Benchpark and Ramble Tutorial

Ramble

HPCIC Tutorial Series

September 3, 2025

HIGH PERFORMANCE COMPUTING
INNOVATION CENTER

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Prepared by LLNL under Contract DE-AC52-07NA27344.

Tutorial Presenters

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LLNL

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Tutorial Agenda (approximate)

Welcome and Introduction	All	10 min
Benchpark Overview and Basics Hands on: Running an experiment, analyzing performance of a scaling study	Olga	75 min
Ramble Overview and Basics	Doug	25 min
Benchpark System and Experiment Specifications Hands on: Writing an experiment in Benchpark	Olga	60 min
Q&A and Wrap-up	All	10 min

Ramble

Tutorial Materials

Find these slides and associated scripts here:

software.llnl.gov/benchpark/basic-tutorial.html

We also have a channel on Spack slack.
You can join here:

slack.spack.io

Join the **#benchpark-support** channel!

You can continue to ask questions here after the tutorial has ended.

Tutorial Instances: http://bit.ly/4kGQDlc

- We have an AWS instance for the hands-on component of this tutorial
- The instance provides:
  - Pre-installed Benchpark and required dependencies
  - Job scheduler

When logging in to the instance:

- Please use a unique username to avoid resource allocation conflicts
  - First initial followed by last name (e.g., John Doe would be jdoe)
- PW: hpctutorial25

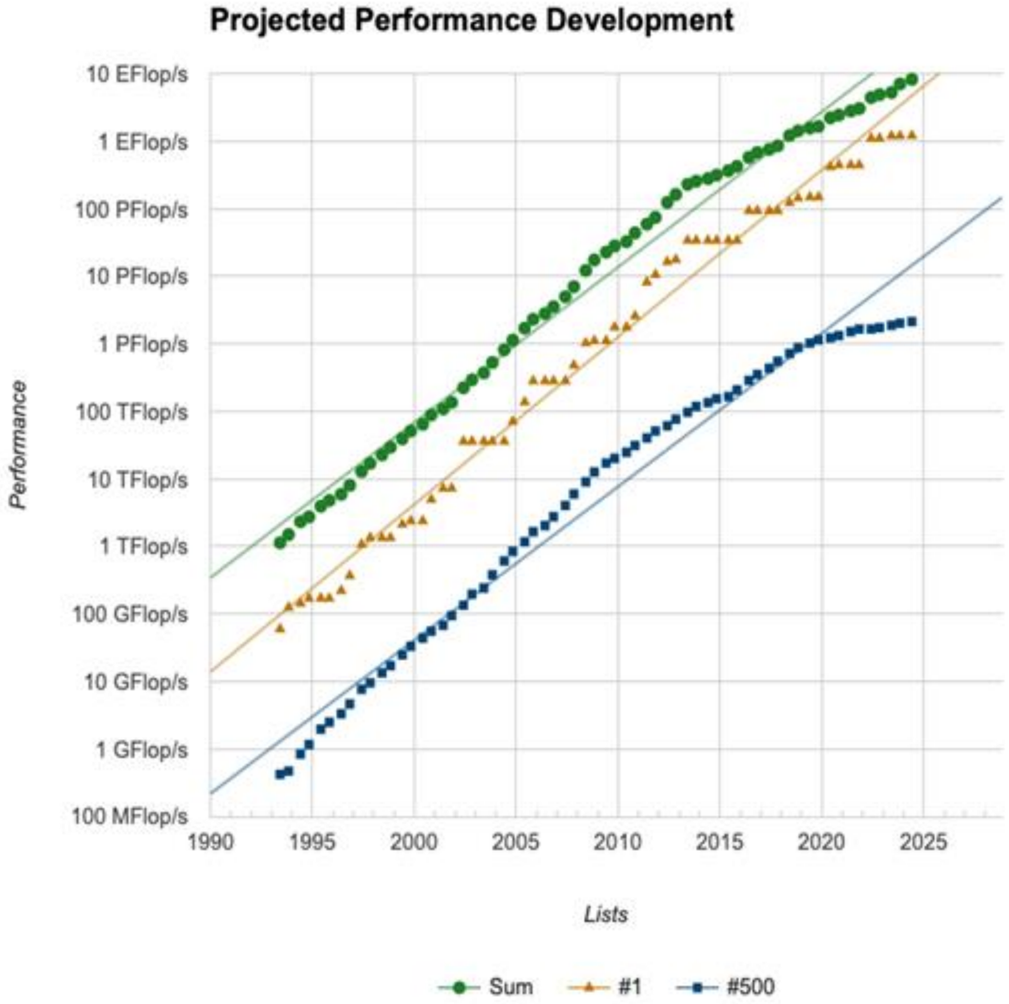
We benchmark HPC systems for many reasons

- Procurements
  - Communicate datacenter workload to vendors
  - Co-design systems, monitor progress
  - System acceptance (contractual specification)
- Validation of software stack, tools
  - Compilers
  - Debuggers
  - Correctness tools
  - Performance tools
- Research
  - Programming models
  - Computational methods
  - Performance across architectures

Benchmarking is challenging

Source: https://www.top500.org/statistics/perfdevel/

- What are we trying to characterize?
- Are we capturing the best the system can do?
- Is something else impacting performance?
- Did we build and run the code in the optimal and reproducible way?



HPC benchmarks run on diverse HPC hardware

Perlmutter
Lawrence Berkeley Nat'l Lab
AMD Zen + NVIDIA

Fugaku
RIKEN **Fujitsu ARM a64fx**

Sierra
Lawrence Livermore Nat'l Lab
IBM Power9 + NVIDIA

El Capitan
Lawrence Livermore Nat'l Lab
AMD Zen + Radeon

Frontier
Oak Ridge National Lab
AMD Zen + Radeon

Aurora
Argonne National Lab
Intel Xeon + Xe

- Benchmark source code
  - Abstraction (OpenMP, RAJA, Kokkos)
  - Hardware-specific (CUDA, ROCm)
- Optimized code for the CPU and GPU
  - Must make effective use of the hardware
  - Can make 10-100x performance difference
- Rely heavily on system packages
  - Need to use optimized communication and MPI libraries that come with machines

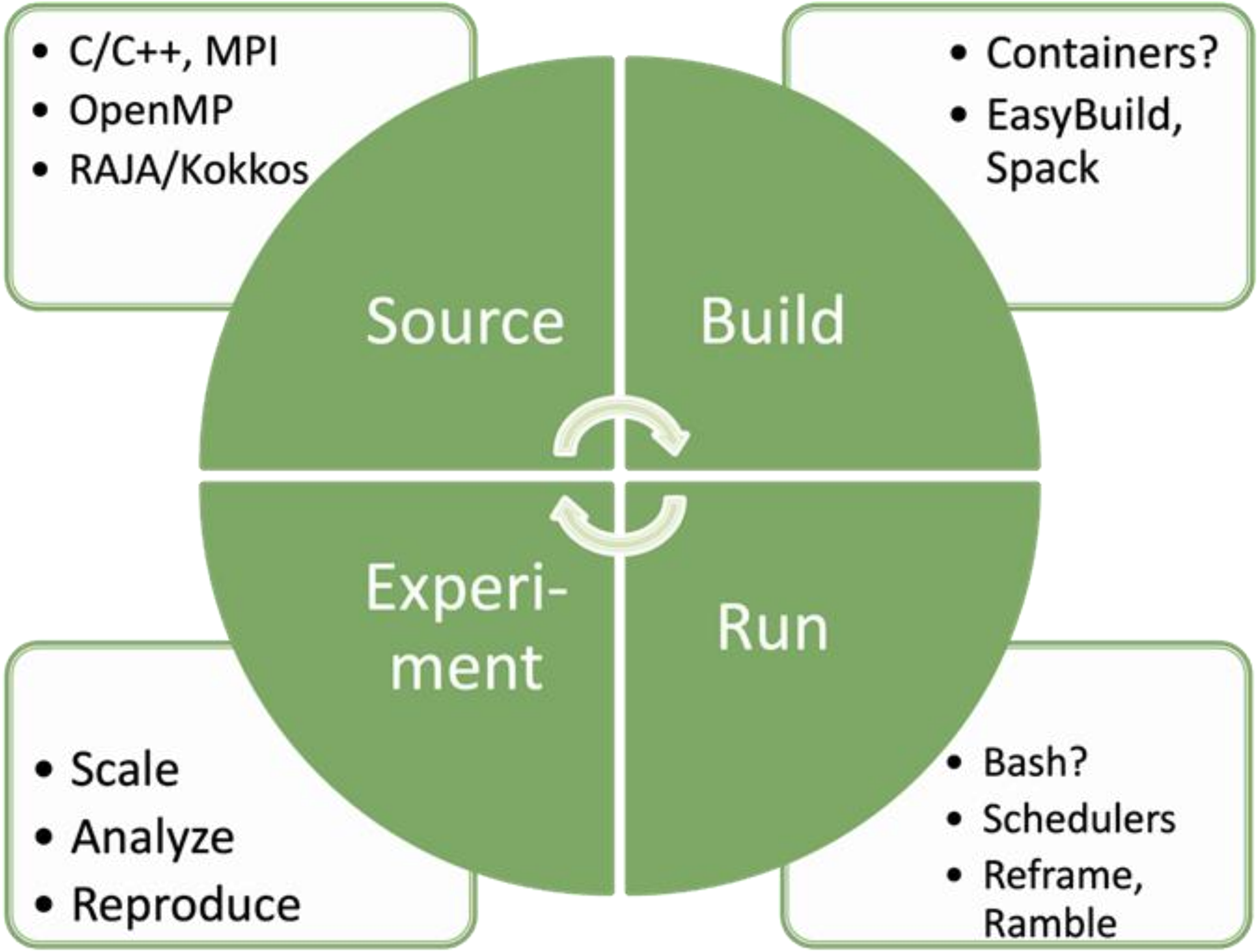
Writing benchmark source code is only the beginning

State-of-the-practice:
HPC system benchmarking is manual!

- Building on each system is different, porting the builds to new systems is manual
- Running on each system is different, porting run scripts to new systems is manual
- Systems keep changing, requiring updates to how we build and run benchmarks
- Triggering builds and runs is manual: benchmark results don't stay up to date
- Performance analysis of results is manual

HPC benchmarks are HPC software

- Portability
- Maintenance
- Testing/CI
- Verification
- Reproducibility



All components must work for your system, focus on explainable performance

Benchpark enables complete specification of HPC benchmarks

Infrastructure-as-code benchmark specification codifies:

- Benchmark build and run instructions
- HPC Systems
- HPC Experiments

Leverage advances in HPC automation

- Source code
- Build specification
- Run specification
- CI

github.com/llnl/benchpark

RUNNER

Ramble

Spack

Every part of the specification is codified: used to communicate, automate

Benchpark enables reproducible specifications of benchmarks

Specify
- How to build and run benchmarks on a system

Run
- Run an experiment on a system

Reproduce
- Re-run an experiment on a system

Replicate
- Run an experiment on a new system

Maintain
- CI: Run experiment on HPC systems

Record
- Perf.measu-rements + *full spec* of experiment

Full specification enables reproducibility, replicability, and automation

HPC System definition for *Performance*

- Resources (CPU cores, GPUs)
- Scheduler (Slurm, flux)
- Process mapping (cores, sockets, GPUs, NICs)
- On-node parallelism (CUDA, ROCM, OpenMP)
- Software stack
  - Compilers (which is best?)
  - MPI implementations (best?)
  - Math libraries

HPC System in Benchpark: *Specify Once*

- systems
  - all_hardware_descriptions
  - aws-pcluster
  - generic-x86
  - lanl-venado
  - llnl-cluster
  - llnl-elcapitan
  - llnl-sierra
  - riken-fugaku

```
class LlnlElcapitan(System):
    variant(
        "rocm",
        default="5.5.1",
        values=("5.4.3", "5.5.1", ”6.2.4"),
        description="ROCm version",
    )
    variant(
        "compiler",
        default="cce",
        values=("gcc", "cce", "rocmcc"),
        description="Which compiler to use",
    )
    def initialize(self):
        super().initialize()
        self.scheduler = "flux”
        self.sys_cores_per_node = "128”
        self.sys_gpus_per_node = "4”
```

benchpark system init --dest=elcap llnl-elcapitan rocm=6.4.2 compiler=cce

System Specifications

The table below provides a directory of information for systems that have been specified in Benchpark. The column headers in the table below are available for use as the `system` parameter in `benchpark setup`.

Search:

name	integrator.vendor	integrator.name	processor.vendor	processor.name	processor.ISA	processor.u
Atos-zen2-A100-Infiniband	Atos	XH2000	AMD	EPYC-Zen2	x86_64	zen2
AWS_PCluster-zen-EFA	AWS	ParallelCluster	AMD	EPYC-Zen	x86_64	zen
DELL-cascadelake-InfiniBand	DELL		Intel	Xeon6248R	x86_64	cascadelake
DELL-sapphirerapids-OmniPath	DELLEMC	PowerEdge	Intel	XeonPlatinum8480	x86_64	sapphirerapi
Fujitsu-A64FX-TofuD	Fujitsu	FX1000	Fujitsu	A64FX	Armv8.2-A-SVE	aarch64
HPECray-haswell-P100-Infiniband	HPECray		Intel	Xeon-E5-2650v3	x86_64	haswell
HPECray-neoverse-H100-Slingshot	HPECray	EX254n	NVIDIA	Grace	Armv9	neoverse
HPECray-zen2-Slingshot	HPECray		AMD	EPYC-7742	x86_64	zen2
HPECray-zen3-MI250X-Slingshot	HPECray	EX235a	AMD	EPYC-Zen3	x86_64	zen3
HPECray-zen4-MI300A-Slingshot	HPECray	EX255a	AMD	EPYC-Zen4	x86_64	zen4
IBM-power9-V100-Infiniband	IBM	AC922	IBM	POWER9	ppc64le	power9
Penguin-icelake-OmniPath	PenguinComputing	RelionCluster	Intel	XeonPlatinum924248C	x86_64	icelake
Supermicro-icelake-OmniPath	Supermicro		Intel	XeonPlatinum8276L	x86_64	icelake
x86_64					x86_64	

HPC systems in Benchpark: July 2025

- 4 in Europe
- 6 in US labs
- 1 in Japan
- 1 at a university
- 2 cloud systems

- all_hardware_descriptions
- aws-pcluster
- common
- csc-lumi
- cscs-daint
- cscs-eiger
- generic-x86
- jsc-juwels
- lanl-venado
- llnl-cluster
- llnl-elcapitan
- llnl-sierra
- riken-fugaku

HPC Experiment definition for *Performance*

- On-node parallelism (CUDA, ROCM, OpenMP)
- Problem sizes
  - Overall problem size, or
  - Per node or per GPU
- Scaling studies
  - How to scale
  - How to decompose
- Resources (cores, GPUs)

Goal: Specify reproducible sets of experiments that map onto specific systems

HPC Experiment in Benchpark: Specify Once

```
class Amg2023(Experiment, OpenMPExperiment, CudaExperiment, ROCmExperiment,
              Scaling(ScalingMode.Strong, ScalingMode.Weak, ScalingMode.Throughput,
               Caliper):
    variant(
        "workload",
        default="problem1",
        values=("problem1", "problem2"),
        description="problem1 or problem2",
    )

    def compute_applications_section(self):
         self.register_scaling_config({
              ScalingMode.Strong: {
                   “n_resources”: lambda var, itr, dim, scaling_factor: var.val(dim) * scale,
                   “problem_size”: lambda var, itr, dim, scaling_factor: var.val(dim) // scale,
              },
              ScalingMode.Weak: {
                   “n_resources”: lambda var, itr, dim, scaling_factor: var.val(dim) * scale,
                   “problem_size”: lambda var, itr, dim, scaling_factor: var.val(dim),
              },
              ScalingMode.Throughput: {
                   “n_resources”: lambda var, itr, dim, scaling_factor: var.val(dim),
```

benchpark experiment init --dest=amg amg2023 +rocm +strong workload=problem2 caliper=mpi,time --system=<system>

Benchmarks and Experiments

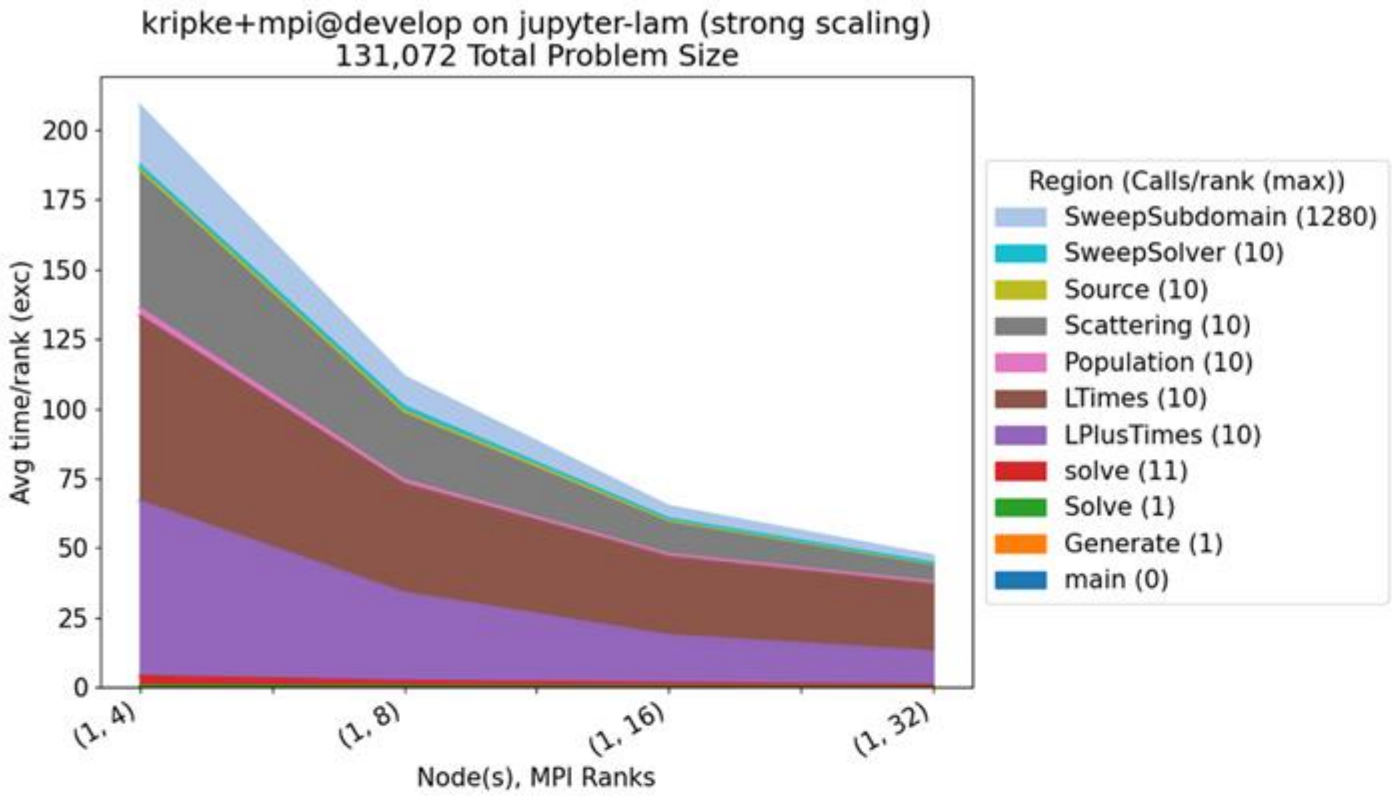
	hpl	hpcg	qws
application-domain	['synthetic']	['synthetic']	['qcc
benchmark-scale	['large-scale']	['large-scale']	['we
communication	['mpi']	['mpi']	['mp
communication-performance-characteristics	['network-collectives', 'network-point-to-point']	['network-point-to-point']	[]
compute-performance-characteristics	[]	[]	[]
math-libraries	['blas']	[]	[]
memory-access-characteristics	[]	[]	[]
mesh-representation	[]	[]	[]
method-type	['dense-linear-algebra', 'solver']	['conjugate-gradient', 'solver', 'sparse-linear-algebra']	[]
programming-language	['c']	['c++']	['c++
programming-model	[]	['openmp']	[]

Experiments in Benchpark: July 2025

- experiments
  - ad
  - amg2023
  - babelstream
  - genesis
  - gpcnet
  - gromacs
  - hpcg
  - hpl
  - ior
  - kripke
  - laghos
  - lammps
  - md-test
  - osu-micro-benchmarks
  - phloem
  - quicksilver
  - qws
  - raja-perf
  - remhos
  - salmon-tddft
  - saxpy
  - smb
  - stream

- HPL, HPCG
- 4 microbenchmarks
- 3 MPI benchmarks
- 8 US, 1 Europe, 2 Japan

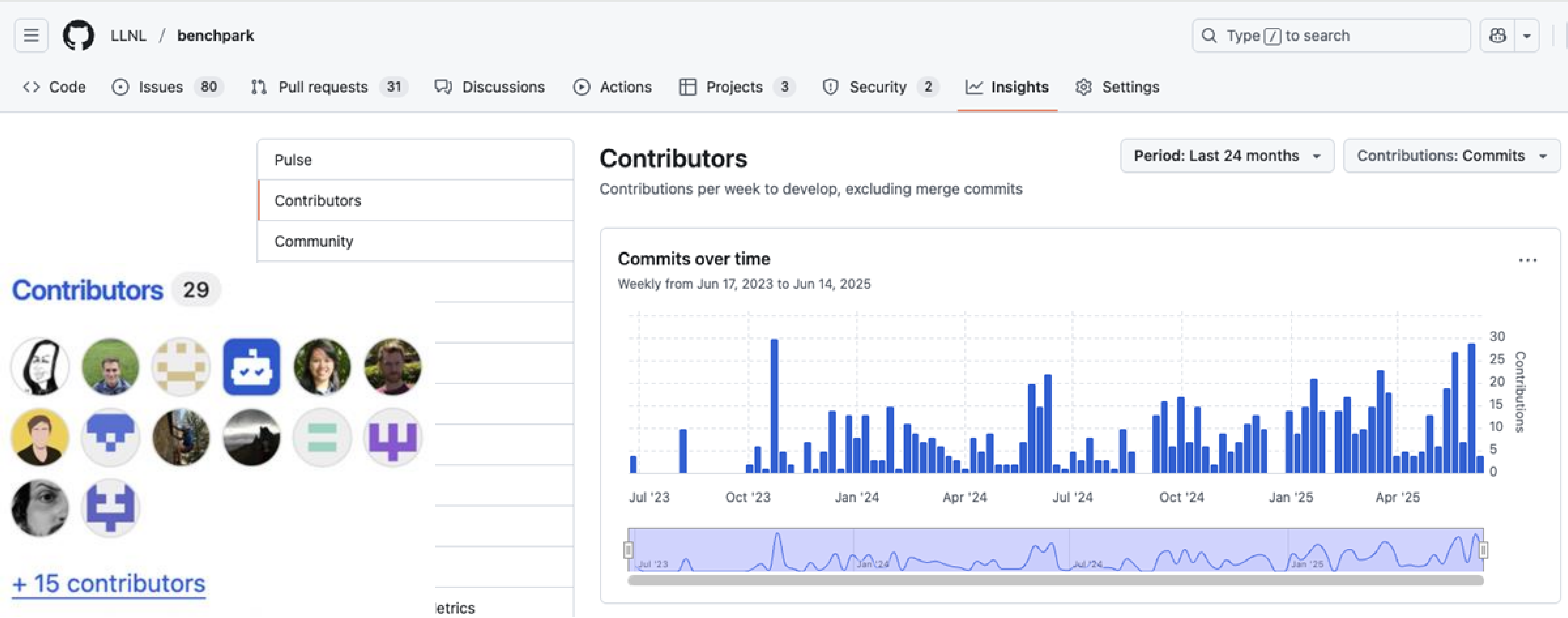
`benchpark analyze` for generating pre-defined analysis charts




```
main
├─ Generate
│  ├─ MPI_Allreduce
│  ├─ MPI_Comm_split
│  └─ MPI_Scan
├─ MPI_Allreduce
├─ MPI_Bcast
├─ MPI_Comm_dup
├─ MPI_Comm_free
├─ MPI_Comm_split
├─ MPI_Finalize
├─ MPI_Finalized
├─ MPI_Gather
├─ MPI_Get_library_version
├─ MPI_Initialized
└─ Solve
   └─ solve
      ├─ LPlusTimes
      ├─ LTimes
      ├─ Population
      │  └─ MPI_Allreduce
      ├─ Scattering
      ├─ Source
      └─ SweepSolver
         ├─ MPI_Irecv
         ├─ MPI_Isend
         ├─ MPI_Testany
         ├─ MPI_Waitall
         └─ SweepSubdomain
```

See https://software.llnl.gov/benchpark/benchpark-analyze.html

Contributions from 11 organizations (60% non-LLNL)



All Dashboards My CDash Logout

Benchpark

PREV LATEST

Dashboard Calendar Project Settings

Public CDash dashboard for CI tests

Nightly [benchpark-develop] *30 builds* [view timeline]

		Update	Test			
Site	**Build Name**	**Revision**	**Not Run**	**Fail**	**Pass**	**Start Time**
dane6	dane/kripke caliper=mpi scaling=weak scaling-iterations=2 compiler=oneapi	74bb04	0	0$_{-1}$	1^{+1}	4 hours ago
dane1	dane/kripke caliper=mpi scaling=strong scaling-iterations=2 compiler=oneapi	74bb04	0	0	1	4 hours ago
dane16	dane/laghos caliper=mpi scaling=strong scaling-iterations=2	74bb04	0	0	1	4 hours ago
dane1	dane/stream	74bb04	0	0	1	4 hours ago
dane7	dane/smb	74bb04	0	0	1	5 hours ago
dane3	dane/remhos	74bb04	0	0	1	5 hours ago
dane6	dane/phloem	74bb04	0	0$_{-1}$	1^{+1}	5 hours ago
dane3	dane/osu-micro-benchmarks	74bb04	0	0	1	5 hours ago
dane6	dane/laghos	74bb04	0	0	1	5 hours ago
dane4	dane/kripke	74bb04	0	0	1	5 hours ago

Tuolumne HPECray-zen4-MI300A-Slingshot [benchpark system init --dest=tuolumne-system llnl-elcapitan cluster=tuolumne] *30 builds* [view timeline]

		Update	Test			
Site	**Build Name**	**Revision**	**Not Run**	**Fail**	**Pass**	**Start Time**
tuolumne2150	tuolumne/kripke +rocm scaling=strong scaling-iterations=2 gpumode=CPX	9edf8b	0	1^{+1}	0$_{-1}$	10 hours ago
tuolumne2149	tuolumne/raja-perf +rocm	e1a1c5	0	0	1	12 minutes ago
tuolumne2149	tuolumne/kripke +rocm scaling=strong scaling-iterations=2 gpumode=TPX	e1a1c5	0	0	1	19 minutes ago
tuolumne2149	tuolumne/amg2023 +rocm	e1a1c5	0	0	1	20 minutes ago
tuolumne2149	tuolumne/laghos +rocm scaling=strong scaling-iterations=2 gpumode=TPX	e1a1c5	0	0	1	26 minutes ago
tuolumne2150	tuolumne/laghos +rocm scaling=strong scaling-iterations=2 gpumode=CPX	e1a1c5	0	0	1	27 minutes ago
tuolumne2149	tuolumne/laghos +rocm	e1a1c5	0	0	1	28 minutes ago
tuolumne1001	tuolumne/amg2023 +rocm scaling=strong scaling-iterations=2 gpumode=TPX	e1a1c5	0	0	1	38 minutes ago
tuolumne2149	tuolumne/kripke +rocm scaling=strong scaling-iterations=2 gpumode=CPX	e1a1c5	0	0	1	39 minutes ago
tuolumne2149	tuolumne/kripke +rocm	e1a1c5	0	0	1	40 minutes ago

First Previous 1 2 3 Next Last

Benchpark codifies benchmarking steps

- Benchpark does **not** replace benchmark source, build system, or Spack package
- Benchpark manages benchmark **experiments** and how they map onto **systems** with specified (or default)
  - Compilers
  - MPI/comm libraries
  - Math libraries
- Start running benchmark experiments on your system with just a few commands

```
git clone git@github.com:LLNL/benchpark.git
```

```
benchpark list systems
benchpark system init --dest=elcap llnl-elcapitan
```

```
benchpark list experiments
benchpark experiment init –system=elcap --dest=amg
        amg2023 +rocm +strong
```

```
benchpark setup amg workspace
ramble workspace setup
```

```
ramble on
```

Who does Benchpark target

People who want to use or distribute benchmarks for HPC!

1. End Users of HPC Benchmarks

- Install, run, analyze performance of HPC benchmarks

2. Benchmark Developers

- People who want to share their benchmarks

3. Procurement teams at HPC Centers

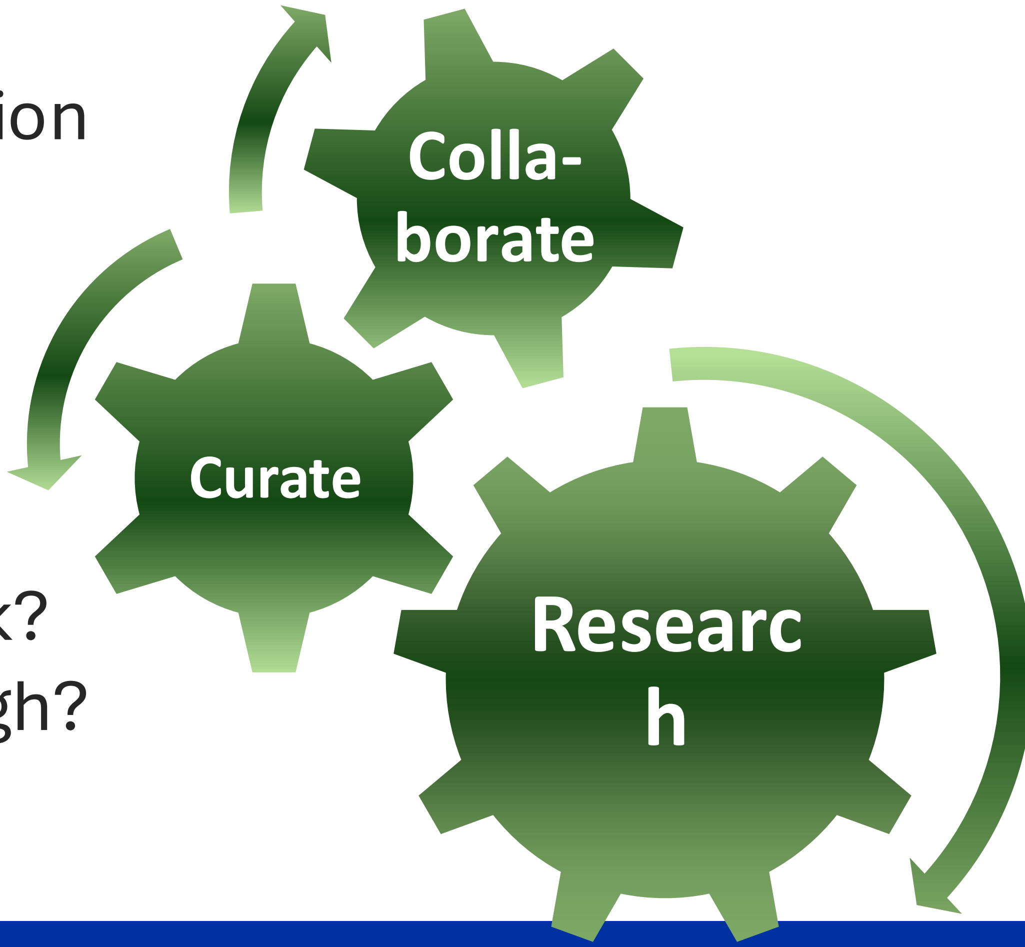
- Curate workload representation, evaluate and monitor system progress

4. HPC Vendors

- Understand the curated workload of HPC centers, propose systems

Catalogued library of *working* benchmarks

- Enables exploration of large configuration space
  - Architectural
  - Software stack
  - Temporal
- What architecture and system configuration is best for my benchmark?
- On my system, is OpenMPI good enough?
- What purpose will Benchpark help you address?



Building a community to contribute/benefit

Benchpark: Open collaborative repository for reproducible specifications of HPC benchmarks

Infrastructure-as-code benchmark specification enables **reproducibility, replicability, and automation**

- HPC Systems
- HPC Experiments

Specify
- How to build and run benchmarks on a system

Run
- Run an experiment on a system

Reproduce
- Re-run an experiment on a system

Replicate
- Run an experiment on a new system

Maintain
- CI: Run experiment on HPC systems

Record
- Perf.measu-rements + *full spec* of experiment

- Tagging, keywords for publications
- Performance metrics, metrics of usefulness
- Dashboards: Archive specs+results

- CI pipelines on PRs from GitHub at data centers across the world and in the cloud

*Olga Pearce et al, Continuous Benchmarking, HPCTests SC|23
*Olga Pearce et al, Repeat, Replicate, Reproduce, ACM REP 2025

Full specification enables reproducibility, replicability, and automation

Benchpark roadmap and community engagement

Future directions:

- Suite curation: Reproducible specification of an entire suite
- Tagging: Keywords for publications, finding benchmarks
- Metrics: Performance, usefulness
- Dashboards: Archive+share *specs*+results, Slices in configuration space
- CI pipelines at data centers across the world and in the cloud

Community Engagement:

- Co-design / vendors on board, but incentive for app teams? (carrot or stick?)
- Who owns which parts of the specification and approves changes?
- Who finances R&D and maintenance?
- ROI for the people working on it? → think about post docs, researchers, etc.

Collaboration, reproducibility, fully-specified public results

Hands On Session 1
Running an existing benchmark on an existing system

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What is Ramble?

What is Ramble?

Ramble is an open-source experimentation framework written in python.

Ramble's primary goals are to:

- Accelerate productivity
- Improve experiment portability
- Increase reproducibility information
- Encoding domain knowledge

Ramble is particularly good at generating parameterized "experiments", but can be used for more than performance focused experiments.

What is Ramble?

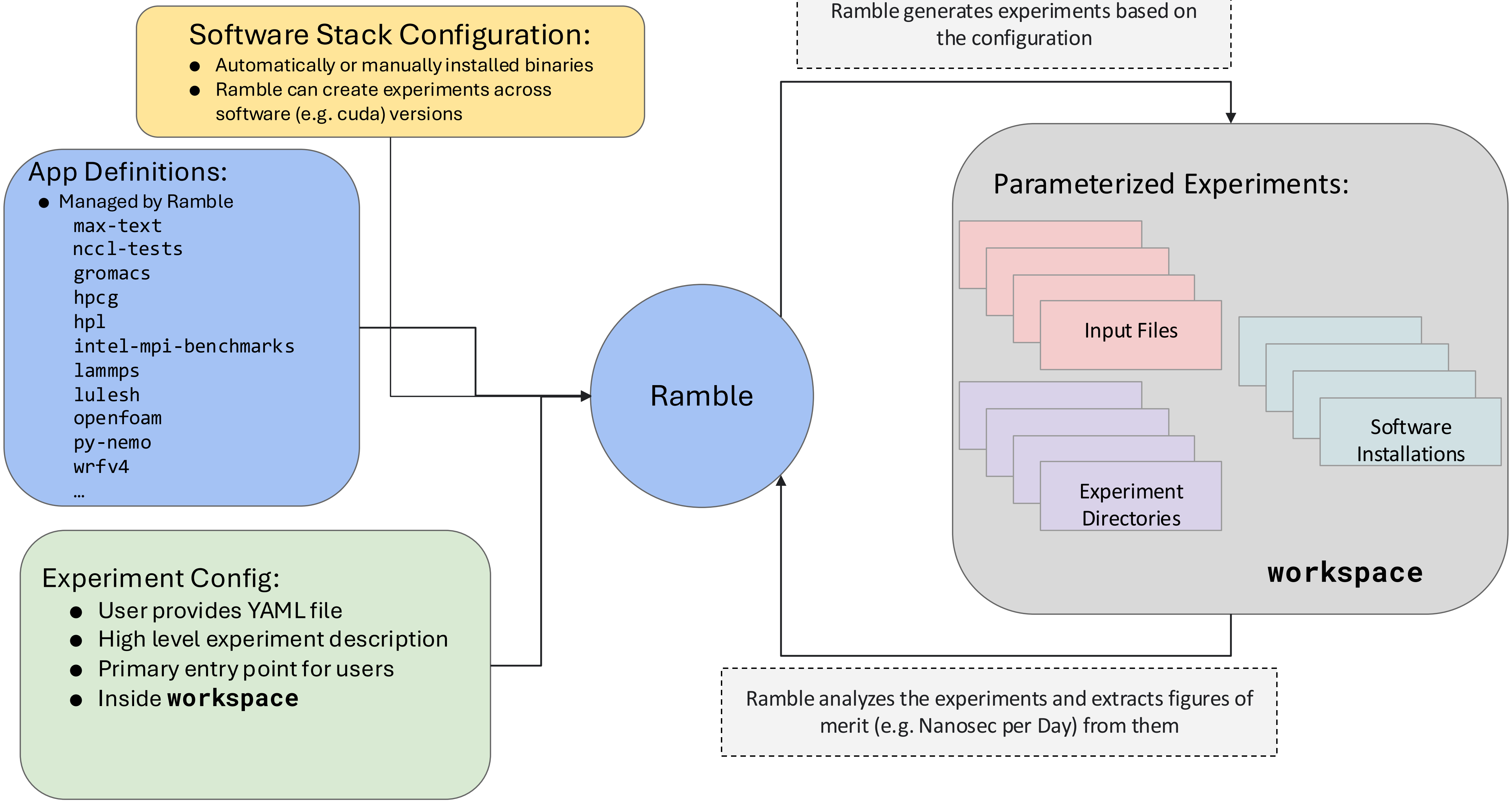
Ramble is:

- Written in python
- Multi-platform
- Heavily based on Spack (Written on top of Spack’s infrastructure)
- An experimentation framework (Related to running experiments like Spack is to building software)
- Open Source: https://github.com/GoogleCloudPlatform/ramble

Ramble provides:

- A flexible templating engine
- A domain specific language for describing an application and its workloads
- Standardized definitions of how workloads are configured and executed

Ramble Architecture



Ramble Components

Object Definitions

Portable definitions written in python, that represent:

Applications:
- Executables (commands to run)
- Input files (things to download)
- Software (things to install)
- Workloads (executables + input files)
- Figures of merit (things to analyze)

Package Managers (spack, eessi)
Workflow Managers (slurm, batch, gke)
Modifiers (lscpu, intel-aps, etc..)

Ramble supports **public** and **private** object definitions through configurable repos.

Does not include experiment or system details.

Experiment Configuration (Workspace)

Self contained directory describing a set of **parameterized** experiments to execute.

Contains:
- YAML File, describes:
    - Experiments
    - Software stack
    - Execution workflow
- Template files

After setup, contains:
- Input files
- Experiment execution directories
- Software environments

Experiment Directory

Each experiment has **their own** execution directory.

These contain:
- Rendered versions of the template files (which can then be executed)

After executing the might contain:
- Links to the input files
- Output files from the experiment to be analyzed

Ramble Components

Software Stack

Ramble supports using a predefined software stack, or generating a new software stack to produce experiments.

Supported software stack workflows in Ramble include:

- Pre-installed software (Considered "Existing")
  - e.g. ISV applications installed in a static location
  - Software installed manually through another mechanism (yum, apt, pip, etc..)
- Driving the creation of a software stack:
  - Using a 3P package manager (currently supports spack, pip, eessi, environment-modules)
  - Can parameterize various aspects of the stack
  - Can use a binary cache to accelerate deployments, and provide binary objects to customers

When Ramble manages the software stack, it can parameterize portions of the stack to generate various studies. This includes:

- Changing compilers
- Changing dependencies (e.g. MPI impl., CUDA vs. ROCM)
- Package versions (e.g. CUDA versions)
- Optimization Targets (e.g. Icelake vs. Zen 3)
- etc...

Allows very flexible descriptions of the software environment

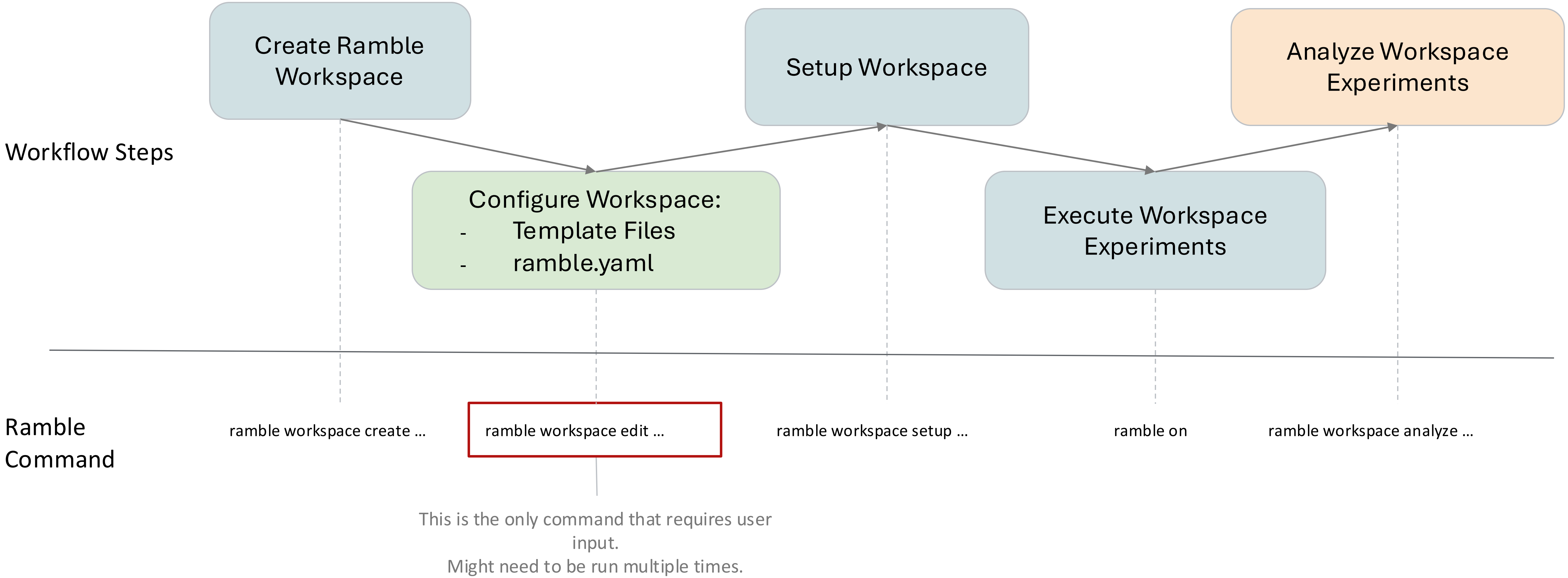
Spack is used to distribute well defined software stacks.

Various organizations provide public spack caches, which can make it faster to deploy a complex software stack.

How does Ramble work?

Ramble Controlled Step
User Input Step
Output Step

What is Ramble's Workflow?



Create Ramble Workspace | Configure Workspace: - Template Files - ramble.yaml | Setup Workspace | Execute Workspace Experiments | Analyze Workspace Experiments

Ramble Workspace:

A workspace is a self contained directory, that contains:

- software environments
- input files
- experiments

Workspaces are independent, and should represent a set of independent experiments you want to execute.

Workspace: my_experiments

```
configs:
└──── ramble.yaml
    execute_experiment.tpl
```

inputs | software | experiments

Workspace Config:

Ramble's workspace config YAML can generate many experiments with only a little syntax.

```
applications:
  wrfv3:                                          ← Application Definition Name
    n_repeats: 5 } Define 5 repeats per experiment
    variables:
      processes_per_node: [30, 56]    } Define two vectors, of length 2.
      partition: ['c2', 'c2d']
      n_ranks: '{processes_per_node}*{n_nodes}'
    workloads:
      CONUS_2p5km:                                ← Workload Name (from Application Definition)
        experiments:
          scaling_study_{partition}_{nodes}nodes:
            variables:
              n_nodes: [1, 2, 4, 8, 16, 32]} Define one vector, of length 6
            matrix:   } Define one matrix, using the n_nodes vector. Shape is 1x6.
            - n_nodes
```

- Vectors that are not used by a matrix are zipped together (must be the same length)
- Zip of vectors are crossed with any matrices
- Result is: 1x6 (matrix) x 2 (vectors) x 5 (repeats) = 60, where each index is a 4-element tuple: (processes_per_node, n_ranks, n_nodes, repeat_idx)

Workspace Config:

In addition to the YAML config, Ramble has a template engine to render scripts:

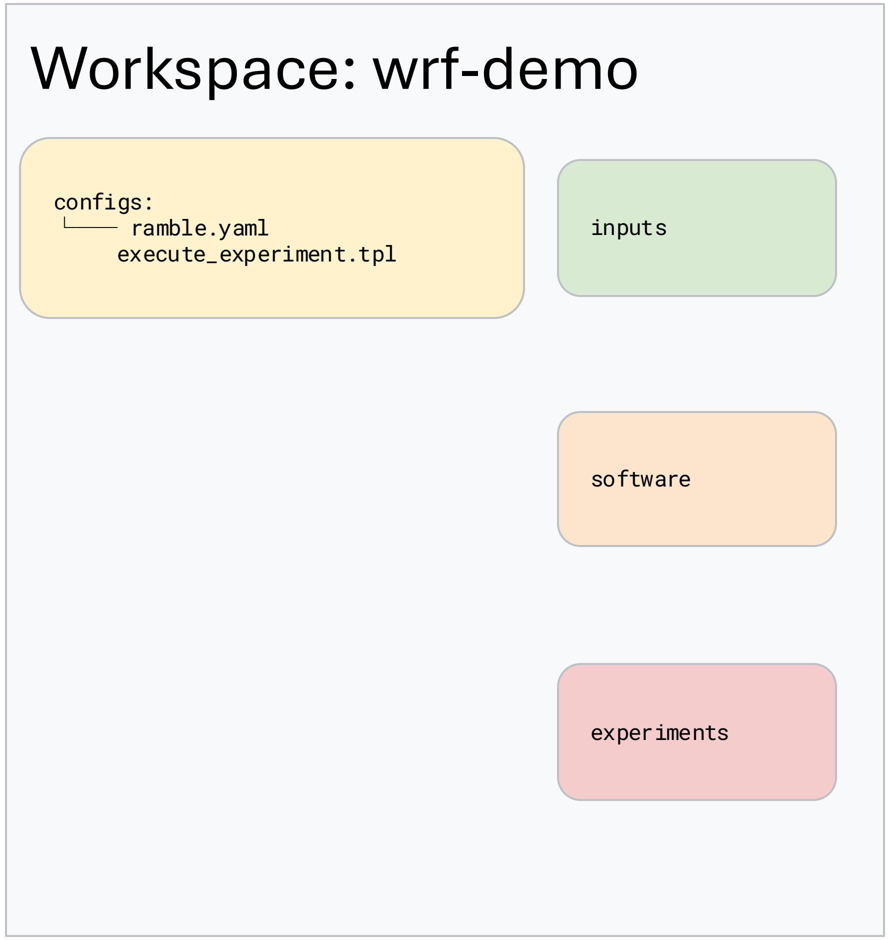
```
#!/bin/bash

{command}
```

```
#!/bin/bash

source <path/to/spack>
spack env activate <path/to/env>
cp <inputs>/* <experiment_dir>/.
mpirun -n <n_ranks> wrf.exe
```

Workspace Setup:



Execute input phases:
- Determine which inputs are necessary
- Download them
- Define variables for referring to these inputs

Execute software phases (Only used on SpackApplications currently):
- Install necessary compilers
- Create spack environments for the experiments
- Using spack, install the required software
- Define variables for referring to the spack environments

Execute experiment creation phases:
- Create experiment execution directories
- Define variables specific to the experiment
- Render any *.tpl files into the execution directories
- Append the experiment to $workspace/all_experiments

Execute Experiments:

Workspace: wrf-demo

```
configs:
└──── ramble.yaml
     execute_experiment.tpl
```

```
software/
└──── wrfv3.CONUS_2p5km
      └──── spack.yaml
```

```
inputs:
└──── ...
```

all_experiments

```
experiments/
└──── wrfv3
      └──── CONUS_2p5km
            ├──── scaling_study_c2_16nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2_1nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2_2nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2_32nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2_4nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2_8nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2d_16nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2d_1nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2d_2nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2d_32nodes
            │     └──── execute_experiment
            ├──── scaling_study_c2d_4nodes
            │     └──── execute_experiment
            └──── scaling_study_c2d_8nodes
                  └──── execute_experiment
```

After setting up a workspace, the experiments can be executed using:
- $workspace/all_experiments
- ramble on (with an activated workspace)

Depending on the ramble.yaml and execute_experiment.tpl this:
- Executes experiments sequentially
- Submits experiments to a workload manager

Analyze Workspace:

After experiments are executed, Ramble can extract their figures of merit.

This is done through:

```
ramble workspace analyze
```

Ramble will process the output files described in an experiment's application.py, and extract success criteria and figures of merit.

These are then written to a file (e.g. results.txt) in the provided format (can be text, yaml, or json).

What other things can you do with Ramble?

Parameterizing Software Definitions

A common workflow in optimizing software is exploring how modifications to a software stack impact performance. Ramble's support of these workflows can be seen below:

```
ramble:
  …
  applications:
    wrfv3:
      workloads:
        CONUS_2p5km:
          experiments:
            '{mpi}_{partition}_{n_nodes}nodes':
              variables:
                n_nodes: [1, 2, 4, 8, 16, 32]
                mpi: ['impi', 'ompi']
                env_name: 'wrf-{mpi}'
              matrix:
              - n_nodes
              - mpi
```

```
[ramble:]
  …
  software:
    packages:
      wrf:
        pkg_spec: wrf@3.9.1.1
      impi:
        pkg_spec: intel-oneapi-mpi@2021.9
      ompi:
        pkg_spec: openmpi@4.1.4
    environments:
      wrf-{mpi}:
        packages:
        - wrf
        - '{mpi}'
```

Parameterizing Software Definitions

A common workflow in optimizing software is exploring how modifications to a software stack impact performance. Ramble's support of these workflows can be seen below:

```
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  …
  applications:
    wrfv3:
      workloads:
        CONUS_2p5km:
          experiments:
            '{mpi}_{partition}_{n_nodes}nodes':
              variables:
                n_nodes: [1, 2, 4, 8, 16, 32]
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                env_name: 'wrf-{mpi}'
              matrix:
              - n_nodes
              - mpi
```

```
[ramble:]
  …
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    packages:
      wrf:
        pkg_spec: wrf@3.9.1.1
      impi:
        pkg_spec: intel-oneapi-mpi@2021.9
      ompi:
        pkg_spec: openmpi@4.1.4
    environments:
      wrf-{mpi}:
        packages:
        - wrf
        - '{mpi}'
```

Defines spack environments

Variable expansion

MPI packages

Performance Analysis Tools

Modifiers all composable definitions to edit the experiment behavior

```
ramble:
  …
  modifiers:
  - name: intel-aps
  applications:
    wrfv3:
      workloads:
        CONUS_2p5km:
          experiments:
            '{mpi}_{partition}_{n_nodes}nodes':
              variables:
                n_nodes: [1, 2, 4, 8, 16, 32]
                mpi: ['impi', 'ompi']
                env_name: 'wrf-{mpi}'
              matrix:
              - n_nodes
              - mpi
```

```
[ramble:]
  …
  software:
    packages:
      wrf:
        pkg_spec: wrf@3.9.1.1
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    environments:
      wrf-{mpi}:
        packages:
        - wrf
        - '{mpi}'
```

Performance Analysis Tools

Modifiers all composable definitions to edit the experiment behavior

```
ramble:
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  - name: intel-aps
  applications:
    wrfv3:
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        CONUS_2p5km:
          experiments:
            '{mpi}_{partition}_{n_nodes}nodes':
              variables:
                n_nodes: [1, 2, 4, 8, 16, 32]
                mpi: ['impi', 'ompi']
                env_name: 'wrf-{mpi}'
              matrix:
              - n_nodes
              - mpi
```

```
[ramble:]
  …
  software:
    packages:
      wrf:
        pkg_spec: wrf@3.9.1.1
      impi:
        pkg_spec: intel-oneapi-mpi@2021.9
      ompi:
        pkg_spec: openmpi@4.1.4
    environments:
      wrf-{mpi}:
        packages:
        - wrf
        - '{mpi}'
```

Performance Analysis Tool

Three Rs in HPC Benchmarking

1. Repeat
2. Replicate
3. Reproduce

Three Rs in HPC Benchmarking

1. Repeat: run on same system
2. Replicate
3. Reproduce

	Component	Repeat
(1)	System H/W	✓
(2)	System S/W	✓
(3)	Application	✓

- Verifying benchmark still builds and runs
- Handing over benchmarking tasks from one user to another
- Evaluating benchmark performance changes as system ages
- Running multiple trials of a benchmark for noise variability

Three Rs in HPC Benchmarking

1. Repeat
2. Replicate: run with a different software stack
3. Reproduce

	Component	Repeat	Replicate
(1)	System H/W	✓	✓
(2)	System S/W	✓	≈
(3)	Application	✓	✓

- Verifying benchmark still builds and runs with update system software
- Validating performance of updated system software
- Evaluating performance differences of different software substitutes (e.g., gcc or icc compilers)

Three Rs in HPC Benchmarking

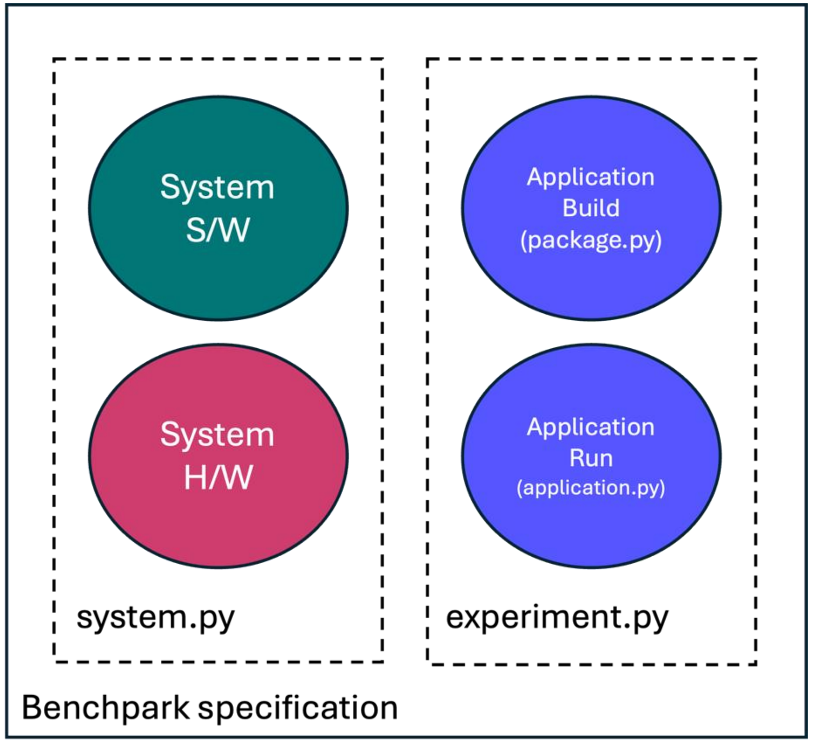
1. Repeat
2. Replicate
3. Reproduce: run on a different system

	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈

- Verifying benchmark builds and runs on diverse hardware
- Evaluating benchmark performance across different hardware
- Exploring potential benefits of hardware upgrades

Benchpark Specification for Three Rs

	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈



Benchpark Specification for the Three Rs

	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈

Repeat as a different user

```
sysa:~ user1$ benchpark system init --dest=sysa intel-cluster
    cluster=sysa
sysa:~ user1$ benchpark experiment init --dest=qs
    quicksilver +openmp +weak
sysa:~ user1$ benchpark setup ./qs ./sysa workspace/
```

```
sysa:~ user2$ benchpark system init --dest=sysa  intel-
    cluster cluster=sysa
sysa:~ user2$ benchpark experiment init --dest=qs
    quicksilver +openmp +weak
sysa:~ user2$ benchpark setup ./qs ./sysa workspace2/
```

Replicate with different SW stack

```
sysa:~ user1$ benchpark system init --dest=sysa1  intel-
    cluster cluster=sysa compiler=gcc1
sysa:~ user1$ benchpark experiment init --dest=qs
    quicksilver +openmp +weak
sysa:~ user1$ benchpark setup ./qs ./sysa1 workspace/
```

```
sysa:~ user2$ benchpark system init --dest=sysa2  intel-
    cluster cluster=sysa compiler=gcc2
sysa:~ user2$ benchpark experiment init --dest=qs
    quicksilver +openmp +weak
sysa:~ user2$ benchpark setup ./qs ./sysa2 workspace2/
```

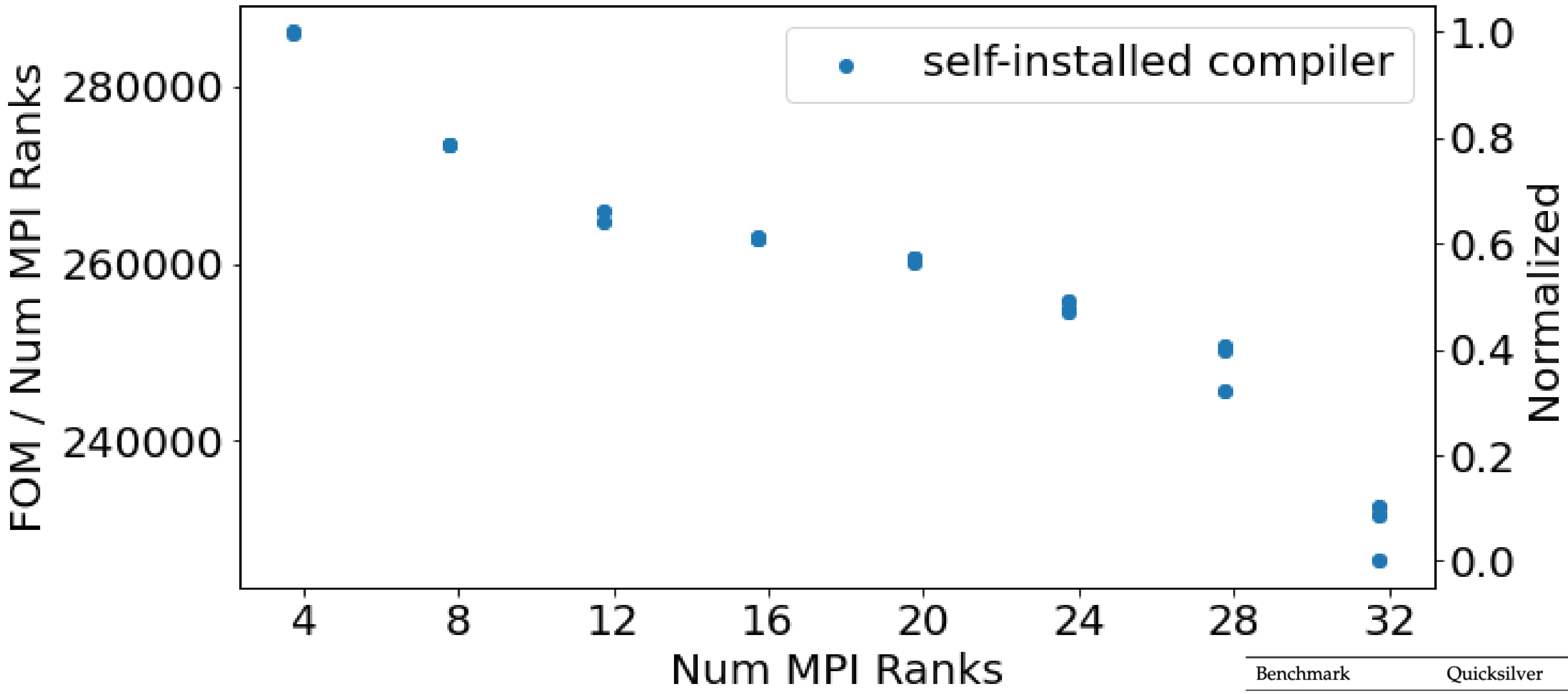
Reproduce on a different system

```
sysa:~ user1$ benchpark system init --dest=sysa  intel-
    cluster cluster=sysa
sysa:~ user1$ benchpark experiment init --dest=qs-openmp
    quicksilver +openmp +weak
sysa:~ user1$ benchpark setup ./qs-openmp ./sysa worksp/
```

```
sysb:~ user2$ benchpark system init --dest=sysb  ibm-cluster
sysb:~ user2$ benchpark experiment init --dest=qs-cuda
    quicksilver +cuda +weak
sysb:~ user2$ benchpark setup ./qs-cuda ./sysb work2/
```

Repeat runs of Quicksilver on Ruby using *same compiler*

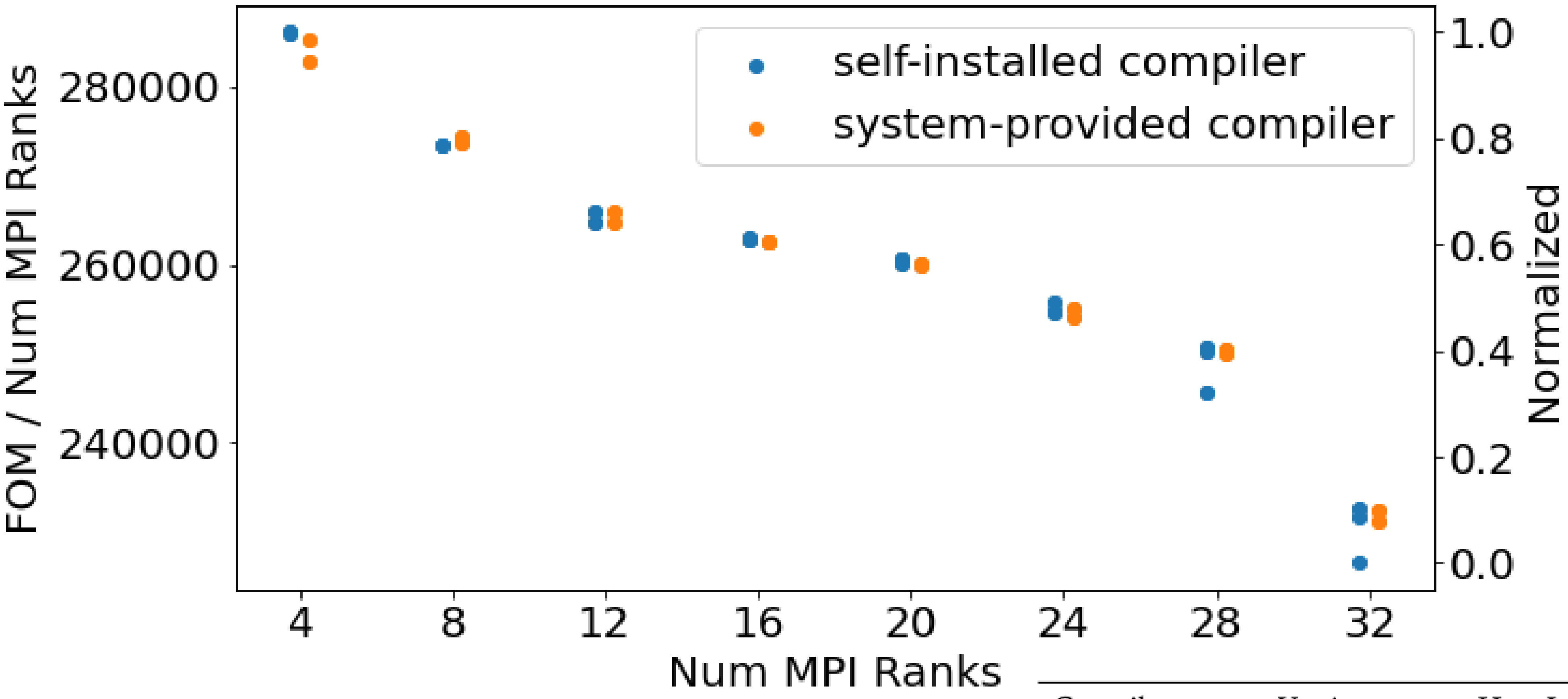
	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈



Benchmark	Quicksilver
Variants	+mpi, +openmp
Num Ranks	4, 8, 12, 16, 20, 24, 28, 32
Num Nodes	1
Scaling	weak
Repetitions	4 (Increase as appropriate for analysis)

Replicate runs of Quicksilver on Ruby with *different compilers*

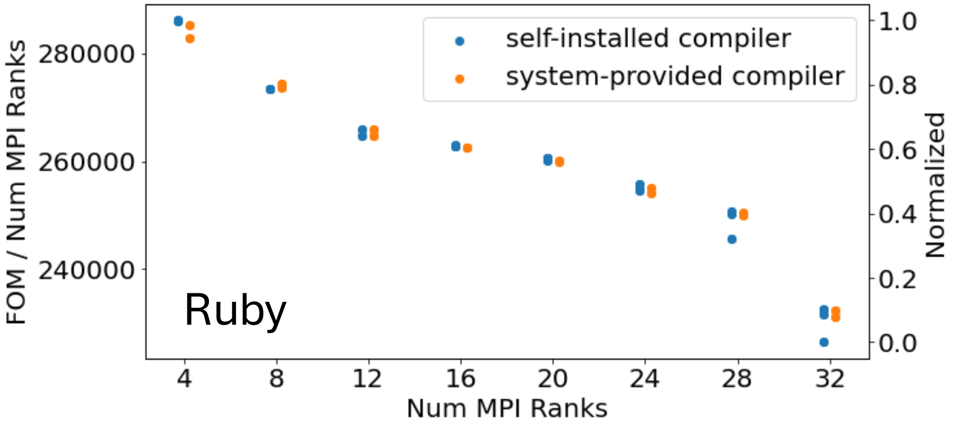
	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈

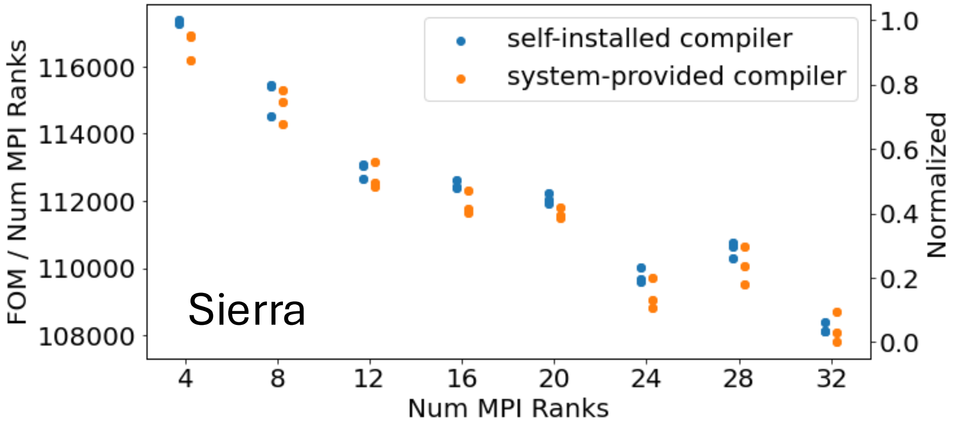


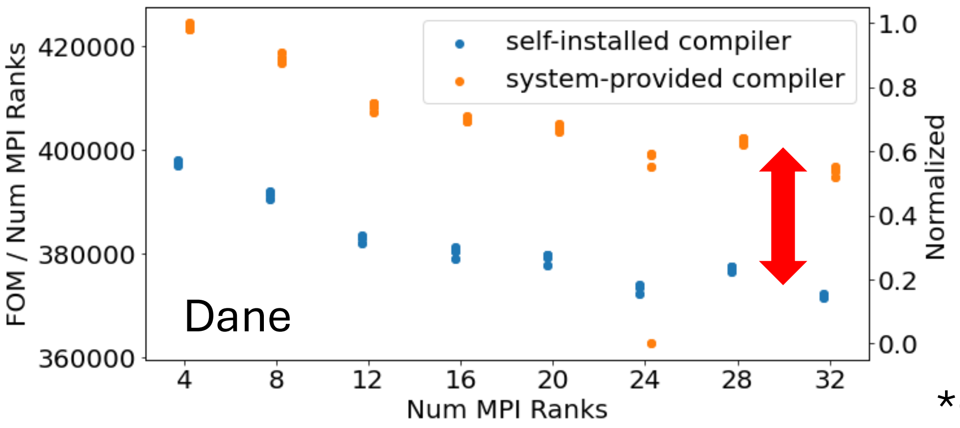
Compiler	Version	How Installed
gcc	12.1.1	system-provided
gcc	12.1.0	self-installed

Reproduce runs of Quicksilver across *different systems*

	Component	Repeat	Replicate	Reproduce
(1)	System H/W	✓	✓	X
(2)	System S/W	✓	≈	X
(3)	Application	✓	✓	≈







System	P-value	Statistically Significant?
Ruby	0.490	No
Sierra	0.349	No
Dane	0.00000105	Yes

System Name	CPU Hardware	Number of Cores
Ruby	Intel Cascade Lake	56
Sierra	IBM Power 9	44
Dane	Intel Sapphire Rapids	112

*Gap on Dane is statistically significant

Analysis of calltrees to understand performance difference

```
0.000 main
└─ 0.134 qs.mainloop
   ├─ 0.019 MPI_Allreduce
   ├─ 0.228 cycleFinalize
   │  ├─ 0.003 MPI_Allreduce
   │  └─ 0.000 MPI_Wait
   ├─ 0.558 cycleInit
   │  ├─ 0.011 MPI_Allreduce
   │  └─ 0.022 MPI_Barrier
   └─ 0.022 cycleTracking
      ├─ 0.000 MPI_Cancel
      ├─ 0.001 MPI_Irecv
      ├─ 0.000 MPI_Wait
      ├─ 230.542 cycleTracking_Kernel
      ├─ 1.158 cycleTracking_MPI
      │  ├─ 0.018 MPI_Irecv
      │  ├─ 0.023 MPI_Isend
      │  ├─ 0.108 MPI_Test
      │  ├─ 0.046 MPI_Wait
      │  └─ 0.001 cycleTracking_Test_Done
      │     └─ 20.566 MPI_Allreduce
      └─ 0.000 cycleTracking_Test_Done
         └─ 0.000 MPI_Allreduce
```

Self-Installed Compiler

```
0.000 main
└─ 0.135 qs.mainloop
   ├─ 0.025 MPI_Allreduce
   ├─ 0.226 cycleFinalize
   │  ├─ 0.003 MPI_Allreduce
   │  └─ 0.000 MPI_Wait
   ├─ 0.559 cycleInit
   │  ├─ 0.014 MPI_Allreduce
   │  └─ 0.024 MPI_Barrier
   └─ 0.022 cycleTracking
      ├─ 0.000 MPI_Cancel
      ├─ 0.001 MPI_Irecv
      ├─ 0.000 MPI_Wait
      ├─ 219.612 cycleTracking_Kernel
      ├─ 1.165 cycleTracking_MPI
      │  ├─ 0.019 MPI_Irecv
      │  ├─ 0.023 MPI_Isend
      │  ├─ 0.106 MPI_Test
      │  ├─ 0.046 MPI_Wait
      │  └─ 0.001 cycleTracking_Test_Done
      │     └─ 19.478 MPI_Allreduce
      └─ 0.000 cycleTracking_Test_Done
         └─ 0.000 MPI_Allreduce
```

System-Provided Compiler

Legend (Metric: Avg time/rank (exc)
- 207.49 – 230.54
- 161.38 – 207.49
- 115.27 – 161.38
- 69.16 – 115.27
- 23.05 – 69.16
- 0.00 – 23.05

Takeaways

- Formalize how to repeat, replicate, and reproduce HPC benchmarking experiments
- Showcase how Benchpark enables reproducibility through specification of experiments and HPC systems
- Full record of the specification is preserved for introspection and reproducibility

Hands On Session 2
Adding an experiment for a benchmark

Follow script at http://software.llnl.gov/benchpark/add-an-experiment.html

Tutorial Instances: http://bit.ly/4kGQDlc

- We have an AWS instance for the hands-on component of this tutorial
- The instance provides:
  - Pre-installed Benchpark and required dependencies
  - Job scheduler

When logging in to the instance:

- Please use a unique username to avoid resource allocation conflicts
  - First initial followed by last name (e.g., John Doe would be jdoe)
- PW: hpctutorial25

Performance Tools: Caliper

- Caliper is an performance profiling library
- Integrates a performance profiler into your program
  - Profiling is always available
  - Simplifies performance profiling for application end users
- Common instrumentation interface
  - Provides program context information for other tools
- Designed for HPC
  - Supports MPI, OpenMP, CUDA, HIP, Kokkos, RAJA
- software.llnl.gov/Caliper

Performance Tools: Thicket

- Thicket is a toolkit for Exploratory Data Analysis
- Enables exploratory data analysis of multi-run data
- Compose data from diff. sources and types
  - Different scaling (e.g., strong, weak)
  - Different application parameters
  - Different compilers and optimization levels
  - Different hardware types (e.g., CPUs, GPUs)
  - Different performance tools

- Perform analysis on the thicket of runs
  - Manipulate the set of data
  - Visualize the dataset
  - Perform analysis on the data
  - Model data
  - Leverage third-party tools in the Python ecosystem

thicket.readthedocs.io

Ramble modifiers in Benchpark encapsulate reusable patterns to perform a specific configuration of an experiment

- Affinity modifier for pinning threads
- Allocation modifier to request resources
- Hwloc modifier to capture hardware topology
- Caliper modifier to profile an application

benchpark experiment init --dest=amg amg2023 --system=elcap –rocm workload=problem2 +strong caliper=mpi.time

HIGH PERFORMANCE COMPUTING
INNOVATION CENTER

Join us after the tutorial!

Tutorial material: software.llnl.gov/benchpark/basic-tutorial.html

Connect with us on Spack slack

#benchpark-support

We want your feedback!

Contribute systems, benchmarks, experiments, and features on GitHub

slack.spack.io
#benchpark-support

★ Star us on GitHub!
github.com/llnl/benchpark

HPSF
BENCHMARKING WORKING GROUP