

Portable and Reproducible Benchmarking for Exascale Systems

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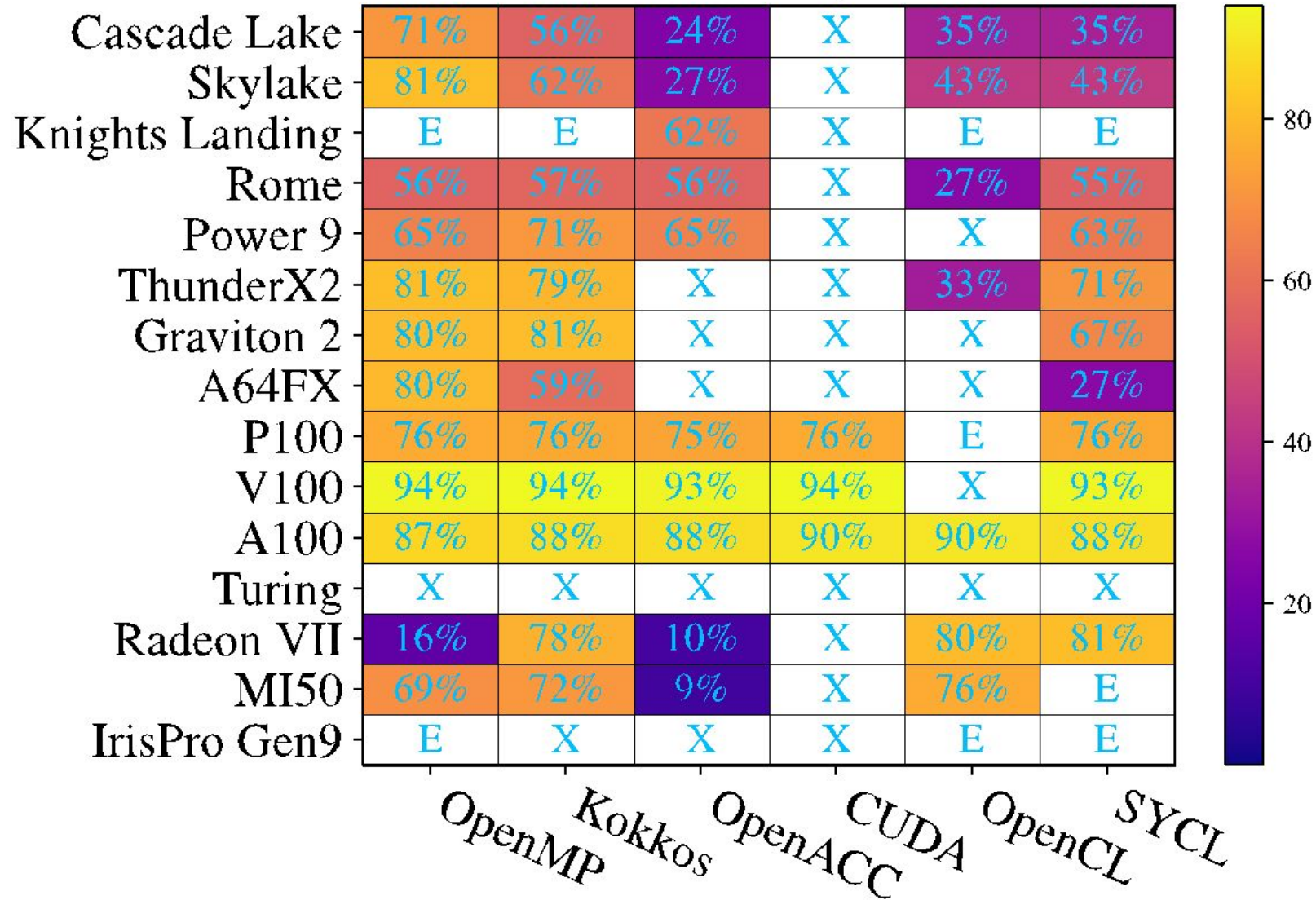
1 - Advanced Research Computing Centre, UCL

2 - Advanced Computer Systems, University of Bristol

3 - Computer Science, University of Reading

4 - Met Office

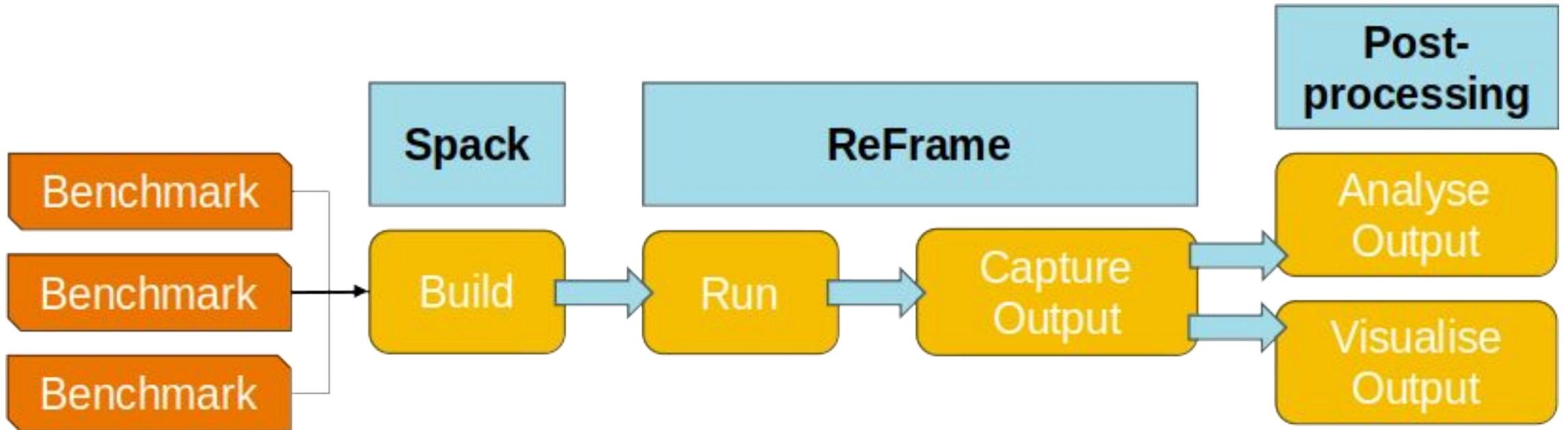
BabelStream Triad array size=2**29



Summary

- It's important to understand how our applications perform on different HPC architectures in order to make informed decisions about **future systems** and **future software**
- Benchmarking, as it's traditionally done, requires a lot of manual effort, is time-consuming, **error prone and difficult to reproduce**
- **Tools exist** in the community to automate the manual effort – recording and documenting in the process.
- We've developed a framework using **Spack** and **ReFrame** to automate portable building and running of benchmarks.
- There is an initial price to pay, but the increase in productivity should be **worth it!** More collaborators are welcome.

Building Blocks of a Benchmarking Workflow



ExCALIBUR Portable Benchmarking Framework v1.0.0



Framework for automating builds, runs and data collection of benchmarks across HPC systems

It contains

- ReFrame configuration and Spack environments for UK HPC systems
- Benchmark applications from collaborators
- Analysis and Visualisation tools
- Documentation and Tutorials
- Python packaging

It is **not**

- An authoritative collection of benchmarks
- A benchmarking campaign



<https://github.com/ukri-excalibur/excalibur-tests>

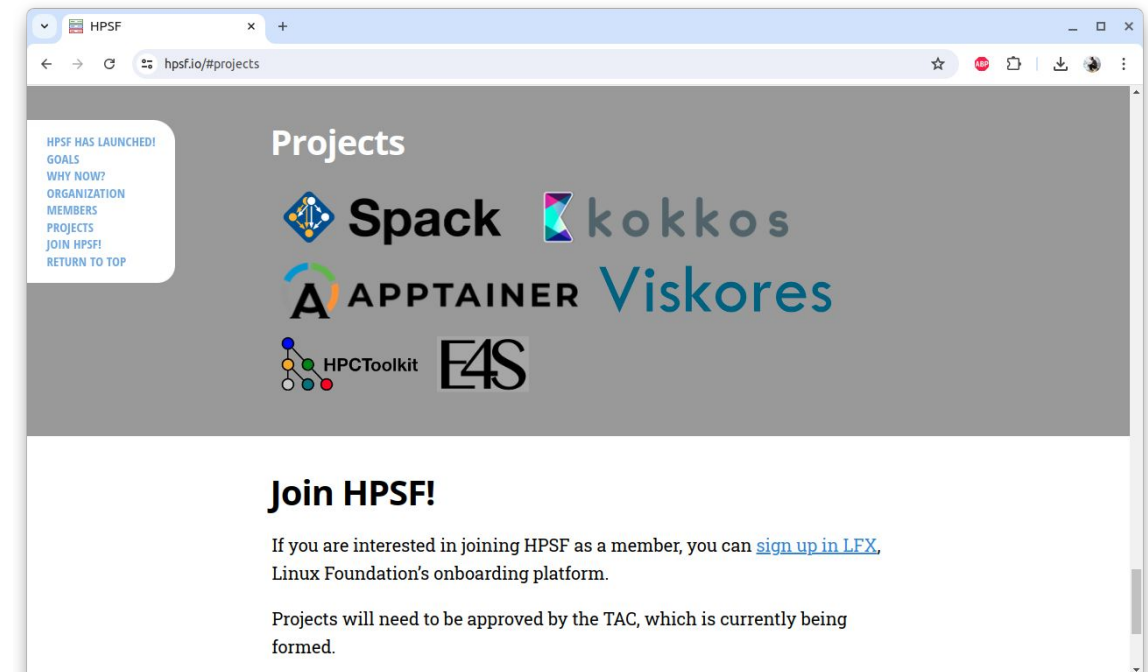
Using Spack for building benchmarks

Spack manages dependencies and automates builds

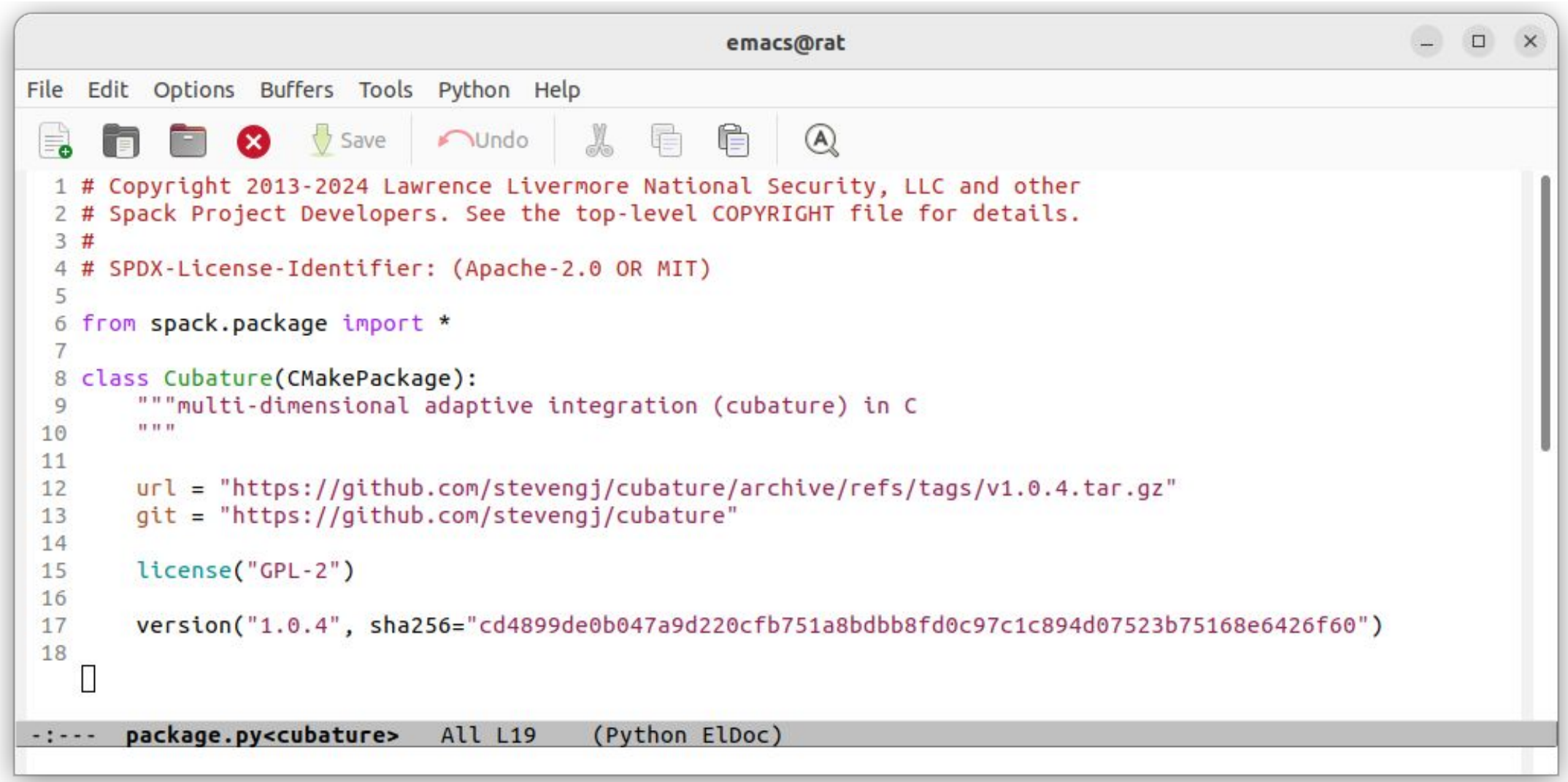
- Developed in US national labs, used heavily in ECP
- Supports a variety of build systems
- Build steps are recorded
- Maintains a repository of build recipes
- Customizable virtual environments
- Flexible python interface
- Easy to install and run with user permissions



github.com/spack/spack



Spack recipe example (1/2)

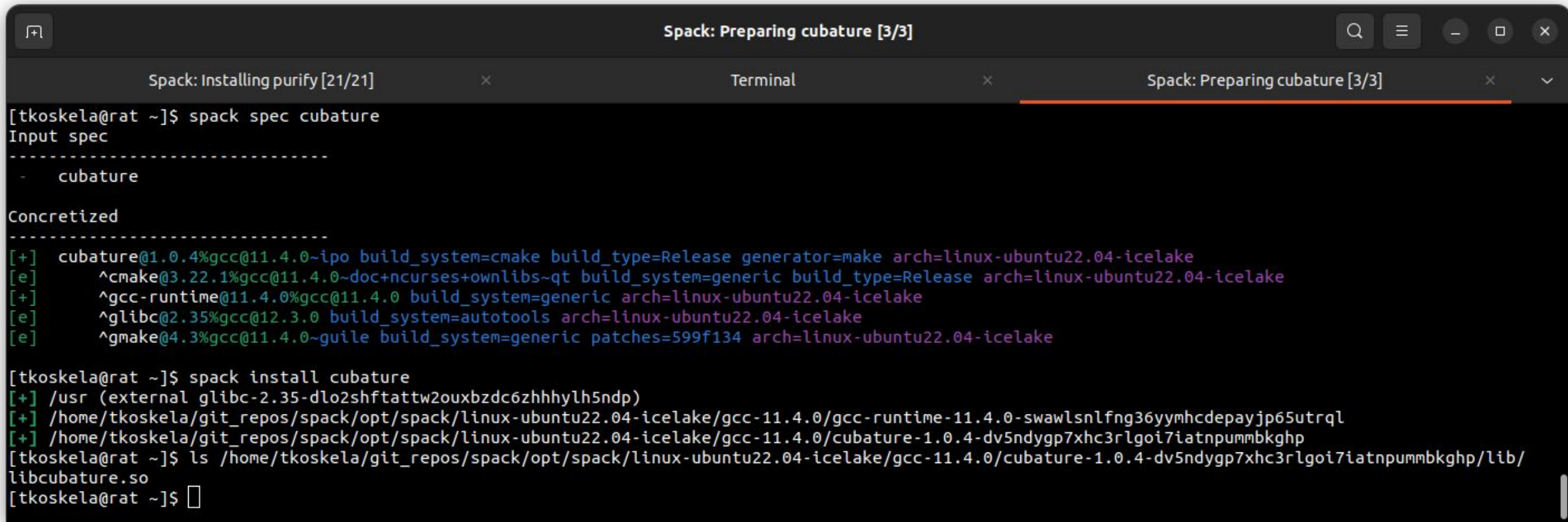


The screenshot shows an Emacs editor window titled 'emacs@rat'. The menu bar includes 'File', 'Edit', 'Options', 'Buffers', 'Tools', 'Python', and 'Help'. The toolbar contains icons for file operations (new, open, save, close), editing (undo, redo, cut, copy, paste), and search. The main text area displays a Python script for a Spack package recipe. The script includes copyright information, license details, and the package definition class 'Cubature' which inherits from 'CMakePackage'. The class defines the source URL, git repository, license, and version with a SHA256 checksum. The status bar at the bottom indicates the current file is 'package.py' for the 'cubature' package, at line 19, with Python syntax highlighting and ElDoc enabled.

```
1 # Copyright 2013-2024 Lawrence Livermore National Security, LLC and other
2 # Spack Project Developers. See the top-level COPYRIGHT file for details.
3 #
4 # SPDX-License-Identifier: (Apache-2.0 OR MIT)
5
6 from spack.package import *
7
8 class Cubature(CMakePackage):
9     """multi-dimensional adaptive integration (cubature) in C
10     """
11
12     url = "https://github.com/stevengj/cubature/archive/refs/tags/v1.0.4.tar.gz"
13     git = "https://github.com/stevengj/cubature"
14
15     license("GPL-2")
16
17     version("1.0.4", sha256="cd4899de0b047a9d220cfb751a8bdbb8fd0c97c1c894d07523b75168e6426f60")
18
19
```

-:--- package.py<cubature> All L19 (Python ElDoc)

Spack recipe example (2/2)



```
Spack: Preparing cubature [3/3]
Spack: Installing purify [21/21]
Terminal
Spack: Preparing cubature [3/3]

[tkoskela@rat ~]$ spack spec cubature
Input spec
-----
- cubature

Concretized
-----
[+] cubature@1.0.4%gcc@11.4.0~ipo build_system=cmake build_type=Release generator=make arch=linux-ubuntu22.04-icelake
[e]   ^cmake@3.22.1%gcc@11.4.0~doc+ncurses+ownlibs~qt build_system=generic build_type=Release arch=linux-ubuntu22.04-icelake
[+]   ^gcc-runtime@11.4.0%gcc@11.4.0 build_system=generic arch=linux-ubuntu22.04-icelake
[e]   ^glibc@2.35%gcc@12.3.0 build_system=autotools arch=linux-ubuntu22.04-icelake
[e]   ^gmake@4.3%gcc@11.4.0~guile build_system=generic patches=599f134 arch=linux-ubuntu22.04-icelake

[tkoskela@rat ~]$ spack install cubature
[+] /usr (external glibc-2.35-dlo2shftattw2ouxzbzdc6zhhyh5ndp)
[+] /home/tkoskela/git_repos/spack/opt/spack/linux-ubuntu22.04-icelake/gcc-11.4.0/gcc-runtime-11.4.0-swawlsnlfng36yymhcdepayjp65utrql
[+] /home/tkoskela/git_repos/spack/opt/spack/linux-ubuntu22.04-icelake/gcc-11.4.0/cubature-1.0.4-dv5ndygp7xhc3rlgoi7iatnpumbkgph
[tkoskela@rat ~]$ ls /home/tkoskela/git_repos/spack/opt/spack/linux-ubuntu22.04-icelake/gcc-11.4.0/cubature-1.0.4-dv5ndygp7xhc3rlgoi7iatnpumbkgph/lib/
libcubature.so
[tkoskela@rat ~]$
```


Using ReFrame for running performance benchmarks

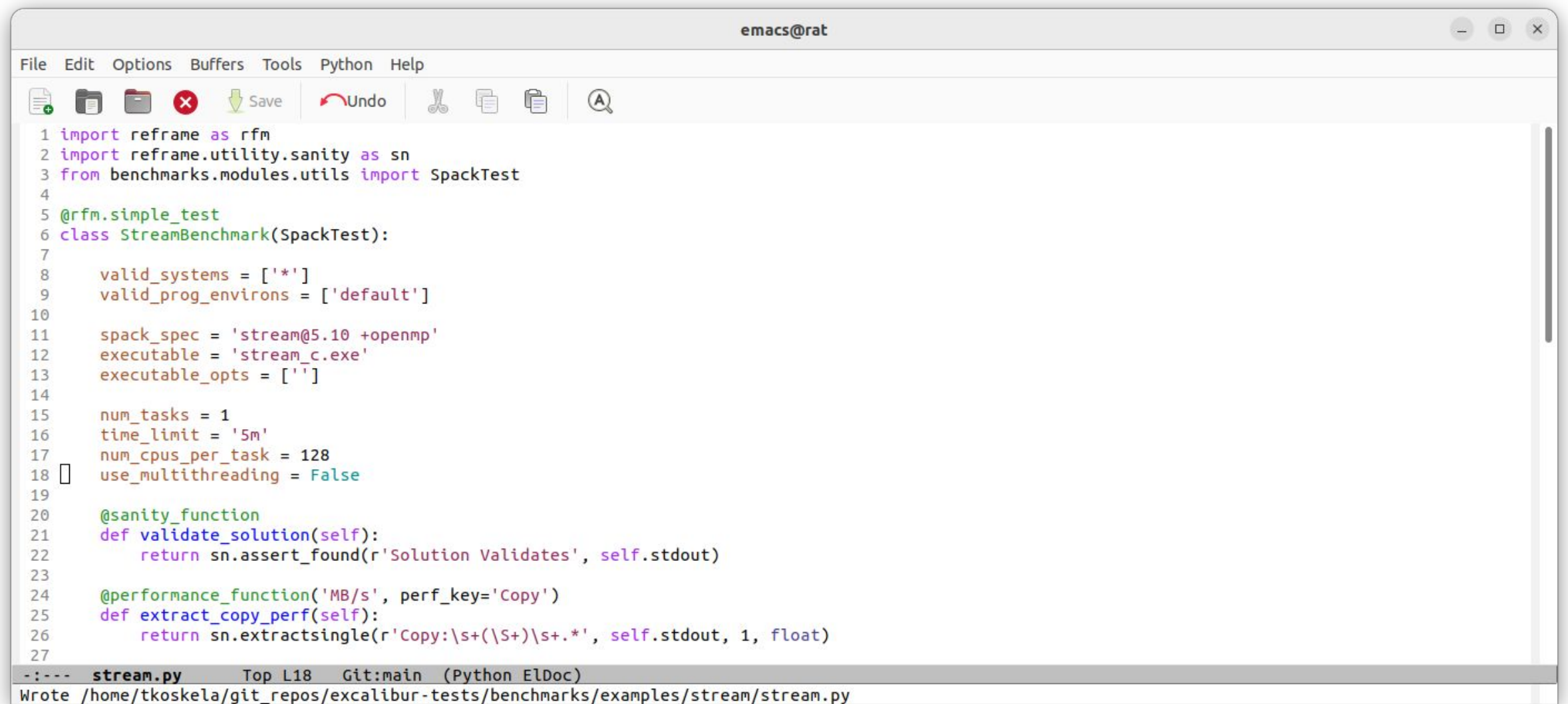
ReFrame

github.com/reframe-hpc/reframe

Framework for regression tests and benchmarks for HPC systems

- From CSCS and ETH Zurich
- Python interface to write benchmarks in a declarative way
- Abstracts interactions with the scheduler and build system
- Tailored for HPC systems
- Supports multidimensional test parametrisation
- Supports many build systems, integrates with spack
- Logs performance, helps keep records

ReFrame class example



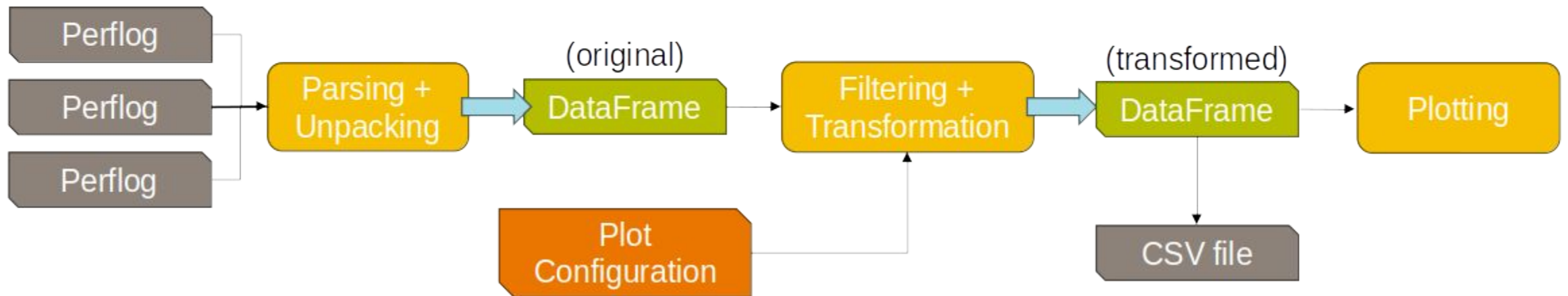
The screenshot shows an Emacs editor window titled 'emacs@rat'. The menu bar includes 'File', 'Edit', 'Options', 'Buffers', 'Tools', 'Python', and 'Help'. The toolbar contains icons for file operations (new, open, save, close), editing (undo, redo, cut, copy, paste), and search. The main text area displays a Python script for a ReFrame benchmark class named 'StreamBenchmark'. The script imports 'reframe as rfm', 'reframe.utility.sanity as sn', and 'from benchmarks.modules.utils import SpackTest'. It defines a class 'StreamBenchmark(SpackTest)' with attributes for 'valid_systems', 'valid_prog_environs', 'spack_spec', 'executable', and 'executable_opts'. It also sets 'num_tasks = 1', 'time_limit = '5m'', 'num_cpus_per_task = 128', and 'use_multithreading = False'. The class includes a '@sanity_function' decorator for 'validate_solution' and a '@performance_function' decorator for 'extract_copy_perf'. The status bar at the bottom shows the file path, line number (L18), and Git information.

```
1 import reframe as rfm
2 import reframe.utility.sanity as sn
3 from benchmarks.modules.utils import SpackTest
4
5 @rfm.simple_test
6 class StreamBenchmark(SpackTest):
7
8     valid_systems = ['*']
9     valid_prog_environs = ['default']
10
11     spack_spec = 'stream@5.10 +openmp'
12     executable = 'stream_c.exe'
13     executable_opts = []
14
15     num_tasks = 1
16     time_limit = '5m'
17     num_cpus_per_task = 128
18     use_multithreading = False
19
20     @sanity_function
21     def validate_solution(self):
22         return sn.assert_found(r'Solution Validates', self.stdout)
23
24     @performance_function('MB/s', perf_key='Copy')
25     def extract_copy_perf(self):
26         return sn.extractsingle(r'Copy:\s+(\S+)\s+.*', self.stdout, 1, float)
27
28 --- stream.py      Top L18   Git:main (Python ElDoc)
Wrote /home/tkoskela/git_repos/excalibur-tests/benchmarks/examples/stream/stream.py
```

Analysis and Visualisation Workflow

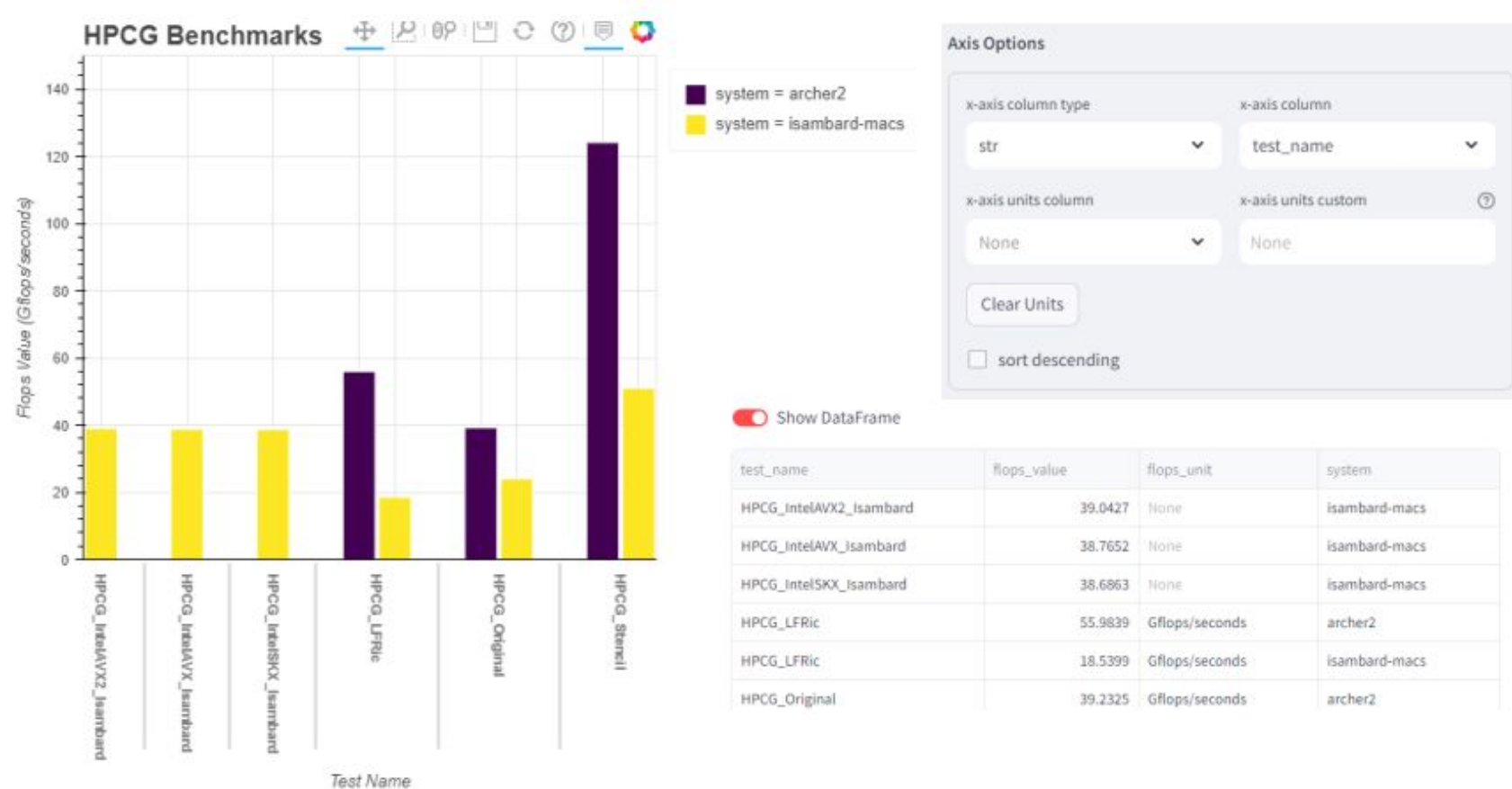


```
python post_processing.py log_path config_path
```



Visualisation GUI

- Post-processing can be run as a web app via **Streamlit**.
- Plot config is now an optional argument because it can be created from scratch in the UI.



Future Plans

- Maintain the suite and support benchmark and system additions.
- Post-processing feature development
- Systematic deployment – include framework as CI on key HPC systems
- Platform for hosting data – curate and store benchmark results

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Thanks! (Demo)



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