyone could test and verify the scaled-down model. Even if the results are off, this ensures that the experiment has no *logical problem*, and it can be taken to an HPC system with more confidence. This automatic scaling down might even prove useful for the original inquiry to simulate higher fidelity with fewer resources.

Another specific work is to tune the error thresholds on continuous results from computational experiments[6].

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