Thicket: Seeing the performance experiment forest for the individual run trees

RADIUSS Tutorial Series 2023

CASC
Center for Applied Scientific Computing

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Go to: https://software.llnl.gov/radiuss/event/2023/07/11/radiuss-on-aws/ to learn more about our other tutorials and documentation!

Upcoming Tutorials

Date	Time (Pacific)	Project
August 3, 2023	9:00a.m.–11:00a.m.	Build, link, and test large-scale applications with **BLT**
August 8–9 2023	8:00a.m.–11:30a.m. both days	Learn to install your software quickly with **Spack**
August 10, 2023	9:00a.m.–11:00a.m.	Use **MFEM** for scalable finite element discretization application development
August 14, 2023	9:00a.m.–12:00p.m.	Integrate performance profiling capabilities into your applications with **Caliper** Analyze hierarchical performance data with **Hatchet** Optimize application performance on supercomputers with **Thicket**
August 17, 2023	9:00a.m.–11:00a.m.	Use **RAJA** to run and port codes quickly across NVIDIA, AMD, and Intel GPUs Discover, provision, and manage HPC memory with **Umpire**
August 22, 2023	9:00a.m.–11:00a.m.	Visualize and analyze your simulations in situ with **Ascent**
August 24, 2023	9:00a.m.–11:00a.m.	Leverage robust, flexible software components for scientific applications with **Axom**
August 29, 2023	9:00a.m.–11:00a.m.	Analyze runs of your code with **WEAVE**
August 31, 2023	9:00a.m.–11:00a.m.	Learn to run thousands of jobs in a workflow with **Flux**

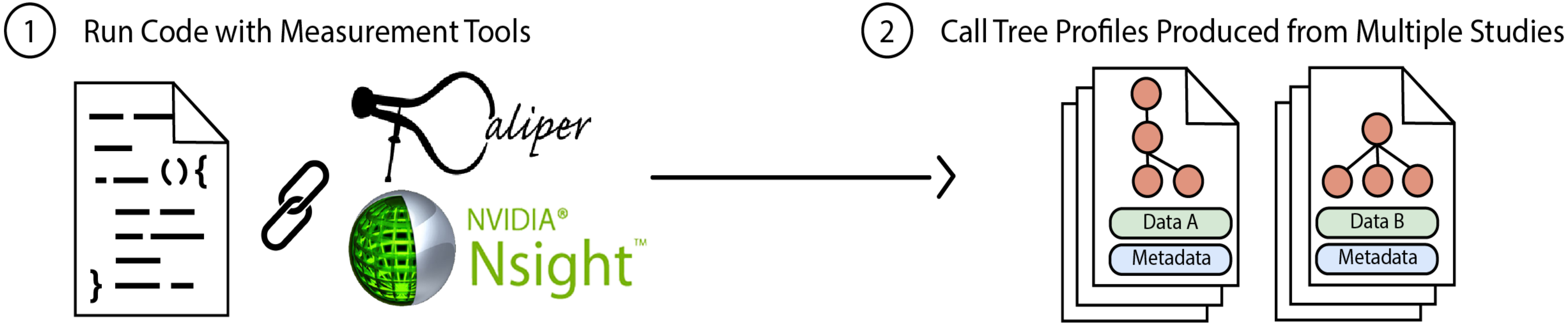
Thicket Tutorial Materials

- The container includes example Jupyter notebooks, Thicket install, and RAJA Performance Suite datasets
  - Alternatively, the Jupyter notebooks and the RAJA Performance Suite datasets are available directly at https://github.com/llnl/thicket-tutorial in a self-contained Binder environment with all dependencies
  - Join our mailing list! https://bit.ly/caliper-thicket-users

- We'll use this material in the hands-on portion of the tutorial.

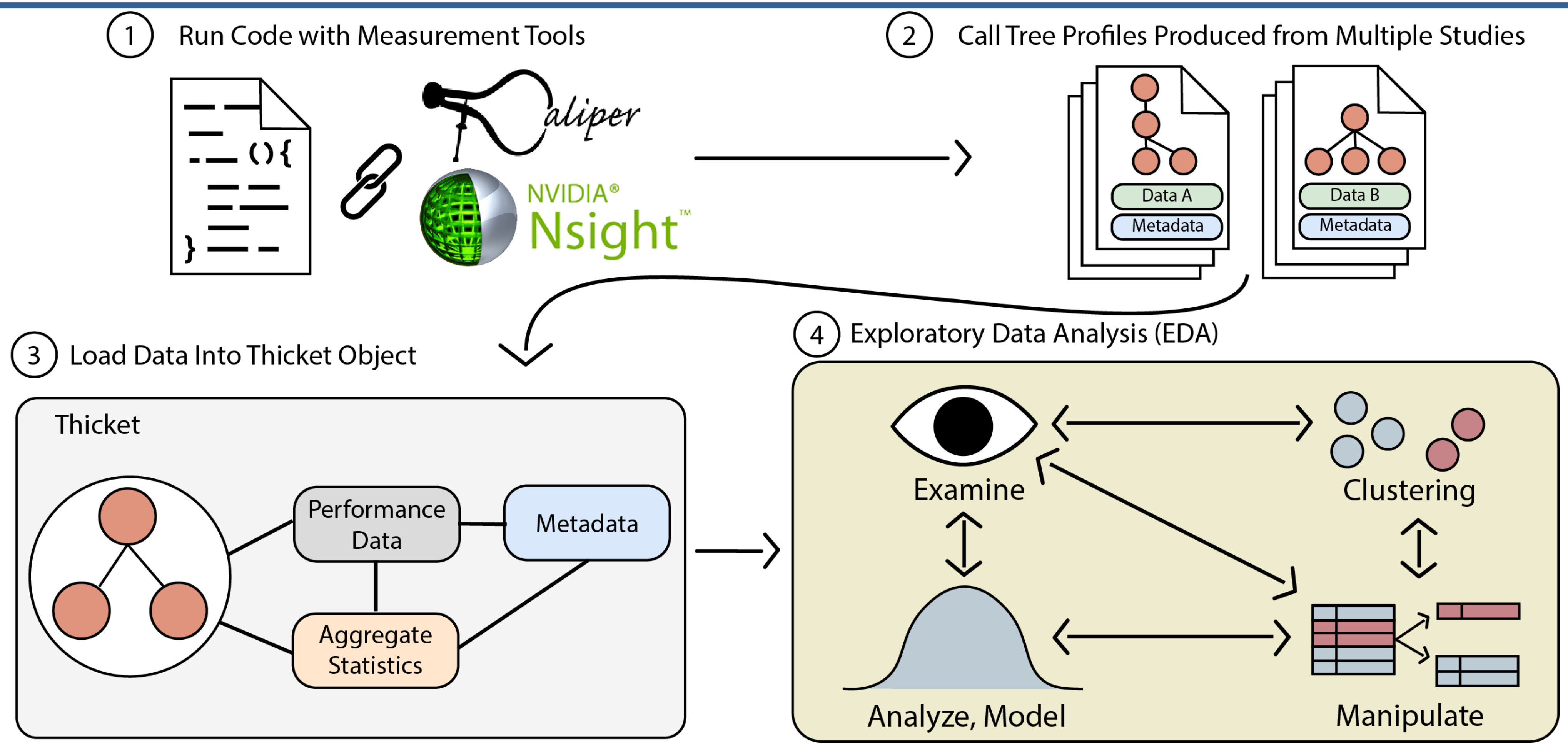
Challenge: Performance analysis in complex HPC ecosystem

- HPC software and hardware are increasingly complex. Need to understand:
  - Strong scaling and weak scaling of applications
  - Impact of application parameters on performance
  - Impact of choice of compilers and optimization levels
  - Performance on different hardware architectures (e.g., CPUs, GPUs)
  - Different tools to measure different aspects of application performance



Goal: Analyze and visualize performance data from different sources and types

Our big picture solution for analyzing and visualizing performance data from different sources and type



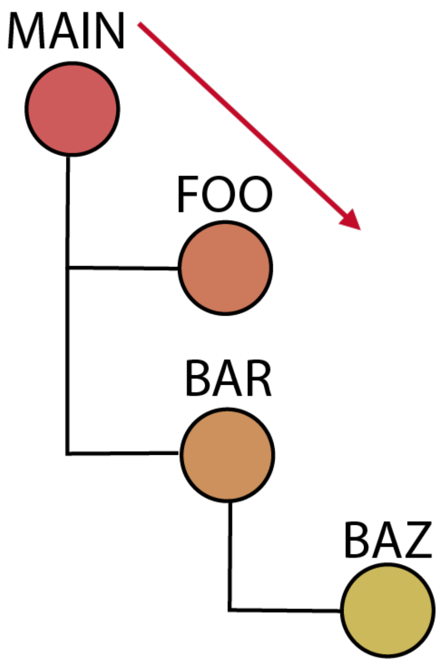
Documentation: **thicket.readthedocs.io**

https://github.com/LLNL/thicket
https://github.com/LLNL/thicket-tutorial

What do profiling tools collect per run?

e.g., Caliper

1) Call Tree



2) Performance data

Node	Cache Misses
MAIN	
FOO	
BAR	
BAZ	

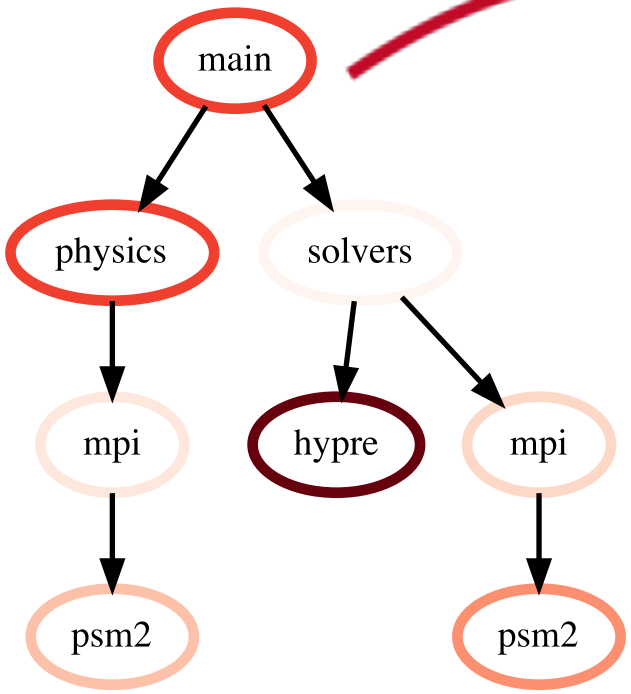
- Time, FLOPS
- Cache misses
- Memory accesses

3) Metadata per run

User	Platform

- Batch submission (user, launch date)
- Hardware info (platform)
- Build info (compiler versions/flags)
- Runtime info (problem parameters, number of MPI ranks used)

Thicket builds upon Hatchet's *GraphFrame*: a Graph and a Dataframe



Graph: Stores relationships between parents and children

node	name	nid	node	time	time (inc)
main	main	0	main	40.0	200.0
physics	physics	1	physics	40.0	60.0
mpi	mpi	2	mpi	5.0	20.0
psm2	psm2	3	psm2	15.0	15.0
solvers	solvers	4	solvers	0.0	100.0
hypre	hypre	5	hypre	65.0	65.0
mpi	mpi	6	mpi	10.0	35.0
psm2	psm2	7	psm2	25.0	25.0

Pandas Dataframe: 2D table storing numerical data associated with each node (may be unique per rank, per thread)

Visualizing Hatchet's GraphFrame components

```
>>> print(gf.tree())      # print graph
>>> print(gf.dataframe)   # print dataframe
```

```
0.000 foo
├─ 6.000 bar
│   └─ 5.000 baz
├─ 0.000 qux
│   └─ 5.000 quux
│       ├─ 10.000 corge
│       ├─ 15.000 garply
│       └─ 1.000 grault
└─ 15.000 waldo
    ├─ 3.000 fred
    │   └─ 5.000 plugh
    └─ 15.000 garply
```

```
Legend (Metric: time)
■ 13.50 – 15.00
■ 10.50 – 13.50
■ 7.50 – 10.50
■ 4.50 – 7.50
■ 1.50 – 4.50
■ 0.00 – 1.50

name User code    ◀ Only in left graph    ▶ Only in right graph
```

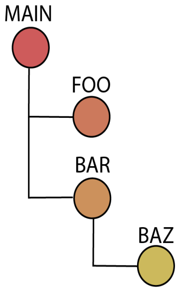
node	name	time	time (inc)
{'name': 'foo'}	foo	0.0	130.0
{'name': 'bar'}	bar	5.0	20.0
{'name': 'baz'}	baz	5.0	5.0
{'name': 'grault'}	grault	10.0	10.0
{'name': 'qux'}	qux	0.0	60.0
{'name': 'quux'}	quux	5.0	60.0
{'name': 'corge'}	corge	10.0	55.0
{'name': 'bar'}	bar	5.0	20.0
{'name': 'baz'}	baz	5.0	5.0
{'name': 'grault'}	grault	10.0	10.0
{'name': 'garply'}	garply	15.0	15.0
{'name': 'grault'}	grault	10.0	10.0

Use Thicket to *compose* performance profiles in Python

P1

Metadata

User	Platform



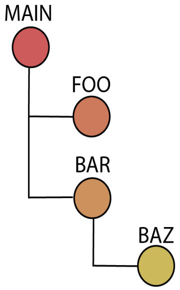
Performance metrics

Node	Cache Misses
MAIN	24
FOO	
BAR	
BAZ	

P2

Metadata

User	Platform



Performance metrics

Node	Cache Misses
MAIN	16
FOO	
BAR	
BAZ	

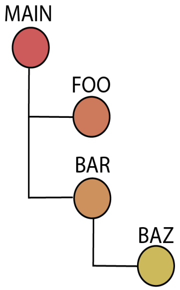
Use Thicket to *compose* performance profiles in Python

1 Compose functions w/matching call trees

P1

Metadata

User	Platform



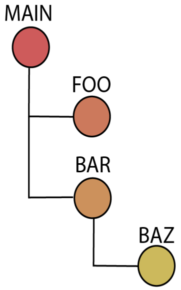
Performance metrics

Node	Cache Misses
MAIN	24
FOO	
BAR	
BAZ	

P2

Metadata

User	Platform



Performance metrics

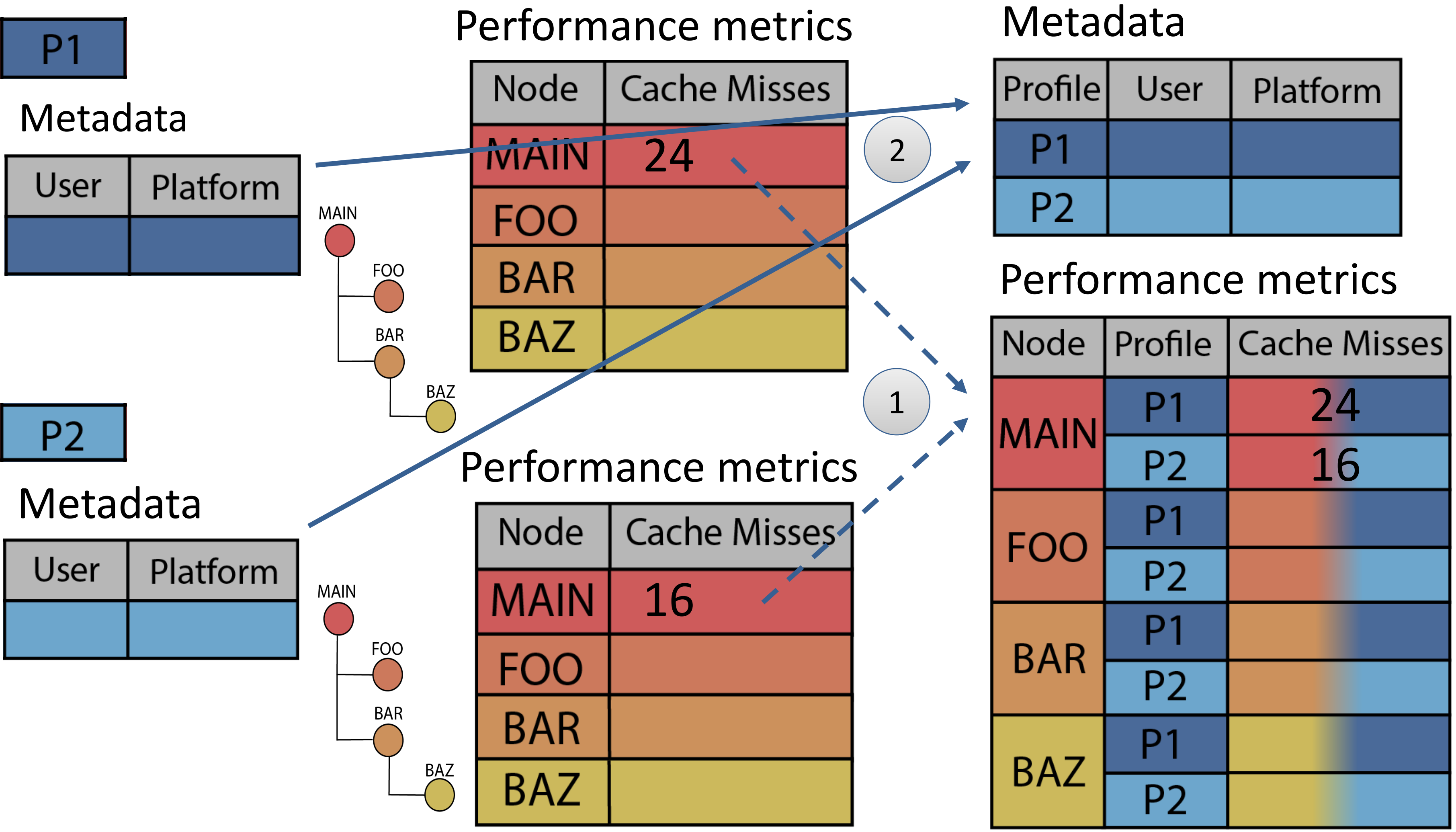
Node	Cache Misses
MAIN	16
FOO	
BAR	
BAZ	

1

Performance metrics

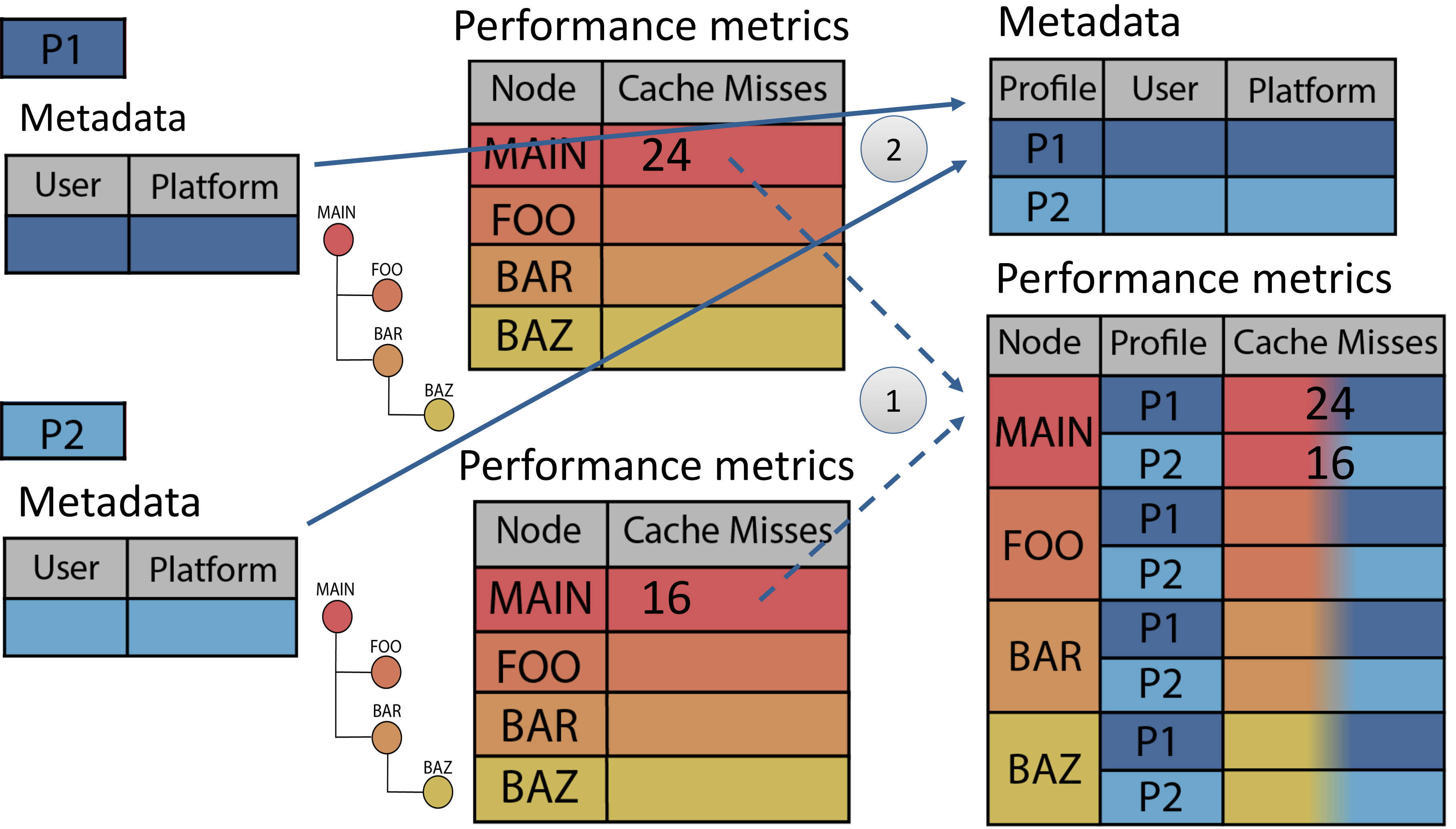
Node	Profile	Cache Misses
MAIN	P1	24
	P2	16
FOO	P1	
	P2	
BAR	P1	
	P2	
BAZ	P1	
	P2	

Use Thicket to *compose* performance profiles in Python



1. Compose functions w/matching call trees
2. Compose metadata with all fields

Use Thicket to *compose* performance profiles in Python



1. Compose functions w/matching call trees
2. Compose metadata with all fields
3. Aggregate statistics (order reduction)

3

Node	Avg. Cache Misses
MAIN	20
FOO	
BAR	
BAZ	

Thicket components are *interconnected*

Metadata

Profile	User	Platform
P1	Jon	lassen
P2	Bob	lassen

Performance metrics

Node	Profile	Cache Misses
MAIN	P1	
	P2	
FOO	P1	
	P2	
BAR	P1	
	P2	
BAZ	P1	
	P2	

Filter on metadata:
platform==“lassen" &&
user==“Bob”

Filtered Metadata

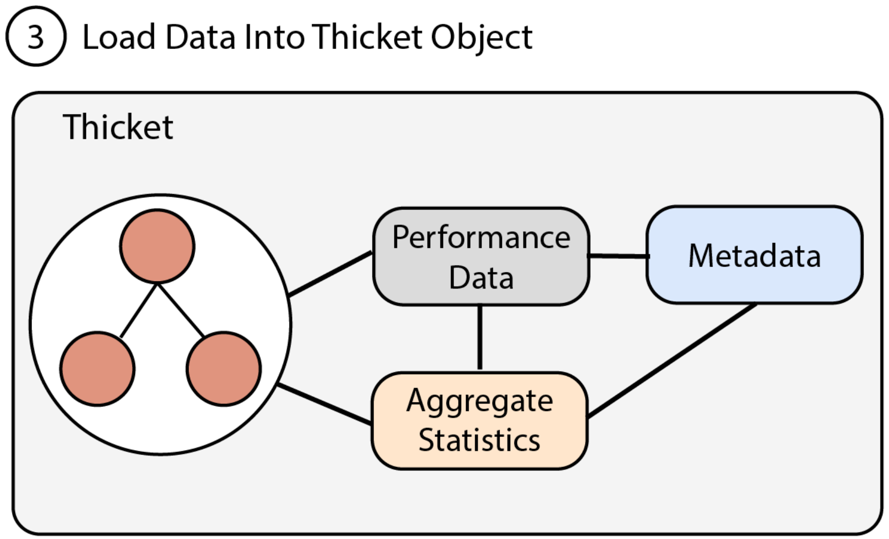
Profile	User	Platform
P2	Bob	lassen

Filtered Performance metrics

Node	Profile	Cache Misses
MAIN	P2	
FOO	P2	
BAR	P2	
BAZ	P2	

Metadata fields useful for understanding and manipulating thicket object!

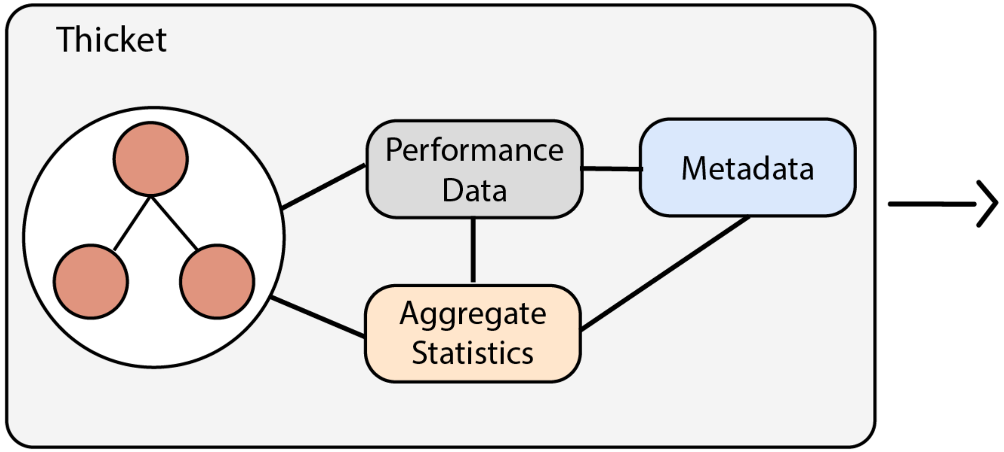
Thicket enables exploratory data analysis of multi-run data



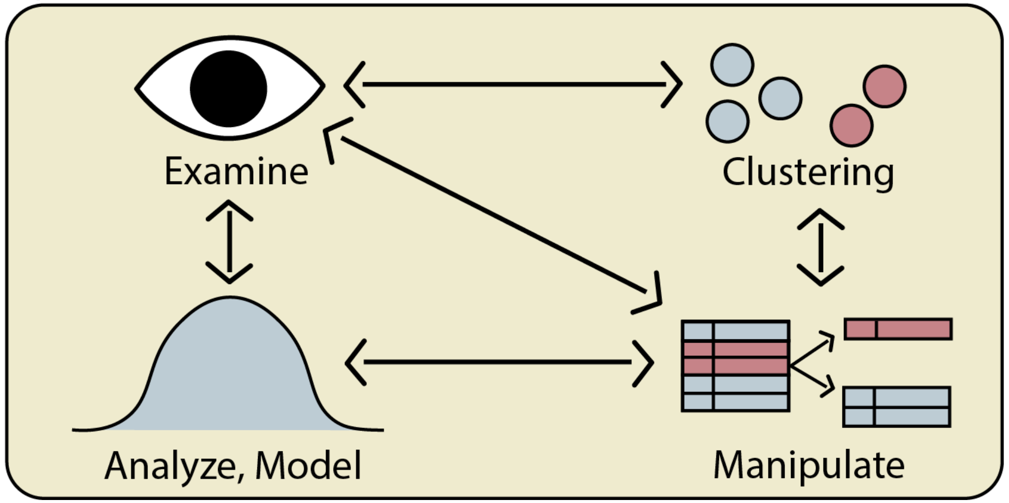
- Compose data from diff. sources and types
  - Different scaling (e.g., strong, weak)
  - Different application parameters
  - Different compilers and optimization levels
  - Different hardware types (e.g., CPUs, GPUs)
  - Different performance tools

Thicket enables exploratory data analysis of multi-run data

③ Load Data Into Thicket Object



④ Exploratory Data Analysis (EDA)



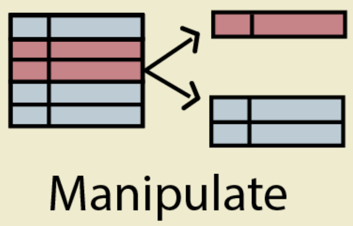
- Compose data from diff. sources and types
  - Different scaling (e.g., strong, weak)
  - Different application parameters
  - Different compilers and optimization levels
  - Different hardware types (e.g., CPUs, GPUs)
  - Different performance tools
- Perform analysis on the thicket of runs
  - Manipulate the set of data
  - Visualize the dataset
  - Perform analysis on the data
  - Model data
  - Leverage third-party tools in the Python ecosystem

Case Study 1: RAJA Performance Suite

- Open-source suite of loop-based kernels commonly found in HPC applications showcasing performance of different programming models on different hardware
- 560 runs/profiles:
  - 2 clusters (CPU, CPU+GPU)
  - 4 problem sizes
  - 3 compilers, 4 optimizations
  - 3 programming models (sequential, OpenMP, CUDA)
  - 3 performance tools (Caliper, PAPI, Nsight Compute)

	cluster	systype build	problem size	compiler	compiler optimizations	omp num threads	cuda compiler	block sizes	RAJA variant	#profiles
0	quartz	toss_3_x86_64_ib	[1M, 2M, 4M, 8M]	clang++-9.0.0	[-O0, -O1, -O2, -O3]	1	N/A	N/A	Sequential	160
1	quartz	toss_3_x86_64_ib	[1M, 2M, 4M, 8M]	g++-8.3.1	[-O0, -O1, -O2, -O3]	1	N/A	N/A	Sequential	160
2	quartz	toss_3_x86_64_ib	[1M, 2M, 4M, 8M]	clang++-9.0.0	-O0	72	N/A	N/A	OpenMP	40
3	quartz	toss_3_x86_64_ib	[1M, 2M, 4M, 8M]	g++-8.3.1	-O0	72	N/A	N/A	OpenMP	40
4	lassen	blueos_3_ppc64le_ib_p9	[1M, 2M, 4M, 8M]	xlc++_r-16.1.1.12	-O0	1	nvcc-11.2.152	[128, 256, 512, 1024]	CUDA	160

Use Thicket to *compose* multi-platform, multi-tool data



Thicket object composed of 2 profiles run on CPU

node	problem_size	time (exc)	Reps	Retiring	Backend bound
Apps_NODAL_ACCUMULATION_3D	1M	0.204583	100	0.144928	0.783786
	4M	0.795511	100	0.139002	0.788017
Apps_VOL3D	1M	0.067061	100	0.402238	0.510525
	4M	0.241508	100	0.400775	0.515976

Thicket object composed of 2 profiles run on GPU

node	problem_size	time (gpu)	gpu__compute_memory_throughput	gpu__dram_throughput	sm__throughput
Apps_NODAL_ACCUMULATION_3D	1M	0.007478	70.689752	46.724767	7.330745
	4M	0.026951	74.275834	51.257993	7.688628
Apps_VOL3D	1M	0.006028	81.012826	67.751194	35.676942
	4M	0.021422	91.929933	70.122011	35.386470

		CPU				GPU			
node	problem_size	time (exc)	Reps	Retiring	Backend bound	time (gpu)	gpu__compute_memory_throughput	gpu__dram_throughput	sm__throughput
Apps_NODAL_ACCUMULATION_3D	1M	0.204583	100	0.144928	0.783786	0.007478	70.689752	46.724767	7.330745
	4M	0.795511	100	0.139002	0.788017	0.026951	74.275834	51.257993	7.688628
Apps_VOL3D	1M	0.067061	100	0.402238	0.510525	0.006028	81.012826	67.751194	35.676942
	4M	0.241508	100	0.400775	0.515976	0.021422	91.929933	70.122011	35.386470

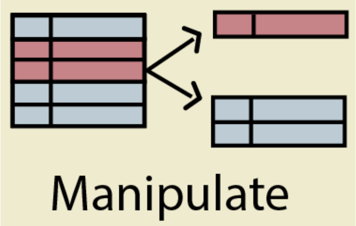
Analyze multi-architecture/multi-tool data

Examine

- Dataset: 4 types of profiles side-by-side to compare CPU to GPU performance
  1. Basic CPU metrics from Caliper
  2. Top-down metrics from Caliper/PAPI
  3. GPU runtime from Caliper
  4. GPU metrics from Nsight Compute
- Examples of analysis:
  - Compute CPU/GPU speedup
  - Correlate memory and compute usage on the CPU vs. GPU

		1 CPU			2 CPU top-down		3 GPU	4 GPU Nsight Compute				Derived
Node	Problem size	time (exc)	Bytes/Rep	Flops/Rep	Retiring	Backend bound	time (gpu)	gpu__compute_memory_throughput	gpu__dram_throughput	sm__throughput	sm__warps_active	speedup
Apps_VOL3D	8M	0.498815	282109496	632421288	0.377843	0.540604	0.040761	93.742058	72.140428	36.206767	54.459589	12.237556
Lcals_HYDRO_1D	8M	2.077556	201326600	41943040	0.032965	0.909545	0.242928	92.944968	92.944968	6.595714	95.266148	8.552147

Manipulate: Filter using call path query




```
0.001 Base_CUDA
└─ 0.000 Algorithm
   ├─ 0.000 Algorithm_MEMCPY
   │  ├─ 0.002 Algorithm_MEMCPY.block_128
   │  ├─ 0.009 Algorithm_MEMCPY.block_256
   │  └─ 0.006 Algorithm_MEMCPY.library
   ├─ 0.000 Algorithm_MEMSET
   │  ├─ 0.001 Algorithm_MEMSET.block_128
   │  ├─ 0.004 Algorithm_MEMSET.block_256
   │  └─ 0.003 Algorithm_MEMSET.library
   ├─ 0.000 Algorithm_REDUCE_SUM
   │  ├─ 0.003 Algorithm_REDUCE_SUM.block_128
   │  ├─ 0.004 Algorithm_REDUCE_SUM.block_256
   │  └─ 0.002 Algorithm_REDUCE_SUM.cub
   └─ 0.000 Algorithm_SCAN
      └─ 0.006 Algorithm_SCAN.default
```

Input call tree

Filter on call path:

(1) Node named "Base_CUDA"

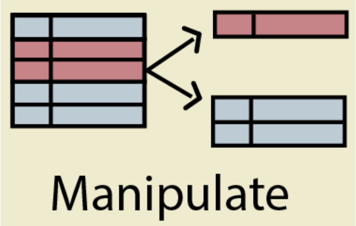
```
0.001 Base_CUDA
```

Output call tree

RAJA

I Lumsden et al. "Enabling Call Path Querying in Hatchet to Identify Performance Bottlenecks in Scientific Applications", e-Science 2022

Manipulate: Filter using call path query




```
0.001 Base_CUDA
└─ 0.000 Algorithm
   ├─ 0.000 Algorithm_MEMCPY
   │  ├─ 0.002 Algorithm_MEMCPY.block_128
   │  ├─ 0.009 Algorithm_MEMCPY.block_256
   │  └─ 0.006 Algorithm_MEMCPY.library
   ├─ 0.000 Algorithm_MEMSET
   │  ├─ 0.001 Algorithm_MEMSET.block_128
   │  ├─ 0.004 Algorithm_MEMSET.block_256
   │  └─ 0.003 Algorithm_MEMSET.library
   ├─ 0.000 Algorithm_REDUCE_SUM
   │  ├─ 0.003 Algorithm_REDUCE_SUM.block_128
   │  ├─ 0.004 Algorithm_REDUCE_SUM.block_256
   │  └─ 0.002 Algorithm_REDUCE_SUM.cub
   └─ 0.000 Algorithm_SCAN
      └─ 0.006 Algorithm_SCAN.default
```

Input call tree

Filter on call path:

(1) Node named "Base_CUDA"

(2) Node with "block_128" in name (and any nodes in between)

```
0.001 Base_CUDA
└─ 0.000 Algorithm
   ├─ 0.000 Algorithm_MEMCPY
   │  └─ 0.002 Algorithm_MEMCPY.block_128
   ├─ 0.000 Algorithm_MEMSET
   │  └─ 0.001 Algorithm_MEMSET.block_128
   └─ 0.000 Algorithm_REDUCE_SUM
      └─ 0.003 Algorithm_REDUCE_SUM.block_128
```

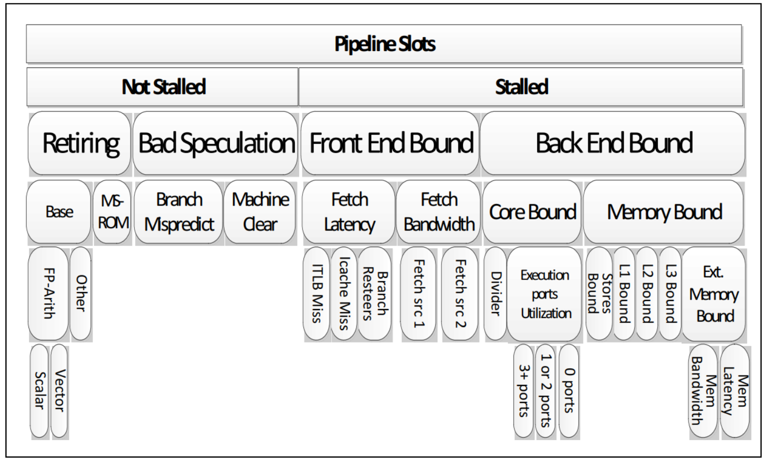
Output call tree

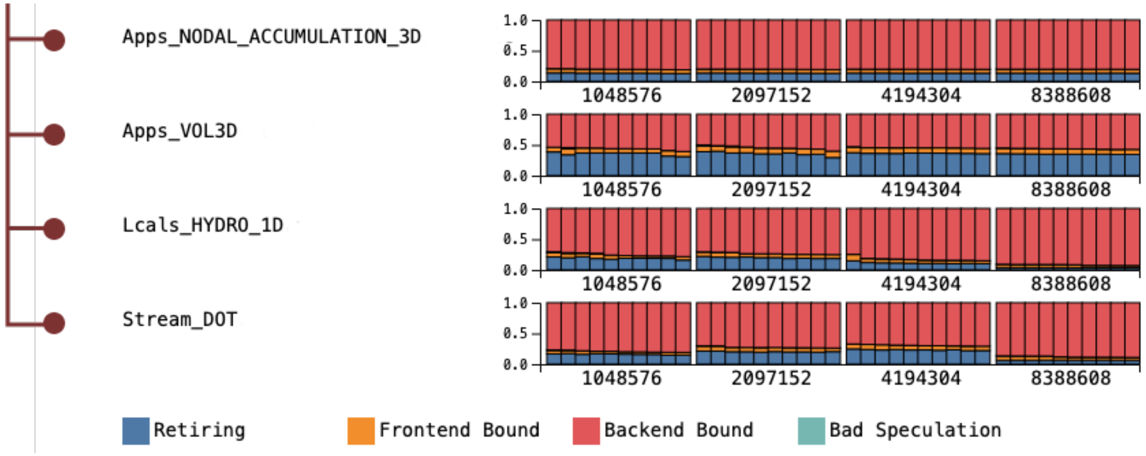
RAJA

I Lumsden et al. "Enabling Call Path Querying in Hatchet to Identify Performance Bottlenecks in Scientific Applications", e-Science 2022

Visualize: Intel CPU top-down analysis

Examine



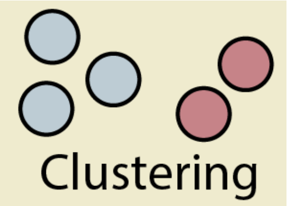


- *Top-down analysis* uses HW counters in a hierarchy to identify bottlenecks*
- Use Caliper's top-down module to derive top-down metrics for call-tree regions

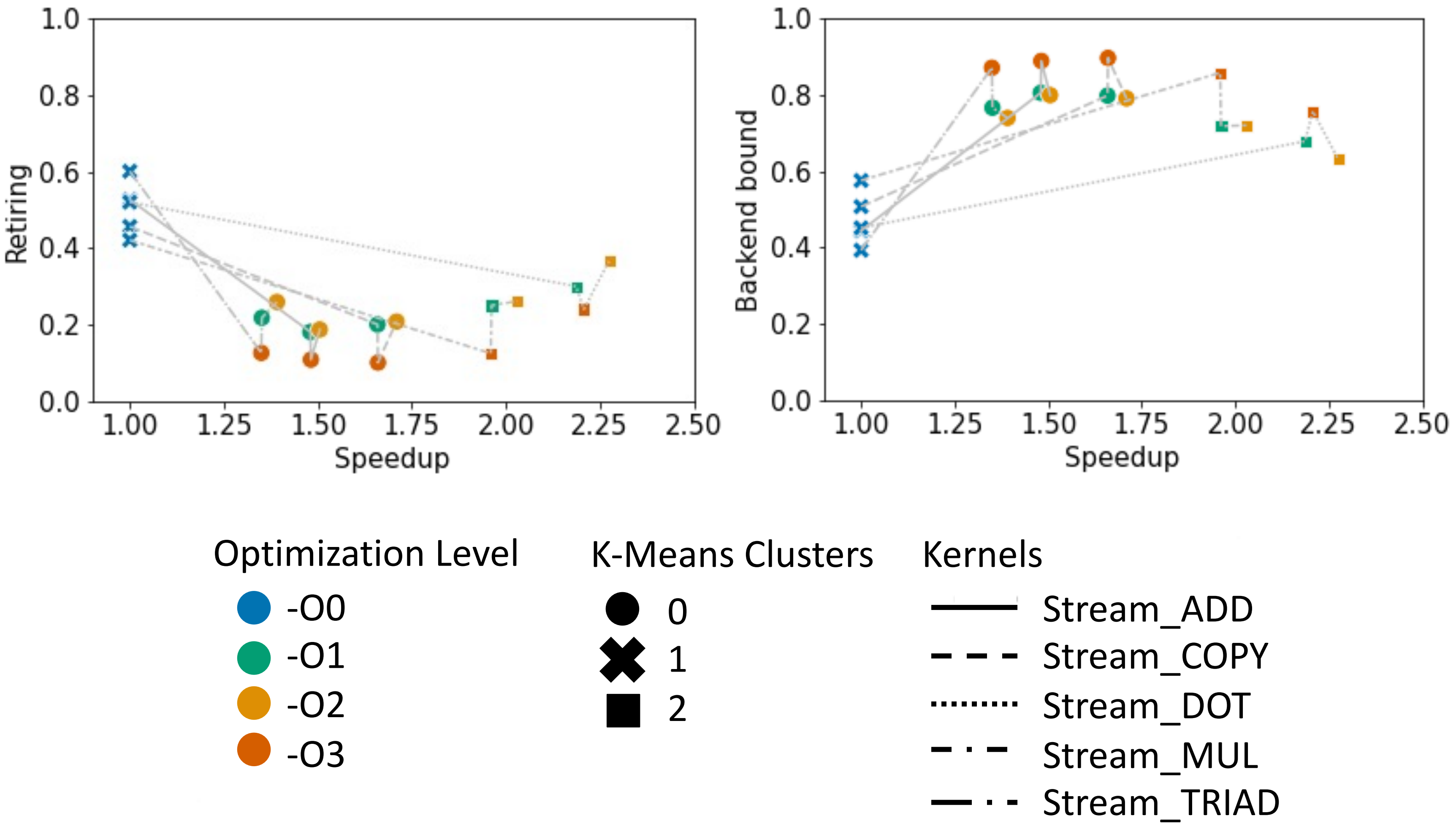
- Thicket's *tree+table* visualization shows top-down metrics as stacked bar charts, each bar is a profile
  - Apps_VOL3D has the highest retiring rates
  - Lcals_HYDRO and Stream_DOT become more backend bound as problem size grows

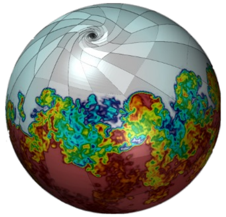
* Yasin, A.: A Top-Down Method for Performance Analysis and Counters Architecture. In: 2014 IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS). pp. 35–44. IEEE, CA, USA (Mar 2014).

Use third-party Python libraries, e.g., Scikit-learn clustering



1. Select data of interest
   - Filter 8M problem size
   - Use query language to extract all implementations of the Stream kernel
2. (optional) Normalize data
3. Apply scikit-learn clustering to top-down analysis metrics of runs with different compiler optimization levels





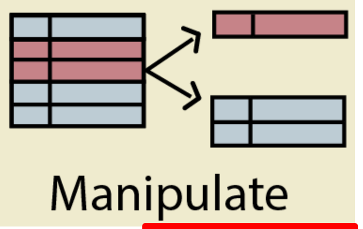
Case Study 2: MARBL multi-physics code

- MARBL is a next-generation multi-physics code developed at LLNL

- 60 runs/profiles:
  - 2 clusters (rztopaz, AWS ParallelCluster)
  - 2 MPI libraries (impi, openmpi)
  - 6 node/rank counts
  - 5 repeat runs per config

	cluster	ccompiler	mpi	version	numhosts	mpi.world.size	#profiles
0	ip----	/usr/tce/packages/clang/clang-9.0.0	impi	v1.1.0-203-gcb0efb3	[1, 2, 4, 8, 16, 32]	[36, 72, 144, 288, 576, 1152]	30
1	rztopaz	/usr/tce/packages/clang/clang-9.0.0	openmpi	v1.1.0-201-g891eaf1	[1, 2, 4, 8, 16, 32]	[36, 72, 144, 288, 576, 1152]	30

Manipulate: Compute noise and scaling

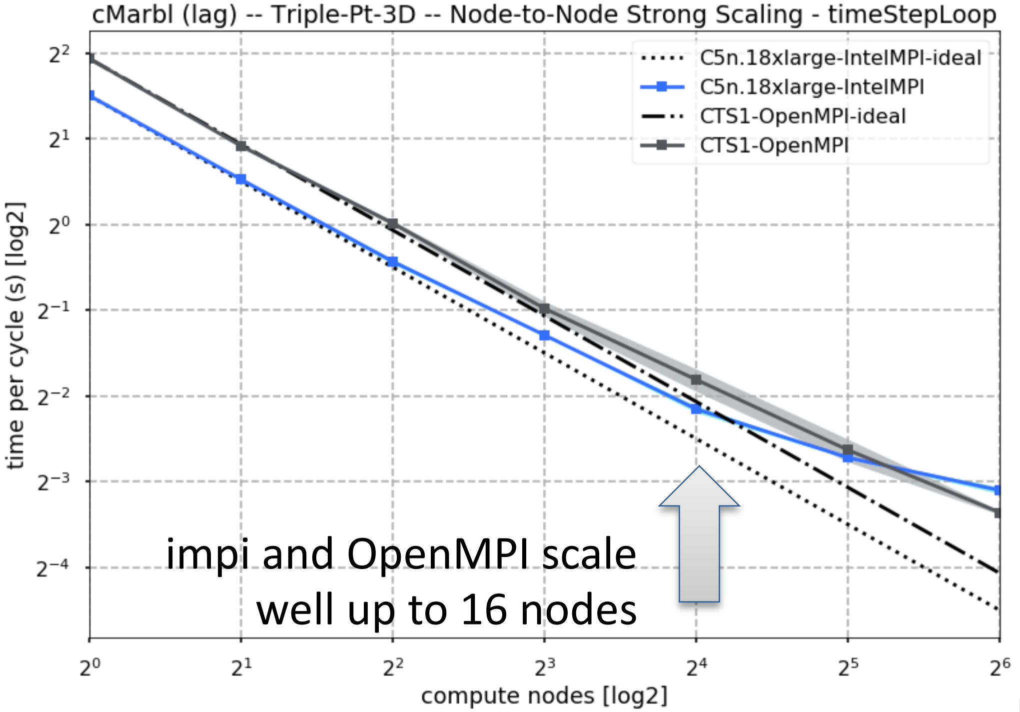


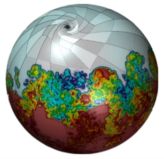
node	profile	Total time	name	mpi.world.size
{'name': 'main', 'type': 'function'}	-8554409769265002864	58036.664552	main	144
	-7335101512240609798	55318.808836	main	36
	-6029692086108825020	156984.246813	main	2304
	-5606382734792961361	64122.371533	main	288
	-4058809097109060732	155040.998627	main	2304
	-3193575964635936033	71010.504038	main	576
	-2978339073585311581	55910.708449	main	72
	-2939704488254773514	157934.204076	main	2304
	-2771797711381234985	56893.512948	main	144
	-2638513839856695106	97432.260966	main	1152

node	profile	Total time	name	mpi.world.size
{'name': 'main', 'type': 'function'}	-7335101512240609798	55318.808836	main	36
	-843517585394879415	55110.656885	main	36
	7720382918482619866	55155.581578	main	36
	8293335926964337960	55139.134916	main	36
	8335957980556391465	55013.682102	main	36

1. Use groupby(mpi.world.size) to generate unique subsets of data which are repeated runs; compute noise

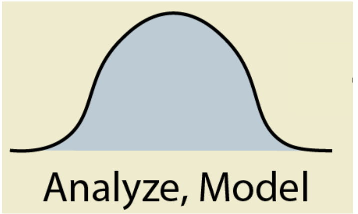
2. Compose runs on different platforms and at different scales





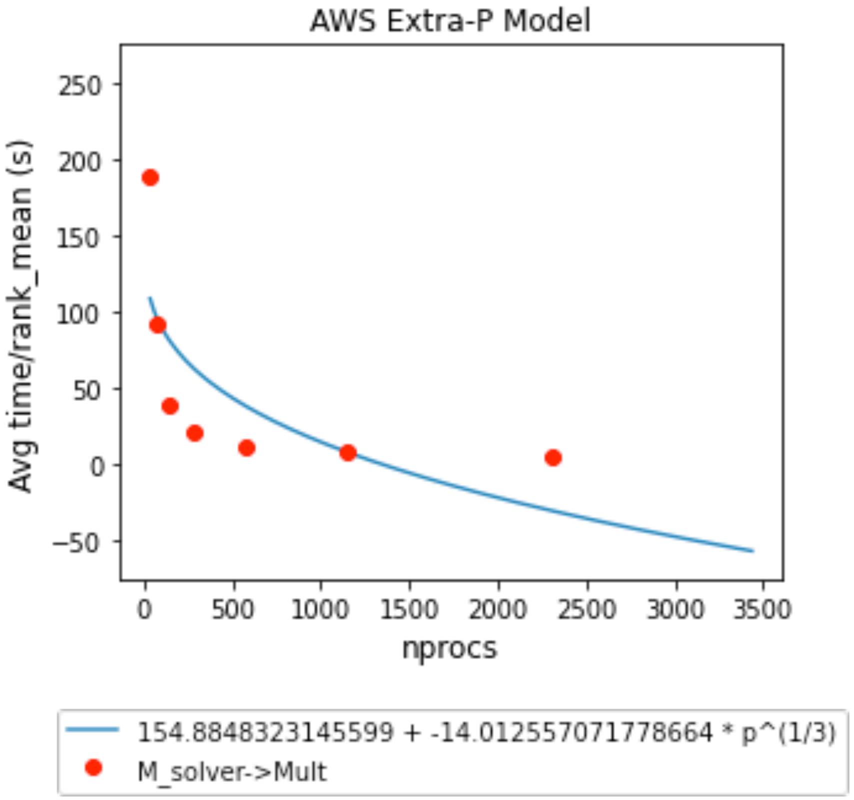
3. Generate strong scaling plot with matplotlib
   — Deviation shown in shaded region, dots are average of 5 runs

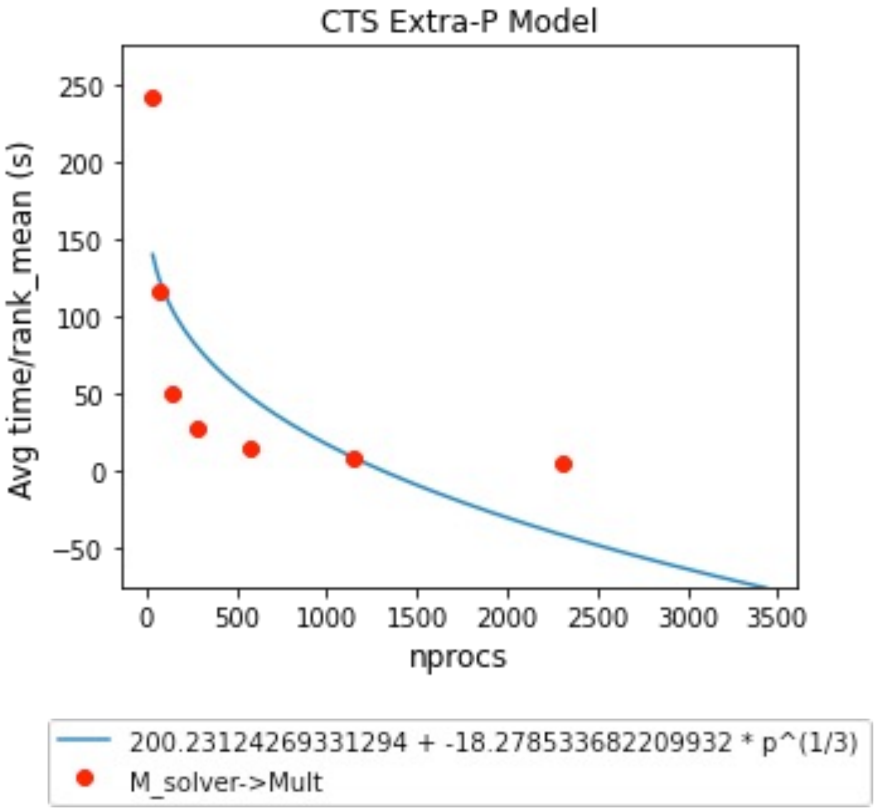
Model: Use third-party Python library, Extra-P

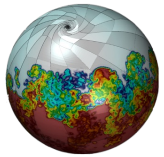


Extra-P derives an analytical performance model from an ensemble of profiles covering one or more modeling parameters http://github.com/extra-p/extrap

- Select functions of interest
- Call Extra-P to model scaling on different hardware types

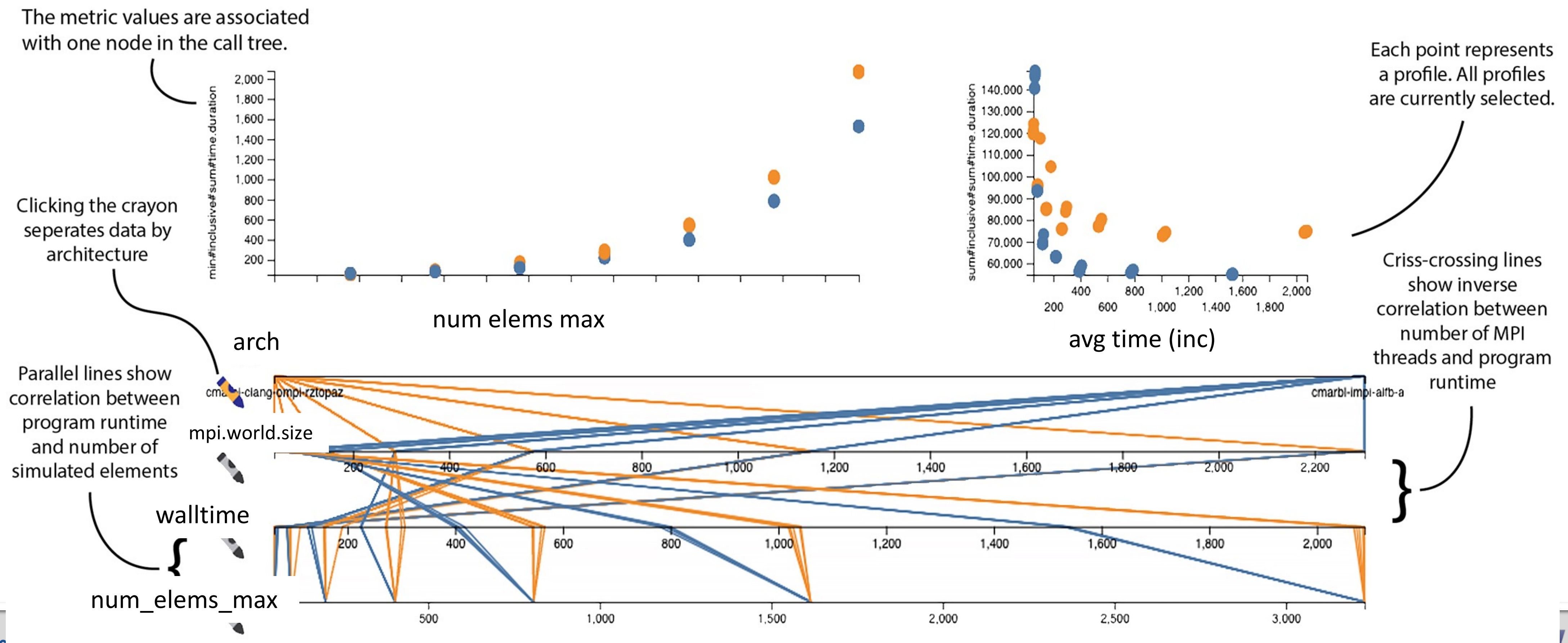


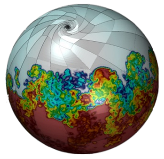




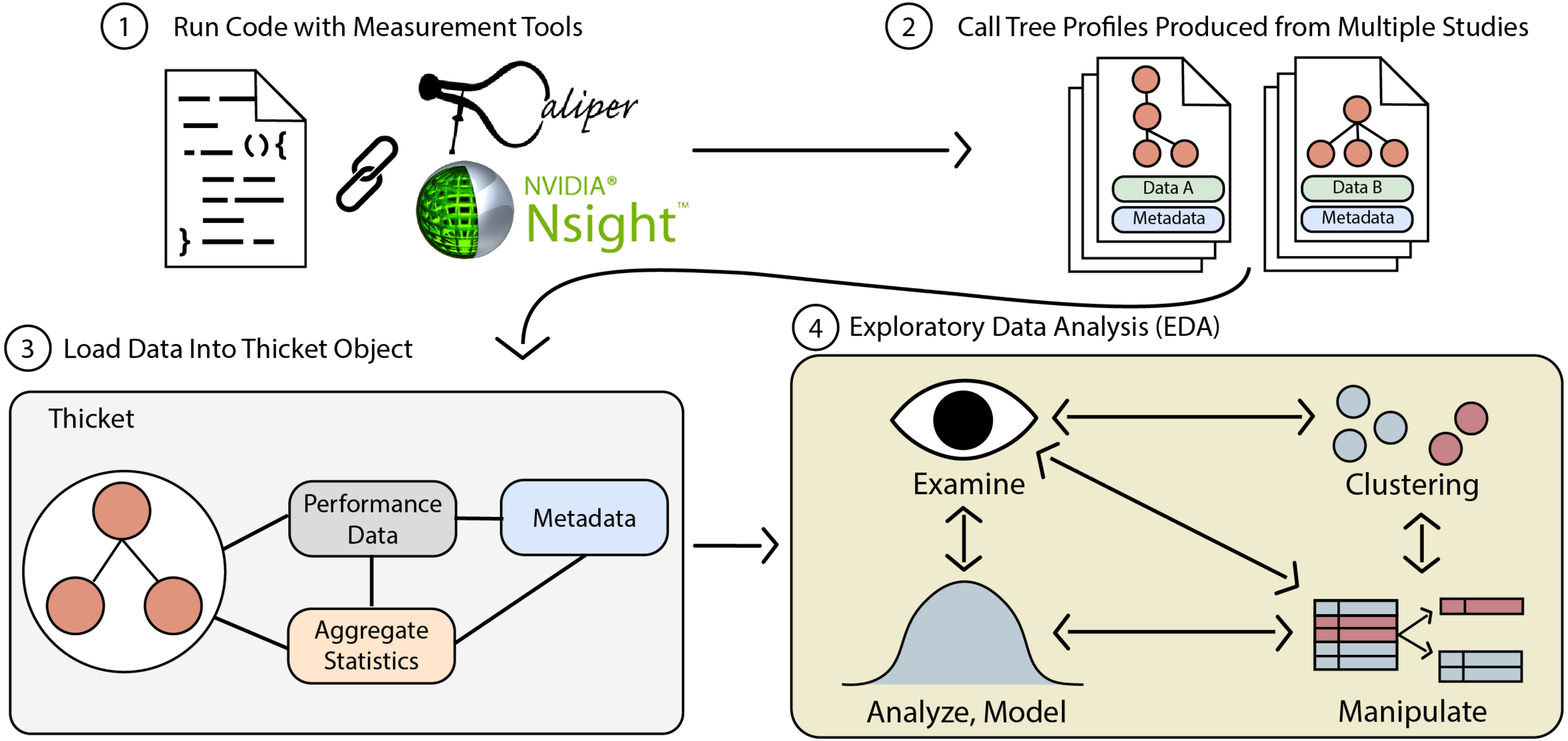
Visualize metadata with parallel coordinates plot

- Thicket's interactive parallel coordinates plot shows relationships between metadata variables, and between metadata and performance data





Thicket is a toolkit for exploratory data analysis of multi-run data



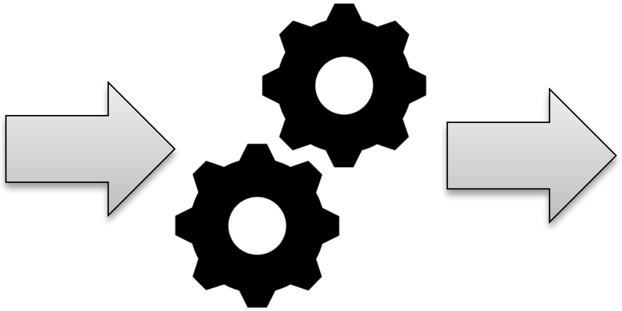
Documentation: **thicket.readthedocs.io**

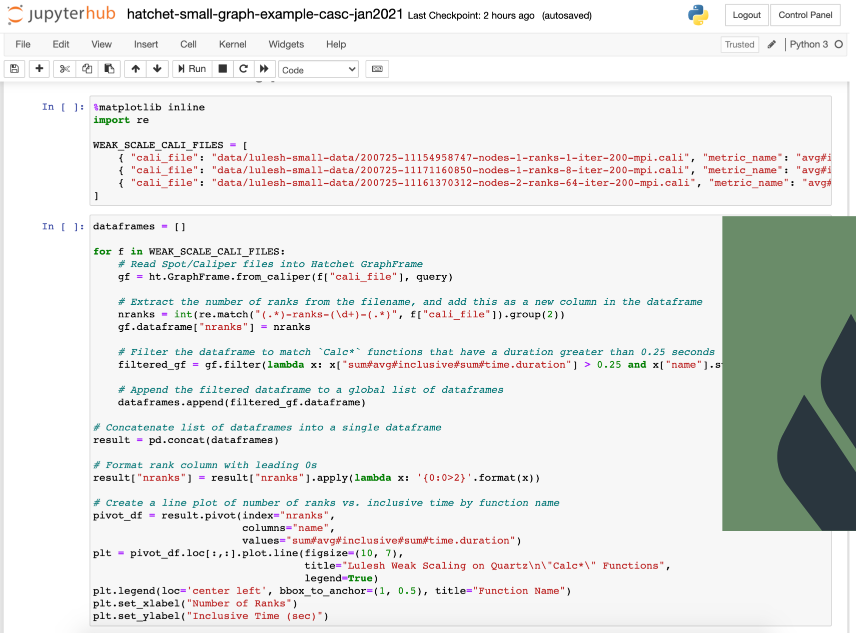
https://github.com/LLNL/thicket
https://github.com/LLNL/thicket-tutorial

On LC Automated Application Performance Analysis Workflow
Go to https://lc.llnl.gov/jupyter

```
#include <caliper/cali.h>

static inline
void LagrangeElements(Domain&
domain, Index_t numElem)
{
    CALI_CXX_MARK_FUNCTION;
// ...
```





Caliper instrumentation in the application

At runtime: Performance and Metadata Collection

Visualization and analysis of caliper datasets using Python in Jupyter notebooks

Caliper

Jupyter and Thicket

c/o D Boehme

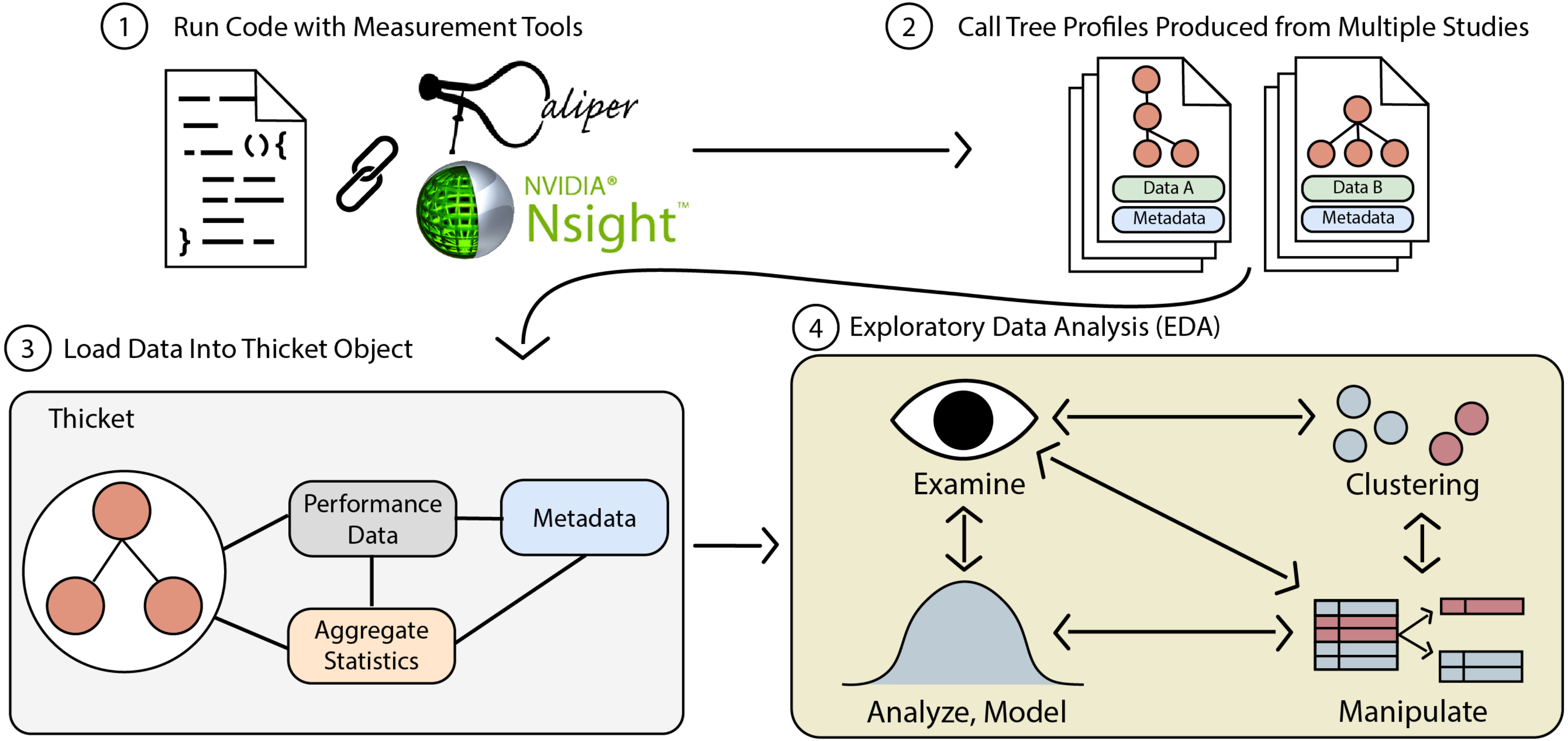
Hands-On Time!

- The container includes example Jupyter notebooks, Thicket 2023.2.0 install, and RAJA Performance Suite datasets
  - Alternatively, the Jupyter notebooks and the RAJA Performance Suite datasets are available directly at https://github.com/llnl/thicket-tutorial in a self-contained Binder environment with all dependencies
  - We expect to update our RAJA Performance Suite tutorial datasets by the end of September
  - Join our mailing list! https://bit.ly/caliper-thicket-users

Steps:

- Login to an instance (see credentials in email)
- Run this command: $ docker run -p 8888:8888 myimage
- Find URL in docker output, copy URL into browser, replace localhost with InstanceIP. It will look similar to: http://<InstanceIP>:8888/?token=9f60c09dcb63a0c6cb9d9e2a436ee541beabf83e67aadcde
- We'll start with notebooks/01_thicket_tutorial.ipynb

Thicket is a toolkit for exploratory data analysis of multi-run data



Join our mailing list! https://bit.ly/caliper-thicket-users

https://github.com/LLNL/thicket
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Documentation: **thicket.readthedocs.io**

CASC

Center for Applied
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