Targeting Real chemical accuracy at the EXascale

Introduction to Verificarlo CI

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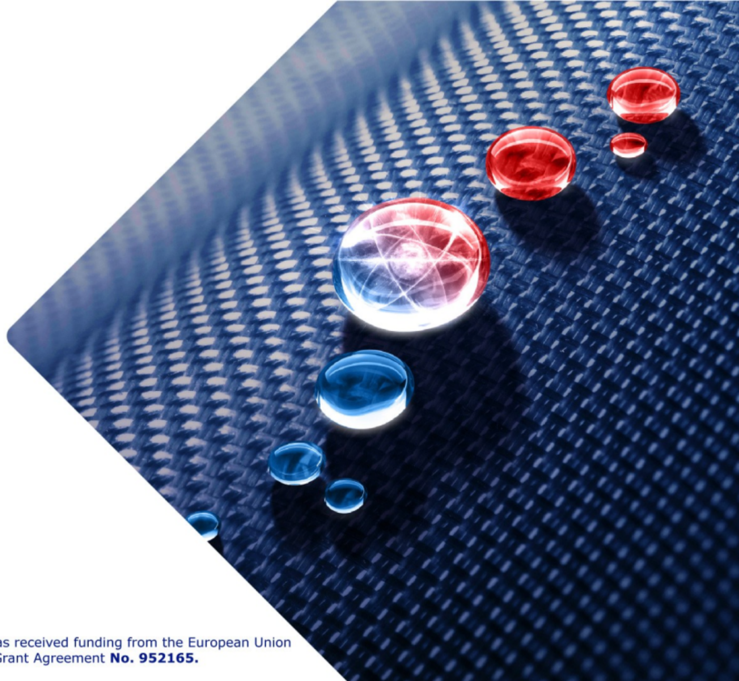
November 21, 2022



Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

Principle of Verificarlo CI

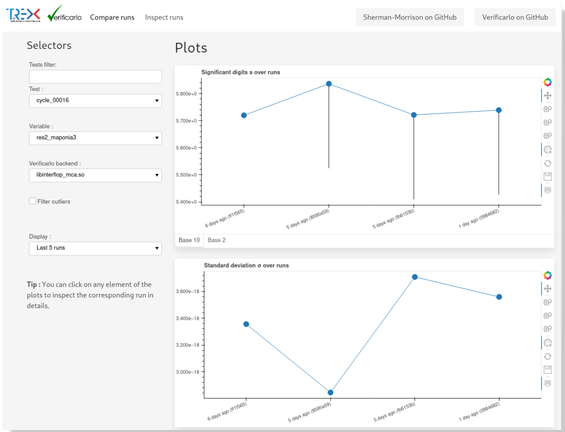
Verificarlo CI is a tool built on top of Verificarlo that lets its user :

- run
- automatize
- visualize

… custom Verificarlo tests.

These tests can be automatized with **Github Actions** or **Gitlab CI/CD**, and their results can then be visualized and shared in **HTML reports**.

Interpreting the report : ”Compare runs” mode



Selectors

Tests filter:

Test : cycle_00016

Variable : res2_maponia3

Verificarlo backend : libinterflop_mca.so

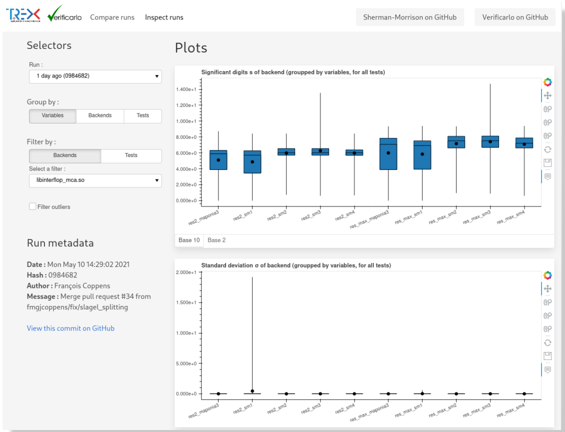
Filter outliers

Display : Last 5 runs

Tip : You can click on any element of the plots to inspect the corresponding run in details.

- Visualize evolution of **one variable over time** (commits)
- Shows significant digits s, standard deviation σ, variable distribution

Interpreting the report : ”Inspect runs” mode



Run : 1 day ago (0984682)

Group by : Variables | Backends | Tests

Filter by : Backends | Tests

Select a filter : libinterflop_mca.so

Filter outliers

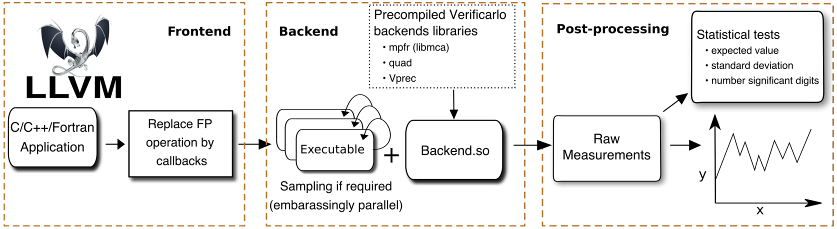
Run metadata

Date : Mon May 10 14:29:02 2021
Hash : 0984682
Author : François Coppens
Message : Merge pull request #34 from fmgjcoppens/fix/slagel_splitting

View this commit on GitHub

- Focus in depth on **one particular run**
- Different group by / filter by options
- For each group, shows distribution of s, σ and compute aggregated variable average

The Verificarlo CI pipeline



LLVM
Frontend
C/C++/Fortran Application
Replace FP operation by callbacks
Backend
Precompiled Verificarlo backends libraries
• mpfr (libmca)
• quad
• Vprec
Executable
+
Backend.so
Sampling if required (embarassingly parallel)
Post-processing
Raw Measurements
Statistical tests
• expected value
• standard deviation
• number significant digits
y
x

Verificarlo CI is integrated into Verificarlo as a **post-processing tool**.

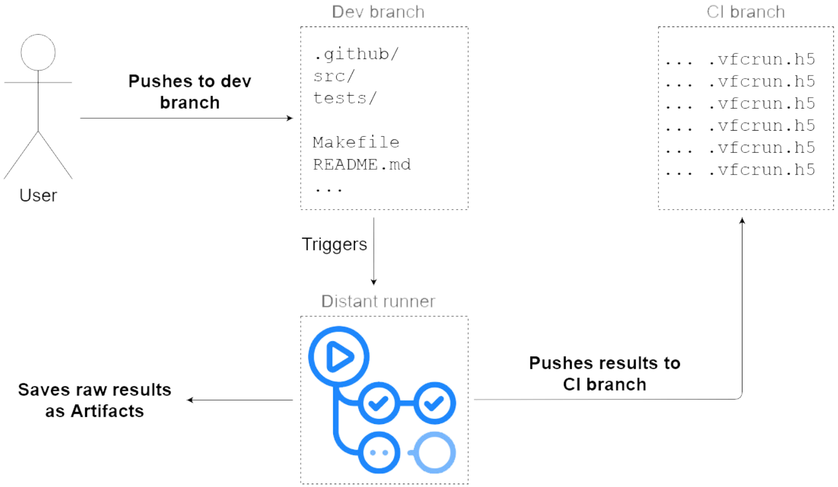
The Verificarlo CI pipeline

The CI integration pipeline relies on two different git branches :

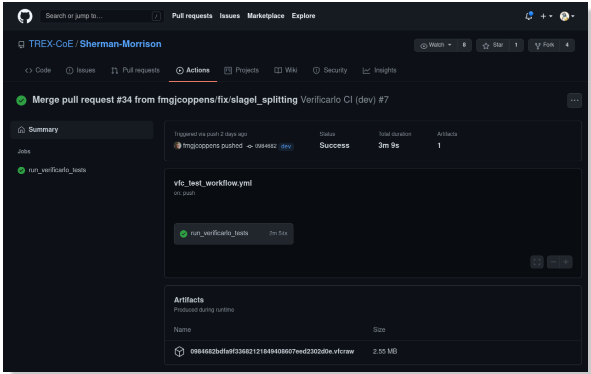
- **the ”dev” branch**, which is pre-existent and contains the project’s source code
- **the ”CI” branch**, which will be automatically be updated with result files, and is completely orphan of the dev branch

Note that while the tool has been **designed to integrate with git and CI systems**, it can still be used **completely independently**, simply as a way to visualize test results.

The Verificarlo CI pipeline



Description of the CI workflow



TREX-CoE / Sherman-Morrison

Merge pull request #34 from fmgjcoppens/fix/slagel_splitting Verificarlo CI (dev) #7

Triggered via push 2 days ago
fmgjcoppens pushed 0984682 dev

Status: Success
Total duration: 3m 9s
Artifacts: 1

Jobs
run_verificarlo_tests

vfc_test_workflow.yml
on: push

run_verificarlo_tests 2m 54s

Artifacts
Produced during runtime

Name	Size
0984682bdfa9f33682121849408607eed2302d0e.vfcraw	2.55 MB

- Workflow runs will be triggered **after each push** by default
- The CI branch will be **updated automatically**
- Raw results will be accessible as **Github Artifacts**
- The CI setup can be automated with the `vfc_ci setup` command

The probes system

In order to export test data from the programs to the tool itself, Verificarlo CI uses a **probes** system which allows the user to :

- **define test variables** (or *probes*) identified by a unique test name / variable name combination
- associate them with an **optional accuracy target** (absolute or relative)

... and **interfaces with Verificarlo CI** itself.

The probes system

- Here is a basic example where we want to store the value of var in a probe called varName belonging to a test testName in **C** :

```
vfc_probe(&probes, "testName", "varName", var);
```

- A **Fortran** interface is also provided using the *ISO_C_BINDING* module:

```
vfc_probe(probes,
"testName//C_NULL_CHAR",
"varName//C_NULL_CHAR",
 var);
```

The `vfc_ci` CLI

Verificarlo CI is accessed through a single command-line interface, *`vfc_ci`*. It provides 3 different subcommands :

- *`setup`* : an helper script to initialize the **CI workflow**
- *`test`* : start a **test run**
- *`serve`* : launch a server giving access to the **HTML report**

Tests configuration file

The *vfc_ci test* command manages the tests runs. It is configured with the *vfc_tests_config.json* file :

```
{
  "make_command": "make tests",
  "executables": [
    {
      "executable": "bin/test",
      "parameters" : "foo",
      "vfc_backends": [
        {
          "name": "libinterflop_mca.so --precision=53",
          "repetitions": 20
        }
    }, [...]
}
```

The `vfc_ci test` command

After executing the tests and gathering the results, the **postprocessing pipeline** is executed. For stochastic backends, we compute for each probe :

- the **empirical average** μ and the *standard deviation* σ
- the **number of significant digits** s_2, s_{10}
- the distribution's **quantiles**

The accuracy checks (with a target t) are evaluated as follows :

- if the check is **absolute**, $\sigma < t$?
- if the check is **relative**, $\frac{\sigma}{|\mu|} < t$?

To reproduce the tutorial: Links

- The **Verificarlo CI tutorial**, can be found at *`https://github.com/verificarlo/vfc_ci_tutorial`*
- For more details, the **Verificarlo CI documentation** can be found at *`https://github.com/verificarlo/verificarlo/blob/master/doc/06-Postprocessing.md#verificarlo-ci`*
- If you plan to use either Singularity or Docker, you will need to run the following script just before starting your server to update some Python packages (follow the instructions) : *`https://gist.github.com/PurplePachyderm/2ae9fedf7f458bdae7534adc0d5862e0`*

To reproduce the tutorial: Singularity

- If you plan to use the **Singularity image on CALMIP** while connecting with the VPN, you can set up port forwarding with :

```
> ssh -L [port]:127.0.0.1:[port]
-p 11300 [username]@127.0.0.1
```

- Then, to load the Verificarlo Singularity image:

```
> module load singularity
> singularity run /usr/local/trex/verificarlo/ver [...] .sif
```

To reproduce the tutorial: Docker

- If you plan to use the **Docker image**, you can download it and setup a container with port forwarding :

```
> docker pull verificarlo/verificarlo
> docker run -it -p [port]:[port]
verificarlo/verificarlo /bin/bash
```

- You can optionally set up a shared directory when creating the container:

```
-v [/path/to/host/dir]:[/path/to/docker/dir]
```